Sunday Afternoon, November 8, 2026

AVS Quantum Science Workshop (ALL-INVITED SESSION)
Room 304 - Session AQS-SuA

AVS Quantum Science Workshop Session (ALL-INVITED SESSION)

Moderators: Dr. Ekta Bhatia, NY CREATES, **Dr. Dave Pappas**, Rigetti Computing, **Dr. Charles R. Eddy, Jr.**, Office of Naval Research Global - London, **Dr. Aranya Goswami**, Nokia Labs

3:00pm **AQS-SuA-1 Fabrication of Superconducting Qubits: Challenges and Opportunities in Scaling of Quantum Computing Circuits***, **Hossein Taghinejad**,* Rigetti Computing **INVITED**

Building fault-tolerant quantum computers requires scaling quantum processors from tens to ultimately millions of qubits while maintaining exceptionally low error rates and high gate fidelity. Achieving this goal is not simply a matter of increasing qubit count; it demands a level of fabrication precision, process uniformity, materials control, and manufacturing yield that far exceeds what is required for small-scale quantum devices. Among the leading hardware platforms, superconducting qubits based on Josephson junctions (JJs) offer a compelling path toward large-scale systems. At the same time, the extreme sensitivity of JJs to nanometer-scale variations in dimensions, tunnel-barrier quality, interfaces, and materials presents formidable challenges to achieving wafer-scale uniformity, high-yield fabrication, and precise qubit frequency control. In this sense, the future of superconducting quantum computing is increasingly a manufacturing problem rather than solely a qubit-physics problem.

In this talk, I will discuss the fabrication of superconducting JJ qubits from the perspective of scalable manufacturing. Particular emphasis will be placed on two major fabrication approaches: single-step shadow (angled) evaporation and multi-step normal-angle deposition. I will examine the advantages and limitations of each approach, focusing on key scaling metrics including qubit frequency variability, junction yield, process reproducibility, and compatibility with large-scale circuit integration. I will further discuss the importance of frequency allocation and precise frequency targeting in multi-qubit processors, highlighting post-fabrication tuning techniques such as alternating-bias-assisted annealing (ABAA) and laser trimming.

* Rigetti Computing Team:

Hossein Taghinejad (Presenter: htaghinejad@rigetti.com), David P. Pappas, Pradeep Manandhar, Cameron Kopas, Xiaqia Wang, Hilal Cansizoglu, Kameshwar Yadavalli, Andrew Bestwick, Josh Mutus.

3:30pm **AQS-SuA-3 Invited Paper***, **Ignace Jarrige**,* Amazon Web Services **INVITED**

4:00pm **AQS-SuA-5 The Capital of Quantum***, **Corey Stambaugh**,* Capital of Quantum **INVITED**

Quantum innovation is increasingly shaped by strong regional ecosystems that contribute to national progress and global momentum. The *Capital of Quantum* represents one such hub: a coordinated Maryland-based ecosystem linking universities, startups, established industry, and government partners. This presentation will situate the Capital of Quantum within the broader U.S. and international landscape, highlight emerging opportunities, and examine how regional strengths can accelerate scalable quantum technologies.

4:45pm **AQS-SuA-8 Invited Paper***, **Prineha Narang**,* UCLA **INVITED**

5:15pm **AQS-SuA-10 Quantum Transduction for Heterogeneous Integration of Quantum Information Systems***, **Matthew LaHaye**,* Air Force Research Laboratory, Information Directorate **INVITED**

The Quantum Information Sciences and Technology (QIST) branch at the Air Force Research Laboratory's Information Directorate (Rome Lab) performs cutting-edge experimental and theoretical research in a multitude of topics at the frontiers of quantum computing and quantum networking. Conducted in support of Air Force strategic objectives in quantum information processing and entanglement distribution, the QIST branch has numerous active research efforts in quantum algorithms and quantum technologies such as trapped-ion systems, integrated quantum photonics, and superconducting quantum circuitry. In this talk, I will give an overview of the research efforts at Rome Lab to develop quantum interconnects between the different quantum technologies (a.k.a. heterogeneous quantum interfaces) and highlight plans to establish a quantum networking testbed for fundamental investigations of entanglement distribution and heterogeneous network design.

5:45pm **AQS-SuA-12 Invited Paper***, **Andrew David Baczewski**,* Sandia National Laboratory **INVITED**

6:15pm **AQS-SuA-14 AQS Panel Discussion and Reception**

Biomaterials Plenary (ALL-INVITED SESSION)
Room 317 - Session BP+BI-SuA

Biomaterials Plenary Session (ALL-INVITED)

Moderators: Dr. Christopher So, Naval Research Laboratory, **Prof. Rong Yang**, Cornell University

3:00pm **BP+BI-SuA-1 Bio-Inspired Design of Multifunctional Materials***, **Kenan Fears**,* US Naval Research Laboratory **INVITED**

Biology serves as an inspiration for researchers due to the countless examples of nature evolving elegant solutions to complex problems humans have difficulty overcoming with engineered materials. For example, acorn barnacles, known for their ability to form a robust underwater cement that withstands harsh marine environments, have also evolved methods to compromise the attachment of the fouling organisms. We discovered barnacles secrete a phase-separating material at their basal interface that oxidizes and lifts off microbial biofilms ahead of growth and cement deposition. Proteomics analysis and confocal microscopy indicate haloperoxidases are present and active at the barnacle's adhesive interface.

Inspired by this approach to combating biofouling, we devised materials and coatings that mimic surface cleaning processes evolved by barnacles. These novel antifouling materials are comprised of surface-active glasses, that is, glasses that intentionally degrade in aqueous environments. We demonstrate the glasses deter marine biofouling by a combination of mechanisms: 1) deterring macrofouler settlement by elevating the concentration of potassium and magnesium ions, which are naturally abundant in seawater, and 2) compromising the adhesion of microbial foulers through the formation of reaction layers that generate reactive oxygen species.

3:30pm **BP+BI-SuA-3 Synthetic Brochosomes: From Biomimicry to Function***, **Tak-Sing Wong**,* The Pennsylvania State University **INVITED**

Leafhopper-produced brochosomes are hollow, buckyball-like nanostructures with distributed nanoscale cavities, representing a unique class of biological optical materials. Inspired by these architectures, we develop synthetic brochosomes with demonstrated broadband, omnidirectional antireflective performance and optical camouflage capabilities [1-3]. This talk highlights recent advances in elucidating geometry-driven optical functionality of brochosomes, where hierarchical pore structures and particle size synergistically suppress reflection across ultraviolet–visible wavelengths [4]. We further discuss scalable manufacturing via droplet microfluidics and interfacial self-assembly, enabling high-throughput production of synthetic brochosomes with tunable architectures [5]. These results position synthetic brochosomes as a versatile platform for optical coatings, signature management, and photonic applications.

References:

[1] L. Wang, J.S. Choi, T.-S. Wong, *Nano Res.* **17**, 734-742 (2024).

[2] S. Yang, N. Sun, B. B. Stogin, J. Wang, Y. Huang, T.-S. Wong, *Nat. Commun.* **8**, 1285 (2017).

[3] Z. Li, L. Wang, X. Liu, J. Li, H.S. Yun, Z. Wang, X. Zhang, T.-S. Wong, S. Sheng, *Sci. Adv.* **10**, eadl4027 (2024).

[4] L. Wang, Z. Li. S. Sheng, T.-S. Wong, *Proc. Natl. Acad. Sci. USA.* **121**, e2312700121 (2024).

[5] J. Choi, T.-S. Wong, *ACS Nano* **19**, 42175-42187 (2025).

4:00pm **BP+BI-SuA-5 Gas Bubble-Encapsulating Microcapsules (GEMs): Pressure-Triggered Drug Delivery and AI-Enabled Fabrication***, **Daeyeon Lee**,* University of Pennsylvania **INVITED**

Pressure-triggered drug delivery holds significant promise for treating pathologies characterized by sudden increases in localized hydrostatic pressure, such as traumatic brain injury and orthopedic injuries.

Conventional microcapsules designed for compression-triggered release are liquid-filled, rendering them intrinsically insensitive to pressure. To address this limitation, we develop Gas Bubble-Encapsulating Microcapsules (GEMs), which incorporate gas bubbles via osmotic cavitation, endowing them with the compressibility necessary for pressure-sensitive mechanical response. To systematically optimize GEM structure, we develop an AI-empowered Automated Droplet Library (ADLib) generator that integrates convolutional neural network-based object detection with real-time microfluidic feedback control, autonomously generating 25 distinct monodisperse double-emulsion populations within 2–3 hours, compared to weeks of manual effort. Using ADLib, we identify two critical structural parameters governing the transition from non-destructive buckling to shell rupture: the shell thickness-to-diameter ratio and the gaseous volume fraction. We establish quantitative design principles that link GEM structure to pressure sensitivity and release kinetics, providing a generalizable platform for pressure-responsive microstructures in targeted drug delivery.

Nanoscale Science and Technology Plenary Session (ALL-INVITED SESSION)

Room 320 - Session NSP-SuA

Nanoscale Science and Technology Plenary Session (ALL-INVITED SESSION)

Moderators: Prof. Deep Jariwala, University of Pennsylvania, **Dr. Marek Kolmer**, Ames National Laboratory

3:00pm **NSP-SuA-1 AFM – after 40 Years Still an Evolving Playground***,* ***Sidney R. Cohen***[1]*,* Weizmann Institute of Science, Israel **INVITED**

In 1986, a brief report in Physical Review Letters by Binnig, Quate and Gerber introduced the atomic force microscope (AFM). Although the original design was quickly modified and improved to exceed the 3 nm lateral and 0.1 nm vertical resolution shown there, the utility and versatility of the instrument were accurately predicted at the time, suggesting the capability to measure any kind of force with sensitivity of atto-Newtons, on both conductors and insulators. This, and subsequent developments turned AFM into the main engine driving the burgeoning field of nanoscience and associated technologies. In the ensuing years, the technique has accomplished feats which would have fit the realm of science-fiction before its invention. I entered the field 2 years after the first report, in 1988, as a post-doc studying nano-scale tribology. The exciting possibilities AFM provides kept me with it until now. In this talk, I will cover our own scientific work which exploited developments of the technique in several areas, including photovoltaics, nanolithography, nanomechanics, “nanoacrobatics”. and surface interactions.The talk will also emphasize the important role of image/data analysis and how that has evolved over the years.

3:30pm **NSP-SuA-3 NS Graduate Award Finalists Presentations**

4:00pm **NSP-SuA-5 NS Early Career Award Finalists Presentations**

4:45pm **NSP-SuA-8 Nanoscale Science and Technology Plenary Award Winner Announcement and Reception**

[1] **NSTD Nanotechnology Recognition Award**

Monday Early Morning, November 9, 2026

Plenary Lecture

Room Ballroom BC - Session PL-MoPL

Plenary Session

Moderator: Prof. Mark Losego, Georgia Institute of Technology

8:30am **PL-MoPL-1 Plenary Lecture***, **Akihisa Sekiguchi,*** Tokyo Electron Limited **INVITED**

Biomaterial Interfaces

Room 321 - Session BI-MoM

Biofilms, Biofouling, and Biomolecules at Interfaces

Moderators: Prof. Sapun Parekh, University of Texas at Austin, **Prof. Rong Yang**, Cornell University

10:00am **BI-MoM-1 Peptide Based Liquid-Liquid Coacervates for Biosensing, Degradation Resistance, and as Biofoundries**, ***Sebastian Diaz***, US Naval Research Laboratory **INVITED**

Nature utilizes various materials such as peptides, nucleotides, and lipids to create order within complex environments such as cell interiors. Imitating nature, we combine DNA nanotechnology with peptide nanotechnology, specifically peptide based liquid-liquid phase separations, to access advanced functionalities. Peptide-based liquid-liquid phase separated domains, also known as coacervates, are neither pure homogenous liquid phase nor a heterogenous aggregate, displaying varying degrees of order. Coacervates are of keen interest in cell biology, where they function as membraneless organelles, dynamically colocalizing enzymes and other biomolecules (e.g. RNA) to enhance translation and other operations. We recently demonstrated that sequestration of DNA biosensors within coacervates allows for i) a greater than 20-fold reduction of the limit of detection within coacervates when compared to control buffer solutions; ii) an increase in the kinetics, equilibrium was reached more than 4-times faster in coacervates; and iii) enhancement in the dye fluorescent quantum yields within the coacervates, resulting in greater signal-to-noise. We have also found that coacervates protect DNA from nuclease degradation while subsequently allowing for release from the coacervate upon proper stimuli, which could have implications for nucleotide delivery applications. We hypothesize that the strong peptide-DNA interaction within the coacervates inhibits degradation and have preliminary evidence that this can be applied to other biological moieties, e.g. enzymes. In a third demonstration, enzymatic cascades are sequestered into coacervates improving product flux through the system by exploiting enzyme stabilization and intermediate channeling.

10:30am **BI-MoM-3 Tailoring the Inert Properties of Zwitterionic Coatings**, *Jana Karthäuser, Lisa Schardt, Katrin Ademmer,* Ruhr University Bochum, Germany*; Jasper Hansen, Andre Laschewsky,* Potsdam University, Germany*;* ***Axel Rosenhahn****,* Ruhr University Bochum, Germany

Manmade materials in contact with aqueous environments become rapidly colonized by living matter like proteins, macromolecules, bacteria, diatoms, and other fouling species. Frequently failure of devices and substantial maintenance costs are among the penalties associated with fouling processes. As the use of biocides is heavily restricted in many applications, environmentally friendly low-fouling materials are intensively explored [1]. In the recent years zwitterionic materials have emerged as highly promising building blocks with inherent inert properties. We synthesized different molecular architectures and studied the effect of structural variation on their inert properties [2]. The resistance to protein and microbe attachment was correlated with their anti-polyelectrolyte properties using several analytical in-situ methods including SPR, AFM, and spectroscopic ellipsometry [3,4,5]. Based on the obtained data, fundamental structure-property correlations and the implications for inert zwitterionic coatings will be discussed.

[1] M. Callow, J. Callow, Nature Communications 2011, 2, 244[2] A. Laschewsky, A. Rosenhahn, Langmuir 2018, 35, 1056[3] J.F. Karthäuser, D. Gruhn, A.M. Guajardo, R. Kopecz, N. Babel, U. Stervbo, A. Laschewsky, R. Viebahn, J. Salber, A. RosenhahnFrontiers in Bioengineering and Biotechnology 2024, 12, 1403654[4] L. Schardt, S. Da Vela, A. Martínez Guajardo, M. Jaugstetter, K. Tschulik, A. Laschewsky, A. RosenhahnAdvanced Materials Interfaces 2025, 12, 2400610[5] J. Karthäuser, J. Hansen, A. Smajlji, K.Z. Hunsucker, Y. Tenzin, C. Braga, T. Patschorke, G. Swain, A. Rosenhahn, A. LaschewskyLangmuir 2025, 41, 4545, 10.1021/acs.langmuir.4c04351

10:45am **BI-MoM-4 Graphene Oxide Coatings Enhance Biofilm Formation and Robustness in 3D-Printed Bioreactors**, ***Maryssa Beasley***, *Christopher Green, Megan Pitz,* US Naval Research Laboratory*; K.A. Shiral Fernando, Iman Eizadynejad, Oscar Ruiz,* Air Force Research Laboratory*; Rebecca Mickol,* US Naval Research Laboratory

Here we demonstrate that both graphene oxide (GO)-coated and GO-impregnated bioreactors result in faster growth and more robust biofilm formation than uncoated bioreactors when inoculated with *Marinobacter atlanticus*. GO is a nanomaterial typically used as either an irreversible binding substrate to trap microbial cells or as an antimicrobial coating, often dependent on GO concentration. Here, GO was incorporated either prior to the final resin cure or as a coating to 3D-printed bioreactors in order to increase cellular adhesion, enhance biofilm formation, and ultimately, increase bioproduction capabilities. Initial assays showed dense biofilm formation on bioreactor segments coated 10x with 0.1 wt% GO-in-water, compared to other solutions. In contrast, crystal violet biofilm assays demonstrated maximum biofilm formation on segments coated only 1x, indicating that high GO concentrations transition from biofilm-promoting to antimicrobial. In bioreactor experiments, effluent oxygen concentrations and final protein concentrations demonstrated that *M. atlanticus* biofilms colonized and grew faster in GO-coated or GO-impregnated systems than in uncoated bioreactors. Recovery, defined as the highest effluent oxygen concentration measured immediately following inoculation, reached only 40.5±13.3% oxygen and 55.5±5.7% oxygen in GO-impregnated and GO-coated bioreactors, respectively, compared to uncoated bioreactors (89.6± 4.1% oxygen). Similarly, biofilms within GO-impregnated and GO-coated bioreactors grew to maximum biomass (here, measured as effluent oxygen concentration < 2%) in less time (3.5±0.8 h and 10.5±2.3 h, respectively) than biofilms within uncoated bioreactors (15.2±3.9 h). Additionally, the same total biomass (as measured by protein concentration) was achieved in half the time with GO-impregnated bioreactors than with uncoated bioreactors (50 h vs. 100 h). When *M. atlanticus* was inoculated into bioreactors with medium that did not contain trace minerals, biofilm growth was fastest in GO-coated bioreactors than in GO-impregnated or uncoated bioreactors, with maximum biomass achieved within 13.9±2.5 h. These results suggest that GO can promote microbial growth, potentially through electron transfer, as previously seen with GO-modified electrodes, although more research is necessary. These data indicate a complex relationship between GO concentration and microbial growth, which requires further investigation to improve and optimize GO coatings for enhanced microbial production.

11:00am **BI-MoM-5 Zwitterionic Polymers for Antifouling Surfaces in Soft Devices**, ***Abdon Pena-Francesch***, University of Michigan **INVITED**

Despite recent advances in medical device technology, seamless integration in biological environments remains a challenge. When interfacing with biological environments, devices are prone to the accumulation of fouling proteins, microorganisms, and biofilms that lead to inflammation, infections, foreign body response, and failure or rejection. Thus, there is an urgent need for long-lasting, highly-stable solutions to prevent biofouling to the wide range of materials, designs, and length scales that comprise medical devices. In this talk, we will present the design of zwitterionic polymer coatings as a bioinspired surface engineering approach to avoid the attachment of proteins, bacteria, and other microorganisms to soft devices. We have recently developed surface functionalization methods compatible with medical-grade silicones (which are typically inert and difficult to functionalize), as well as zwitterionic photoresin formulations compatible with 3D-printing technology, that we have implemented in soft anti-biofouling devices. We will demonstrate their application in two case studies: (i) zwitterionic polymer coatings in urinary catheters that reduce >99% bacterial attachment and the formation of biofilms, outperforming state-of-the-art commercial antimicrobial catheter devices, and (ii) 3D-printed microrobots that avoid immune recognition and clearance by macrophages, significantly prolonging the functional lifetime of medical microrobots.

11:30am **BI-MoM-7 Molecular Shape and Peeling-Stretching Mechanics of Collagen Adsorbed on Silicate Surfaces**, ***Bruno Zappone***, Consiglio Nazionale delle Ricerche - Istituto di Nanotechnology (CNR-Nanotec), Italy **INVITED**

Collagen is the most abundant protein in mammals and plays a critical role in tissue formation, stability, and mechanics, closely linked to its unique triple-helix structure. We used atomic force microscopy (AFM) and the surface forces apparatus (SFA) to study fibril-forming type I and III human collagen absorbed on atomically smooth mica surfaces. The two-dimensional contours of individual collagen molecules showed non-uniform curvature for both types, which persisted after drying the surface and dehydrating the molecules. This finding suggests that collagen either has an intrinsic three-dimensional curvature in solution, or it acquires a two-dimensional curvature due to a particularly strong interaction with the surface. The former case has direct relevance to the self-assembly and elasticity of collagen fibrils, whereas the latter has potential implications for biomaterial design and tissue engineering.

SFA measurements showed strong adhesion between a collagen-coated and an uncoated mica surface, and repulsion between equally coated

surfaces, suggesting that collagen-mica interaction is mainly electrostatic. Moreover, AFM force measurements showed a large adhesive force for a single collagen molecule being peeled by one end from the mica surface. Interestingly, a collagen molecule could be pulled and stretched without failing to a contour length of up to 900 nm—nearly three times its native length—over thousands of stretching cycles until the triple-helix started unravelling. During this process, the alpha-chains slipped progressively, irreversibly, and almost entirely past each other, before being caught by strong physical interactions between overlapping chain ends. These findings indicate that a controlled slippage mechanism at the molecular scale underpins the exceptional toughness of collagen fibrils and collagen-rich tissues such as tendons and skin.

Advances in EUV Lithography
Room 316 - Session EUV-MoM

Advances in EUV Lithography II

Moderators: Prof. Alain Diebold, University at Albany-SUNY, **Mr. Lior Huli**, TEL, **Prof. Gregory Denbeaux**, University at Albany-SUNY, **Dr. Kandabara Tapily**, TEL

10:00am **EUV-MoM-1 Pushing the Limits of High-Volume Manufacturing with EUV Litthography***, **Mike Lercel**,* ASML **INVITED**

EUV lithography has transitioned from an emerging technology to a core manufacturing enabler for advanced logic and memory. Continued innovation with EUV will sustain semiconductor scaling through the next decade. EUV is now established for critical layers in high-volume manufacturing, delivering a step-change in resolution relative to DUV and enabling continued transistor density scaling, while its evolution to higher numerical apertures (0.33 NA to 0.55 NA and beyond) will further improve resolution, simplify patterning, and reduce process complexity and cost through single-exposure solutions. Productivity, availability, and source power are continuing to evolve to make EUV cost effective while improvements in overlay and imaging continue EUV into future nodes. EUV is positioned within a holistic lithography strategy—integrating computational lithography, metrology, and systems—to control edge placement error and enable cost-effective scaling as device architectures evolve toward 3D integration. Overall, EUV for manufacturing will remain central to sustaining Moore's Law and enabling AI-driven semiconductor growth, with expanding opportunities across both 2D scaling and emerging 3D integration schemes.

10:30am **EUV-MoM-3 High NA EUV Challenges and Opportunities***, **Christopher Penny**,* IBM Research **INVITED**

The recent demonstrations of High NA EUV lithography provide significant opportunities to extend scaling for future technology nodes. While many of the key capabilities of High NA EUV have been demonstrated, there remain many significant challenges that must be resolved for High NA EUV to be fully adopted in manufacturing. For example, initial demonstrations have demonstrated single expose patterning for interconnects at 21nm pitch and below; however, further co-optimization of the lithography and etch processes will be required to achieve yield and defectivity levels required for manufacturing. One specific challenge is the introduction of metal oxide resists, and the subsequent process optimization in resist, develop and etch that will be required. Minimizing defectivity (line breaks and bridges) and LER/LWR will continue to be challenging as pitches scale with High NA EUV. The introduction of new materials and processes, such as subtractive Ru patterning, may offer an alternate path to utilize High NA EUV for continued scaling.

11:00am **EUV-MoM-5 Climate-Aware Semiconductor Manufacturing:the Pivotal Role of Lithography***, **Emily Gallagher**,* imec **INVITED**

The semiconductor industry is built on technological innovation, historically guided by familiar metrics: power, performance, area, and cost. Today, increasing emphasis on reducing electrical power demand and improving supply-chain resilience drives growing awareness of environmental impacts. Connecting manufacturing choices to climate impact can be challenging, particularly across highly complex process flows comprising more than 1,000 individual process steps. Addressing the processes that consume demands modelling. To this end, imec has developed a framework based on a bottom–up, virtual fab model to represent a high–volume manufacturing fab.

This "virtual fab" is used to identify global trends in semiconductor manufacturing and the dominant role that lithography plays. Through illustrative, lithography–focused examples, we demonstrate how design, process, and operational decisions influence impacts., and how quantified insights can guide lower–emissions manufacturing. Since performance optimization remains essential, we highlight the need to treat environmental impacts as co-optimized engineering objectives.

11:30am **EUV-MoM-7 EUV Pattern Rectification by the Directed Self-Assembly (DSA) of Block Copolymers***, **Dustin Janes**, Jon-L Innocent-Dolor,* Tokyo Electron America, Inc.

Leading edge manufacturing customers are installing 0.55 NA EUV tools into development fabs, but their resist selection is still uncertain. Interest exists in finding ways to extend chemically amplified resist (CAR) usage to tighter pitch while maintaining a robust etch budget for pattern transfer. EUV rectification by DSA is one strategy to achieve that goal while increasing scanner throughput. Positive-tone developed CAR patterns were rectified by an integrated process flow containing intermediate etch and wet cleans process steps. The exemplary process benefit of DSA at 24 nm line-and-space pitch is achieving uLWR 3σ = 1.6 nm and healing >99% of stochastic defects.

11:45am **EUV-MoM-8 Real-Time Monitoring of Chemical Evolution in Vapor-Deposited Zn-Based Hybrid EUV Resists***, **Thi Thu Huong Chu**, Dan N. Le, Minjong Lee, Dushyant M. Narayan,* University of Texas at Dallas, USA*; Nikhil Tiwale,* Brookhaven National Laboratory*; Oleg Kostko,* Lawrence Berkeley National Laboratory*; Chang-Yong Nam,* Brookhaven National Laboratory*; Jiyoung Kim,* University of Texas at Dallas, USA

Extreme ultraviolet (EUV) lithography is a key enabling technology for sub-10 nm metal half-pitch semiconductor nodes.[1] However, establishing a clear relationship between EUV resist chemistry and lithographic performance remains critical for advancing next-generation patterning with enhanced sensitivity, resolution, and stochastic control.[2] The inherently transient and environment-sensitive nature of irradiation-induced chemistry in EUV resists, however, has limited direct experimental access to reaction pathways under realistic processing conditions.

To address this challenge, we report real-time monitoring of chemical evolution in vapor-deposited Zn-based hybrid EUV resists, providing operando insight into resist reaction mechanisms during e-beam/EUV exposure. In particular, we investigate the distinct roles of organic components (aromatic versus aliphatic) in molecular atomic layer-deposited (MALD) Zn-based hybrid resist thin films to elucidate their influence on sensitivity and patterning performance under both EUV and low-energy electron exposures. By combining operando techniques such as Fourier transform infrared (FTIR) spectroscopy and residual gas analysis (RGA), we directly track chemical bond transformations in real time, enabling the identification of key reaction steps associated with crosslinking and bond scission. Our results reveal distinct exposure mechanisms underlying the observed performance differences. Aromatic-based resists predominantly undergo deformation of aromatic rings, as indicated by a dip at the C=C bond in the FTIR spectrum during 80 eV electron exposure. In contrast, aliphatic systems form dense networks through coordination-driven bonding. Furthermore, we conducted complementary in-operando RGA and electron emission measurements under EUV flood exposure, which revealed the major by-products released during EUV exposure. Together, these findings provide a more comprehensive understanding of the chemical transformations that occur under realistic exposure conditions and highlight the value of real-time, operando approaches in linking molecular structure to lithographic behavior.

The insights provide guiding principles for designing next-generation vapor-deposited hybrid EUV resists with improved performance and reduced stochastic variability.

This research was supported by the U.S. DOE Office of Science Accelerate Initiative Award 2023-BNL-NC033-Fund. This research used resources of the Advanced Light Source, which is a DOE Office of Science User Facility under contract no. DE-AC02- 05CH11231.

[1] I. Giannopoulos *et al.,* Nanoscale, **2024**, 16, 15533–15543.

[2] T. Manouras *et al.,* Nanomaterials, **2020**, 10, 1593.

From Ionic Crystals to Ionic Conductivity: An Iconic Celebration of Gary W. Rubloff's 50+ Years in Science
Room 317 - Session GWR-MoM

From Ionic Crystals to Ionic Conductivity: A Special Celebration of Gary W. Rubloffs 50+ Years in Science

Moderators: Prof. Parag Banerjee, University of Central Florida, **Dr. Keith Gregorczyk**, University of Maryland, College Park, **Prof. Alexander Kozen**, University of Vermont

10:00am **GWR-MoM-1 Recent Advances in Electrochemical Memory***, **Alec Talin,*** Sandia National Lab **INVITED**

Over the past several decades, electronics have relied on deterministic, binary states accessed by electrons to store and process information. The challenge of physical scaling of this approach motivates the need for post-CMOS or post-digital analog approaches to increase functional density and energy efficiency. Instead of using only electron motion to encode information, analog electronics can use electrical, thermal and electrochemical gradients in various heterogeneously integrated materials to move electrons, ions, and domains. Understanding the scientific basis of these complex, frequently coupled mechanisms is difficult, resulting in few reliable physics-based models that can be used by circuit and chip designers. These mechanisms also present increased sensitivity to variability, noise, and poorly controlled kinetic processes. As such, despite decades of research and promising laboratory-scale performance, knowledge gaps in the features of analog electronics have led to their consistent failures to meet the stringent requirements needed for their commercialization. In my presentation, I will discuss our recent work to address these challenges using 3-terminal electrochemical random access memory (ECRAM)[1] that encodes information in three dimensional volumes, rather than 2-dimensions channels or 1-dimensional filaments and combines thermodynamic and kinetic mechanisms to stabilize a high density of analog states.

(1) Talin, A. A.; Meyer, J.; Li, J.; Huang, M.; Schwacke, M.; Chung, H. W.; Xu, L.; Fuller, E. J.; Li, Y.; Yildiz, B. Electrochemical Random-Access Memory: Progress, Perspectives, and Opportunities. *Chem. Rev.* **2025**, *125* (4), 1962-2008. DOI: 10.1021/acs.chemrev.4c00512.

10:15am **GWR-MoM-2 Advancing New Semiconductor Materials and Devices Thought Characterization and Metrology***, **Alain Diebold,*** CNSE, University at Albany **INVITED**

In 1994, Gary Rubloff and Michael Liehr started the AVS Manufacturing Science and Technology Group.The first MSTG sessions were all invited talks that provided a thorough look at silicon integrated circuit manufacturing technology and the associated R&D.Characterization and metrology activities enabled materials and process R&D and increased the yield during manufacturing.In the 1990's transistor devices were planar and on-chip interconnect transitioned from planar aluminum wiring.The next step was Damascene copper interconnect.The new metallization technology brought higher aspect ratio structures which required improved processing and metrology.Then 3D FinFET transistors with hafnium based dielectric layers were introduced again pushing characterization and metrology.Today, the most advanced transistors have vertically stacked channels with gate-all-around dielectric metal technology. Memory technology has very high aspect ratio structures with more than 100 layer stacks.This talk will outline some of the advances in characterization and metrology that have critical enablers for today's technology.The methods that will be covered include spectroscopic ellipsometry, high resolution X-Ray diffraction, scanning electron microscopy for critical dimensions, scanning transmission electron microscopy, and associated advances.

10:30am **GWR-MoM-3 Doing Science with Gary: Accuracy, Elegance and Pleasure***, **Mariano Anderle,*** Italian Society for Science and Technology), CNR-ISTP (Institute for Plasma, Science and Technology), Milan, Italy **INVITED**

The scientific cooperation between our research groups has lasted for more than twenty years and has covered topics ranging from semiconductor manufacturing to biotechnology. Examples of this intense collaboration include:

- Rapid thermal CVD growth of polysilicon on silicon oxide under low temperature and ultraclean deposition conditions;
- Fluorine diffusion kinetics in Si, SiO_2 and MOS structures;
- Sub-atmospheric CVD ozone/TEOS process for SiO_2 trench filling;
- Formation and characterization of nanoporous PMSSQ low-K dielectrics;
- Real time sensing and metrology for atomic layer deposition processes;
- Growth and physico-chemical and biological characterization of polysaccharide films as a platform for living cells in BioMEMS systems;
- Micro-combi approach to prototype combinatorial materials discovery.

In my presentation, I will highlight some of the important achievements stemming from the topics just mentioned, emphasizing how Gary's style-his remarkable ability to interact with people, his rigorous method, together with his profound knowledge and broad expertise (not only scientific)-has transformed the work of a researcher like me into an adventure full of fascination and creativity.

10:45am **GWR-MoM-4 Materials, Technologies, and Systems Integration: How Gary Rubloff Inspired Me to Be a Better Microsystem Researcher***, **Reza Ghodssi,*** University of Maryland College Park **INVITED**

It is a distinct honor to participate in this symposium celebrating Prof. Gary Rubloff's extraordinary contributions to science and engineering. As a colleague at the University of Maryland for more than two decades, I have had the privilege of witnessing first-hand Gary's leadership in fostering interdisciplinary research at the intersection of materials science, electrochemistry, energy systems, and microscale technologies. His vision for collaborative, translational research has inspired a vibrant innovation ecosystem and helped shape many of the interdisciplinary directions pursued by my research group.

In this talk, I will highlight the evolution of integrated micro- and nanosystems developed by my group over more than three decades. I will discuss how we have leveraged foundational MEMS technologies, advanced microfabrication techniques, and systems integration methodologies to develop platforms for sensing, actuation, microfluidic bioMEMS, microscale energy storage and harvesting, including three-dimensional battery architectures, microfabricated electrochemical systems, and self-sustaining power solutions for embedded devices.

I will then describe the translation of these technologies into biomedical and clinical applications, including ingestible capsule devices for gastrointestinal sensing, tissue sampling, drug delivery, and physiological monitoring. The focus of this work is to enable in situ diagnostics and therapeutic interventions, toward gastrointestinal health, biofilm monitoring and inhibition, and platform technologies for investigating gut-brain interactions. Together, these research activities demonstrate how advances in systems integration can be translated into impactful solutions for energy, healthcare, and society, reflecting the interdisciplinary spirit and strong mentoring that have characterized Gary Rubloff's distinguished career.

11:00am **GWR-MoM-5 Biofabrication in Microfluidics for Biological and Fuel Cell Challenges: Inspired by Gary's Innovation Path***, **Xiaolong Luo,*** Catholic University of America **INVITED**

In this talk, I will discuss biofabrication in microfluidics, a significant side path in Gary's extraordinary semiconductor career that enables us to tackle some formidable challenges in biology and fuel cells. First, I will introduce biofabrication in microfluidics and the tools developed to integrate biology with microdevices, including electrodeposition, flow assembly at flow interfaces, and electrofabrication with distal electrodes. Second, the presentation will cover some biofabrication-enabled microfluidic platforms addressing biological and biomedical challenges, ranging from lipid bilayer to tissue-on-a-chip, from model biofilms to microbiome-on-a-chip and biofilm sensors, and from bacterial chemotaxis to rapid antibiotic susceptibility testing for timely sepsis treatments. Finally, I will introduce distal electrofabrication of chitosan membranes on printer paper as anion-exchange membranes for direct methanol fuel cells, with the potential to dramatically lower fuel cell costs for broader civil adaptation.

11:15am **GWR-MoM-6 Hidden Chemistry and Unexpected Pathways in Atomic Layer Deposition***, **Theodosia Gougousi,*** UMBC **INVITED**

Atomic Layer Deposition (ALD) is often described as an ideal, self-limiting thin-film growth process governed by simple ligand-exchange reactions. While this simplified reaction scheme is successful, in general, there is growing experimental evidence that real ALD chemistries are far more complex, involving competing and parallel reaction pathways,resulting in unexpected thin-film properties.

In this talk, I will present a series of examples showing how subtle variations in precursor chemistry, process temperature, and substrate surface condition can activate parallel and competing reaction pathways

that strongly influence interfacial quality and structure, as well as film composition and properties. For example, in simple ALD metal oxide chemistries, I will discuss unexpected phenomena such as precursor decomposition during nominal ALD cycles, transport of interfacial species through growing films, and non-monotonic changes in optical and electrical properties within commonly assumed "ALD windows." In situ and ex situ spectroscopic measurements reveal that these effects arise from hidden chemical processes that persist well beyond initial surface coverage and are highly sensitive to both precursor identity and processing conditions.

These results highlight the limitations of overly simplified growth models and underscore the need to consider the complete ALD chemistry when selecting processes and materials for specific applications. Understanding these hidden pathways is essential for improving process control and reproducibility and for exploiting ALD as a platform for discovering new material behavior.

11:30am **GWR-MoM-7 From Stress Gradients to Reaction Fronts: Physics-Based Modeling for Next-Generation Ionic Devices**, ***David Stewart***, *Yueming Song,* University of Maryland, College Park*; Binh Hoang, Chuan-Fu Lin,* Catholic University of America*; Paul Albertus, Gary Rubloff,* University of Maryland, College Park **INVITED**

Electrochemical modeling is essential to the development of advanced energy storage devices. In research and industry, finite element models with standard governing equations are commonly used to predict battery performance with different structural parameters such as particle grain size or porosity. However, electrochemical modeling is far from a static field that can simply be a plug-and-play solution to designing electrochemical devices. In this presentation we will discuss key results from a decade of work in electrochemical modeling, including 3D architecture design, self-regulating behavior, and the opportunities for measuring and leveraging dynamic material properties exhibit by ionic materials.

In the Rubloff group, we have used these governing equations to predict performance metrics for 3D batteries based on thin film manufacturing techniques. 3D structures have been modeled at the level of pure electrochemistry and including various forms of electro-chemo-mechanical coupling and a stark contrast emerged in the forces that governed Li flux. Most importantly, while GPa levels of stress gradients are predicted to form in a cell using brittle TiO_2 and V_2O_5 electrodes, electro-chemo-mechanical coupling can serve as a self-regulating force, diverting Li flux away from the high stress areas and preventing severe stress-delamination.

While these simulations offer important guidance on cell design and experimental measurements, key to an accurate prediction are dynamic material properties such as the ionic diffusivity, partial molar volume, and electrical conductivity which vary with lithiation state. An important example are FeF_3 electrodes, which exhibit a variable electronic conductivity across several orders of magnitude. The consequence is that the distribution of the lithiated, high conductivity phase, governs the propagation of the electrochemical reaction. We use a patterned current collector to create a 5 mm lateral distribution of Li in thin film FeF_3 electrodes, and show excellent agreement with experimental results. Current concentrates at the reaction front, preventing full lithiation until conductivity equalizes across the electrode, which spreads linearly with time.

We expect these phenomena to play important roles in future ionic device designs such as electrochemical RAM (which leverages dynamic conductivity for in-memory computing). As devices scale, there will be an ongoing competition between self-regulating forces and geometric inhomogeneities which ultimately governs device response. Capturing this competition accurately will require physical and chemical models continuously validated against experiment.

11:45am **GWR-MoM-8 Operando Electrochemical Phase Engineering Platform for Nanocomposite Thin Films**, ***Daniela R. Fontecha***, *Osma J. Gomez, Nam Kim, Sang Bok Lee, Gary W. Rubloff, Keith E. Gregorczyk,* University of Maryland College Park **INVITED**

Nanoscale materials processing advancements have enabled on-chip ionic devices like microbatteries, super capacitors, ion-gated transistors, etc. using standard semiconductor processes (such as atomic layer deposition - ALD) to develop electrochemically active thin films. However, challenges remain in understanding and controlling ionic and electronic transport in nanoscale systems. Nanoscale ionic systems that are tunable at multiple scales (chemical composition, phase distribution, and crystal structure) are critical in understanding how these parameters affect transport and materials properties. In this work we demonstrate a system with these qualities and introduce an additional lever - *operando* electrochemical phase engineering - to systematically control the phase distribution that allows us to study the effects of individual phases on ionic transport in a ternary-phase ALD nanocomposite.

We study a Li-Ti-P-O semicrystalline nanocomposite, which consists of nanocrystalline lithium titanium phosphate (LTP) and anatase TiO_2, both embedded in an amorphous Li-Ti-P-O matrix. This nanocomposite thin film system can be synthesized by alternating between titanium phosphate and lithium oxide ALD sub-processes (resulting film depicted in **Figure 1a**), where changing the ratio of oxide-to-phosphate thickness enables compositional tunability while post-process annealing allows for control of crystalline phases in the system. We demonstrate, through electrochemical phase engineering, a voltage-dependent materials system that converts between high power and high capacity by removing the crystalline LTP phase operando. In the high power voltage window (2.1 V – 3.5 V vs Li^+/Li), depicted in **Figure 1b**, the nanocomposite retains 60 % of its initial capacity (125 mAh/g) at an ultrafast charging rate of 200 C (18 sec). In the high capacity voltage window (0.25 V – 3.5 V vs Li^+/Li), the nanocomposite without crystalline LTP (**Figure 1c**) delivers 1302 mAh/g at 1 C and retains 61.9 % of its initial capacity at a charging rate of 20 C (3 min).

In this talk I will discuss how we combined composition-controlled ALD films with voltage-window-selective cycling to drive controlled evolution of crystal structure, phase distribution, and internal interfaces. Most importantly, we use this control to isolate the contribution of each constituent phase to the overall electrochemical behavior of the system. This work establishes the Li-Ti-P-O nanocomposite as a tunable platform for studying how crystal structure and interfaces govern transport in thin ionic films — with direct relevance to thin film microbatteries & ionic supercapacitors.

Light Source Enabled Science
Room 319 - Session LS-MoM

Light Source Enabled ARPES

Moderators: Dr. Lucía Pérez Ramírez, CEA Saclay, **Dr. Nicholas Strange**, SLAC National Accelerator Laboratory

10:00am **LS-MoM-1 Depth-Resolved X-Ray Spectroscopy of Emergent Electronic and Magnetic States at Oxide Interfaces**, ***Alexander Gray***, Temple University **INVITED**

The emergence of novel electronic and magnetic states at correlated oxide interfaces is governed by a complex interplay of charge transfer, orbital reconstruction, and interfacial magnetism. In this talk, I will demonstrate how the combination of complementary synchrotron-based probes, including hard X-ray photoelectron spectroscopy (HAXPES), angle-resolved photoelectron spectroscopy (ARPES), polarization-dependent X-ray absorption spectroscopy (XAS), and resonant X-ray magnetic reflectivity, enables a comprehensive, depth-sensitive view of these phenomena in buried oxide heterostructures. Using $LaNiO_3/CaMnO_3$, $CaMnO_3/CaRuO_3$, $NdNiO_3/CaMnO_3$, and $VO_2/LaAlO_3/TiO_2$ interfaces as model systems, we reveal how interface engineering, defect chemistry, and interfacial charge transfer can stabilize emergent ferromagnetism and tune electronic phase transitions [1-3]. Looking forward, these synchrotron-enabled insights also establish a foundation for ultrafast studies at X-ray free-electron lasers (FEL), where intense IR or THz electric-field pulses can be used to manipulate interfacial electronic and magnetic states on their intrinsic timescales [4]. These studies highlight the unique power of combining multiple synchrotron techniques to disentangle coupled charge, spin, and orbital interactions at complex interfaces and provide pathways toward controllable oxide-based electronic and spintronic functionalities.

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[1] J. R. Paudel *et al.*, *Phys. Rev. B* **108**, 054441 (2023).
[3] D. Mondal *et al.*, *Nature Comm.* **14**, 6210 (2023).
[3] J. R. Paudel *et al.*, *Nano Letters***24**, 15195 (2024).
[4] A. M. Derrico *et al.*, *Adv. Mater.* **38**, e12328 (2026).

10:30am **LS-MoM-3 Layer-Specific Spin-Polarization in a Triple-Layer Ferromagnetic Oxide**, ***Jonathan Denlinger***, Lawrence Berkeley National Laboratory; *Prosper Ngabonziza,* Louisiana State University; *Alexei Fedorov,* Lawrence Berkeley National Laboratory; *Gang Cao,* University of Colorado Boulder; *James W. Allen,* University of Michigan, Ann Arbor; *G. Gebreyesus,* University of Ghana, Accra, Ghana; *Richard M. Martin,* Stanford University

The transport and magnetic properties of triple-layer oxides can be distinctly affected by the different structural environments of the outer versus central layers. Here we highlight the layer-specific *spin-polarized* electronic structure of the ferromagnetic triple-layer ruthenate $Sr_4Ru_3O_{10}$, using high resolution synchrotron angle- and spin-resolved photoemission spectroscopy (ARPES) [1]. Two separate narrow-band van Hove singularities (vHS) are found ∼30 meV below the Fermi-level at the zone center and at the zone-edge, which exhibit almost pure spin-polarization, but with opposite-sign. Comparison of the ARPES to spin-polarized DFT calculations quantifies the FM exchange splitting energy, and thus the predicted layer-specific spin polarization contributions to the magnetism, which is then indirectly evidenced by ARPES multi-zone matrix element intensities.

Furthermore, the vHS peaks exhibit dramatic Kondo-coherence-like temperature-dependence, that are the result of multi-orbital Hund metal physics. Fine T-dependent effects at various momenta, including oxygen-band spin-polarization and spin-dependent energy and momentum-shifts provide a more refined picture of the itinerant versus localized description of its magnetism. Finally, rotations of oxygen octahedra induce a zone-folded hybridization of opposite spin bands that break up the zone boundary vHS into smaller lower energy scale mini-vHSs that are relevant to the field-induced metamagnetism of the system.

[1] P. Ngabonziza et al. Phys. Rev. B **111**, 115146 (2025)

10:45am **LS-MoM-4 In-situ Strain Tuning of Electronic Order at a Light Source: Insights from μ-ARPES and μ-Diffraction**, ***Yucheng Guo***, Rice University; *Zhaoyu Liu,* Clemson University; *Na Hyun Jo,* University of Michigan, Ann Arbor; *Ji Seop Oh,* Sookmyung Women's University, Korea (Democratic People's Republic of); *Yichen Zhang,* Rice University; *Aaron Bostwick, Chris Jozwiak, Nobumichi Tamura,* Advanced Light Source, Lawrence Berkeley National Laboratory; *Makoto Hashimoto, Donghui Lu,* SLAC National Accelerator Laboratory; *Robert J. Birgeneau,* University of California, Berkeley; *Jiun-Haw Chu,* University of Washington; *Eli Rotenberg,* Advanced Light Source, Lawrence Berkeley National Laboratory; *Ming Yi,* Rice University

In quantum materials, the manipulation of atomic spacing and electron-cloud overlap enables precise control of the many-body Hamiltonian, influencing the material's ground state, excitations, phases, and competing orders. To investigate how these effects are manifested in the electronic band structure, we integrated a piezo-driven stress cell compatible with μ-ARPES and Laue μ-diffraction beamlines at the Advanced Light Source.

Using this capability, we investigate an intriguing phenomenon reported by P. Malinowski *et al.* [1], who demonstrated that continuously applied uniaxial strain can strongly suppress the superconducting transition temperature, Tc, in an optimally doped iron-based superconductor, while the underlying microscopic mechanism remains elusive.

In this presentation, we discuss in-situ uniaxial strain tuning of electronic correlations in an orbital- and momentum-resolved manner, using decoupled strain channels in $BaFe_2(As_{0.7}P_{0.3})_2$. Our results are largely consistent with a nematic quantum critical point scenario.

[1] P. Malinowski *et al.*, *Nature Physics* **16**, 1189–1193 (2020).

11:00am **LS-MoM-5 Large Exciton Binding Energy in a Bulk Van Der Waals Magnet from Quasi-1D Electronic Localization**, ***Shane Smolenski***, *Ming Wen, Qiuyang Li, Eoghan Downey, Adam Alfrey,* University of Michigan, Ann Arbor; *Wenhao Liu, Aswin Kondusamy,* University of Texas at Dallas; *Aaron Bostwick, Chris Jozwiak, Eli Rotenberg,* Advanced Light Source, Lawrence Berkeley National Laboratory; *Liuyan Zhao, Hui Deng,* University of Michigan, Ann Arbor; *Bing Lv,* University of Texas at Dallas; *Dominika Zgid, Emanuel Gull, Na Hyun Jo,* University of Michigan, Ann Arbor

Excitons, bound electron-hole pairs, influence the optical properties in strongly interacting solid-state systems and are typically most stable and pronounced in monolayer materials. Bulk systems with large exciton binding energies, on the other hand, are rare and the mechanisms driving their stability are still relatively unexplored. Here, we report an exceptionally large exciton binding energy in single crystals of the bulk van der Waals antiferromagnet CrSBr. Utilizing state-of-the-art synchrotron-based angle-resolved photoemission spectroscopy and self-consistent ab-initio *GW* calculations, we present direct spectroscopic evidence supporting electronic localization and weak dielectric screening as mechanisms contributing to the amplified exciton binding energy. Furthermore, we report that surface doping enables broad tunability of the band gap offering promise for engineering of the optical and electronic properties. Our results indicate that CrSBr is a promising material for the study of the role of anisotropy in strongly interacting bulk systems and for the development of exciton-based optoelectronics.

11:15am **LS-MoM-6 Probing Domain-Specific Charge Density Wave Dynamics and Strain Tunability in Bulk 1T-VTe2**, ***Pratik Saud***, Carnegie Mellon University, USA; *Sandy Adhitia Ekahana,* Carnegie Mellon University; *Aalok Tiwari,* Carnegie Mellon University, USA; *Mohan Bikram Neupane,* Purdue University, USA; *Sagnik Bajpeyi,* Carnegie Mellon University, USA; *Chris Jozwiak, Eli Rotenberg, Aaron Bostwick,* Advanced Light Source, Lawrence Berkeley National Laboratory; *Arnab Banerjee,* Purdue University, USA; *Simranjeet Singh, Jyoti Katoch,* Carnegie Mellon University, USA

In transition metal dichalcogenides, the emergence of a charge density wave (CDW) is highly sensitive to the material's dimensionality. While bulk and multi-layer 1T-VTe_2 host a robust CDW state, this ordered phase is unexpectedly suppressed in the monolayer limit. This contrast indicates that out-of-plane interactions are fundamental to stabilizing the CDW. Consequently, a rigorous, momentum-resolved investigation of the 3D bulk crystal is a requisite precursor to engineering these states in ultra-thin devices. Here, we utilize advanced synchrotron light sources to systematically investigate the structural and electronic phase transitions of pristine bulk 1T-VTe_2. We employ Laue microdiffraction (beamline 12.3.2) at the Advanced Light Source (ALS) to map local crystallographic symmetries, alongside high-resolution Angle-Resolved Photoemission Spectroscopy with micron-sized spatial resolution (microARPES) at the MAESTRO 7.0.2 beamline to track electronic dispersion. A key objective of this work is to spatially correlate these independent datasets to decouple lattice distortions from the CDW gap formation.

Temperature-dependent ARPES measurements reveal a dramatic phase evolution. At 500 K, the material exhibits a highly symmetric hexagonal Brillouin zone. Cooling to cryogenic temperatures triggers a macroscopic symmetry breaking, forming three distinct structural domains rotated 120 degrees relative to one another. Probing these individual domains enables the observation of highly directional, quasi-one-dimensional electronic features emerging from the symmetric parent state. Furthermore, this multi-domain landscape provides an opportunity to search for localized electronic states residing at the boundaries between these energetically equivalent regions. Next, we will present our work beyond static observation, where we introduce in-operando mechanical strain during photoemission measurements, to actively manipulate domain populations and tune their corresponding electronic signatures. By comprehensively detailing domain formation, boundary phenomena, and strain-engineered responses in the bulk, this research establishes a predictive framework for dimensional crossover effects. Ultimately, these insights lay the critical groundwork for future efforts to isolate, manipulate, and control fragile correlated phases within mechanically exfoliated two-dimensional heterostructures.

11:30am **LS-MoM-7 Observing the Electronic Response of a Mott Insulator at a Current-Induced Insulator-to-Metal Transition Using Transport-ARPES**, ***Cissy Suen***, Max Planck Institute for Solid State Research, University of Britsh Columbia, Germany; *Igor Markovic, Marta Zonno, Niclas Heinsdorf, Sergey Zhdanovich,* University of British Columbia, Canada; *Na Hyun Jo,* Advanced Light Source, Lawrence Berkeley National Laboratory; *Michael Schmid,* Max Planck Institute for Solid State Research, Germany; *Philipp Hansmann,* Friedrich-Alexander-University Erlangen-Nürnberg (FAU), Germany; *Steef Smit, Christine Au-Yeung,* University of British Columbia, Canada; *Valentin Zimmermann,* Max Planck Institute for Solid State Research, Germany; *Berend Zwartsenberg,* University of British Columbia, Canada; *Maximilian Krauloher,* Max Planck Institute for Solid State Research, Germany; *Sergey Gorovikov,* Canadian Light Source, Inc., Canada; *Chris Jozwiak, Aaron Bostwick,* Advanced Light Source, Lawrence Berkeley National Laboratory; *Marcel Franz,* University of British Columbia, Canada; *Eli Rotenberg,* Advanced Light Source, Lawrence Berkeley National Laboratory; *Bernhard Keimer,* Max Planck Insitute for Solid State Research, Germany; *Andrea Damascelli,* University of British Columbia, Canada

The quasi-two-dimensional Mott insulator Ca2RuO4 exhibits a convergence of spin-orbit coupling and electronic correlations that lead to exciting quantum phenomena [1], including a rare insulator-to-metal transition (IMT) induced by a DC current [2]. While structural changes have been tracked by neutron diffraction [3], Raman scattering [4], and x-ray

diffraction [5], the associated electronic changes had not been observed. Here we report angle-resolved photoemission spectroscopy (ARPES) results under DC current, which show a substantial reduction of the Mott gap, along with a change in the Ru t2g band dispersion [6]. We have also captured the high temperature Fermi surface, whose spectral features are unique from the current-induced metallic Fermi surface. In conjunction with a free energy analysis, our results demonstrate that the current-induced phase, albeit thermodynamically equivalent, is electronically distinct from the high-temperature zero-current metallic phase.

Combining ARPES with transport, i.e. transport-ARPES, has been rare given the complexity of disassociating real field- or current-driven physics from the effect of stray electric and magnetic fields on the outgoing photoelectron trajectory. By taking advantage of the micron-sized beam spot at the MAESTRO beamline (7.0.2) at the Advanced Light Source and careful core level spectrum analysis, we show that transport-ARPES can be extended to the study of any ARPES-suitable material. I will include an overview on transport-ARPES, as well as a brief outlook on the exciting prospects of in operando spectroscopy.

[1] A. Jain et al., Nat. Phys. 13 (2017) 633-637

[2] R. Okazaki et al., J. Phys. Soc. Jpn 82 (2013) 103702

[3] J. Bertinshaw et al., Phys. Rev. Lett 123 (2019) 137204

[4] K. Fürsich et al., Phys. Rev. B 100 (2019) 081101

[5] K. Jenni et al., Phys. Rev. Mat 4 (2020) 085001

[6] C.T. Suen et al., Nat. Phys. 20 (2024) 1757–1763

11:45am **LS-MoM-8 Investigation of Momentum Resolved Electronic Structure of Cr1.17Te2***, **Sagnik Bajpeyi,*** Carnegie Mellon University, USA*; Sandy Adhitia Ekahana,* Carnegie Mellon University*; Aalok Tiwari,* Carnegie Mellon University, USA*; Mohan Bikram Neupane,* Purdue University, USA*; Pratik Singh Saud,* Carnegie Mellon University, USA*; Chris Jozwiak, Eli Rotenberg, Aaron Bostwick,* Lawrence Berkeley National Laboratory, US*; Arnab Banerjee,* Purdue University, USA*; Simranjeet Singh, Jyoti Katoch,* Carnegie Mellon University, USA

Chromium tellurides have attracted significant interest due to the strong interplay between electronic correlations and crystal structure. Among them, Cr1.17Te2 is a transition-metal chalcogenide that exhibits complex electronic behavior arising from non-stoichiometry and strong Cr–Te hybridization. Here, we investigate the electronic structure of Cr1.17Te2 using high-spatial-resolution angle-resolved photoemission spectroscopy (microARPES) performed at the MAESTRO Beamline of the Advanced Light Source.

We will present momentum-resolved band dispersion measurements acquired at 10 K using 84 eV photons with varying light polarizations, together with core-level spectroscopy of Cr and Te orbitals and out-of-plane kz dispersion measurements. Potassium surface dosing was further employed to tune the chemical potential and investigate the evolution of electronic states near the Fermi level. Our photon-energy-dependent measurements reveal a periodicity that deviates from expectations based on X-ray diffraction data, suggesting a more complex three-dimensional electronic structure than previously anticipated. These results motivate future soft X-ray ARPES measurements in the 300–700 eV range to further elucidate the intrinsic bulk electronic structure of Cr1.17Te2 and resolve the origin of this discrepancy.

Magnetic Interfaces and Nanostructures
Room 318 - Session MI-MoM

Advanced Magnetic Materials in Low Dimensional Structures I

Moderators: Dr. Valeria Lauter, Oak Ridge National Laboratory, **Prof. Dr. Markus Donath**, Muenster University, Germany

10:00am **MI-MoM-1 Bringing Materials-Specific Clarity to the Debate on Magnetism in RuO_2***, **Bharat Jalan,*** University of Minnesota, USA **INVITED**

RuO_2, a rutile 4d-transition metal oxide, exhibits a unique crystal structure with both edge- and corner-sharing octahedra. This intrinsic anisotropy, when combined with strain engineering, provides a powerful avenue for tuning anisotropic electronic and optical properties. However, from a synthesis perspective, challenges such as variable Ru valence states, Ru/O stoichiometry control, anisotropic strain states, and structural defects can make it difficult to distinguish intrinsic properties from extrinsic effects in RuO_2 thin films – a classic trick in the pursuit of novel functionalities in quantum materials. In this talk, I will highlight our group's efforts in overcoming these synthesis challenges while demonstrating metallicity in epitaxial RuO_2 films down to the unit cell scale. Through a combination of advanced X-ray scattering, X-ray absorption spectroscopy, transmission electron microscopy, temperature-dependent transport, magneto-optical measurements, and density functional theory (DFT) calculations, we uncover robust magnetism in epitaxially strained RuO_2, consistent with an altermagnetic metallic phase [1-4]. Additionally, we reveal a novel polar phase in strained films with significant implications for electrical transport – an unexpected treat in the realm of functional oxides. I will discuss these findings in detail, emphasizing their sensitivity to material defects and structure – key ingredients that are often overlooked but crucial in determining emergent quantum phenomena.

Reference:

1. S. G. Jeong†, I. H. Choi†, S. Nair, L Buiarelli, B. Pourbahari, J. Y. Oh, N. Bassim, A. Seo, W. S. Choi, R. M. Fernandes, T. Birol, L. Zhao, J. S. Lee, and B. Jalan, **Altermagnetic polar metallic phase in ultra-thin epitaxially-strained RuO_2 films**, PNAS 123 (10) e2526641123 (2026) †Equal contribution
2. S. G. Jeong, I. H. Choi, S. Lee, J. Y. Oh, S. Nair, J. H. Lee, C. Kim, A. Seo, W. S. Choi, T. Low, J. S. Lee, and B. Jalan, **Anisotropic Strain Relaxation-Induced Directional Ultrafast Carrier Dynamics in RuO_2 Films**, Sci. Adv. 11, eadw7125 (2025)
3. S. G. Jeong, S. Lee, B. Lin, Z. Yang, I. H. Choi, J. Y Oh, S. Song, S. W. Lee, S. Nair, R. Choudhary, J. Parikh, S. Park, W. S. Choi, J. S. Lee, J. M. LeBeau, T. Low, and B. Jalan, **Metallicity and Anomalous Hall Effect in Epitaxially-Strained, Atomically-thin RuO_2 Films,** PNAS 122(24) e2500831122
4. S. G. Jeong, B. Y. X. Lin, M. Jin, I. H. Choi, S. Lee, Z. Yang, S. Nair, R. Choudhary, J. Parikh, A. Santhosh, M. Neurock, K. A. Stoerzinger, J. S. Lee, T. Low, Q. Tu, J. M. LeBeau, and B. Jalan,**Strain-Stabilized Interfacial Polarization Tunes Work Function Over 1 eV in RuO_2/TiO_2Heterostructures,** *Nat. Commun. 17, 2516 (2026)*

10:30am **MI-MoM-3 Compositionally Tunable Synthesis of High-Entropy Transition Metal Dichalcogenides Exhibiting Above-Room-Temperature Magnetism***, **Xiahua Zhong**, Chen Zhang,* University of Missouri-Columbia*; Zheng Gai, Huan Zhao,* Oak Ridge National Laboratory, USA*; Yingchao Yang,* University of Missouri-Columbia

As silicon-based electronics approach their physical limits, spintronics, leveraging electron spin rather than charge, offers a promising path for next-generation information technologies. Realizing this potential requires two-dimensional (2D) materials with robust and tunable room-temperature magnetism. Here, we report a two-step synthesis strategy for fabricating 2D high-entropy transition metal dichalcogenides (HE-TMDs) incorporating magnetic elements beyond conventional groups 4-6. High-entropy layered double hydroxides (HE-LDHs) are first synthesized via hydrothermal coprecipitation, enabling atomic-level mixing of diverse transition metals across groups 4-12. Subsequent chalcogenization yields 2D HE-TMDs while preserving homogeneous elemental distribution. This approach circumvents the constraints of high-temperature and vapor-phase methods, enabling the synthesis of compositionally complex and structurally controlled 2D magnets. Representative $V_\alpha Cr_\beta Fe_\gamma Co_\delta Ni_{1-\alpha-\beta-\gamma-\delta} S_{2-x}$ exhibits robust ferromagnetism above room temperature, demonstrating the potential of this high-entropy design strategy to expand the family of 2D magnetic materials for spintronic applications.

10:45am **MI-MoM-4 Anomalous Hall Effect in Antiferromagnetic Dirac Semimetal $EuCu_2Sb_2$***, **Souvik Sasmal,*** Argonne National Lab

Magnetic Dirac semimetals—where Dirac fermions are protected by combined crystalline and magnetic symmetries—remain experimentally rare, despite intense theoretical interest. In this work, we identify EuCu2Sb2 as a promising candidate hosting Dirac-like electronic states in proximity to magnetic order. Temperature-dependent transport and magnetization measurements reveal an A-type antiferromagnetic transition at 5.1 K, accompanied by anisotropic resistivity, spin reorientation, and weak anomalous Hall features. Angle-resolved photoemission spectroscopy (ARPES) reveals linear Dirac-like band crossings at the X point, already present in the paramagnetic phase. First-principles calculations support a topological band inversion near the Fermi level and confirm the origin of the Dirac dispersion. These findings establish EuCu2Sb2 as a rare material system that bridges topological band structure with localized magnetism, offering a platform to explore symmetry-protected Dirac states in correlated magnetic materials.

11:00am **MI-MoM-5 Revisiting Altermagnetism in RuO2 and Cr-doped RuO2 Epitaxial Films through THz Spectroscopy and Neutron Scattering**, *David T. Plouff, Nawsher J. Parvez,* Department of Physics and Astronomy, University of Delaware*; Laura Scheuer,* Department of Physics and Astronomy, University of Delaware, Germany*; Shreya Shrestha,* Department of Physics and Astronomy, University of Delaware*; Weipeng Wu,* Department of Physics and Astronomy, University of Delaware, China*; subhash Bhatt,* University of Delaware*; Xinhao Wang,* University of Delaware, China*; Lars Gundlach, M. Benjamin Jungfleisch,* University of Delaware*; Xixiang Zhang,* King Abdulah University of Science and Technology, Saudi Arabia*; Adam A. Aczel,* Oak Ridge National Laboratory, USA*; Jonathan Gaudet,* National Institute for Science and Technology (NIST)*;* ***John Q. Xiao****,* University of Delaware **INVITED**

Altermagnetism has recently emerged as a potentially transformative concept in spintronics, offering the possibility of combining the ultrafast dynamics of antiferromagnets with spin-split electronic structures typically associated with ferromagnets. Among proposed candidates, rutile RuO_2 has attracted intense attention because of predictions of unconventional spin transport. However, despite intense activity, the existence of an intrinsic altermagnetic order in RuO_2 remains highly controversial.

In this talk, we will present our systematic experimental investigation of epitaxial RuO_2 and $Ru_{1-x}Cr_xO_2$ thin films using terahertz and neutron-scattering measurements. Time-domain THz spectroscopy measurements on RuO_2 reveal that previously reported spintronic signatures can be consistently explained by conventional mechanism, including inverse spin Hall effects and anisotropic electronic conductivity associated with the rutile crystal structure, without invoking altermagnetic order. Motivated by theoretical predictions that hole doping may stabilize an altermagnetic state, we further probed magnetic state in $Ru_{1-x}Cr_xO_2$ thin films by using neutron scattering techniques.Our measurements show no evidence of long-range magnetic ordering down to 10 K in $Ru_{0.8}Cr_{0.2}O_2$ thin films, placing important experimental constraints on current theoretical models of altermagnetism in rutile oxides.

Beyond resolving the magnetic ground state, our work also reveals a new THz emission mechanism originating from the interplay between spintronic THz generation and anisotropic electronic transport in RuO_2. This hybrid mechanism enables magnetic-field tuning of the polarization ellipticity of emitted THz radiation, opening new opportunities for functional THz emitters based on correlated oxide materials.

This research was sponsored by NSF DMR-2316664, NSF through the University of Delaware Materials Research Science and Engineering Center (MRSEC), and King Abdullah University of Science and Technology (KAUST), ORFS-2022-CRG11-5031.2.

11:30am **MI-MoM-7 Cobalt Doping on Topological Superconductor $FeTe_{0.55}Se_{0.45}$***,* ***John Drain***[1]*,* University of Wyoming*; Mykola Telychko,* Oak Ridge National Laboratory*; Zheng Gai,* Oak Ridge Natinal Laboratory*; TeYu Chien,* University of Wyoming

$FeSe_xTe_{1-x}$ (FTS) is an iron-based superconductor that has been shown to have non-trivial topology with the correct relative Te/Se content ($FeTe_{0.55}Se_{0.45}$) and relatively high superconducting transition temperature, T_c, of 14.5 K. Majorana zero modes (MZM), a quasiparticle needed for the development of topological quantum computing, have also been observed in magnetic vortices as well as at Fe adatom sites in FTS. Thus, the introduction of new magnetic elements to FTS is of particular interest, due to their potential to influence the formation of MZM and local topology. In this study, the effects of depositing magnetic Co atoms on the FTS surface are explored using scanning tunneling microscopy. We observe an apparent surface reconstruction after cobalt deposition with Co adatoms on top of the surface as well as defects from evident Co absorption. Areas with high concentration of Co defects show suppressed superconductivity. When superconductivity is preserved, in-gap bound states are observed at Co defect sites at either finite energy or zero energy. Furthermore, the energy of these finite energy states shifts to zero as the tunnel-barrier conductance of the STM tip is increased during spectroscopy measurements. The origins of these features as MZM, Yu-Shiba-Rusinov bound states, or Kondo effect will be discussed. These results present a potential prospect for a way to influence FTS properties locally through the introduction of Co to produce conditions ideal for Majorana zero mode and their braiding.

This work was funded by the NSF through Award #: DMR-2228841

11:45am **MI-MoM-8 Magnetic and Magnetostrictive Properties of Multilayer $Fe_{50}Co_{50}$ – Ag with Varied Ag Thickness***,* ***Thomas Mion****,* US Naval Research Laboratory*; Margo Staruch,* US naval Research Laboratory*; Zoey Warecki,* us naval Research Laboratory*; Konrad Bussmann, Peter Finkel,* US Naval Research Laboratory

Temperature stable high magnetostrictive materials are required for microelectromechanical systems (MEMS) devices that seek to function reliably at high temperatures. Due to the immiscibility of Ag with Fe and Co, multilayers of $Fe_{50}Co_{50}$ – Ag will not alloy up to at least 700 C allowing for a stable high magnetostrictive material for MEMS platforms. $Fe_{50}Co_{50}$ is known to be moderately magnetostrictive and with a curie temperature ~1,000 C and a high saturation magnetization. Previous studies have shown with ~10nm $Fe_{50}Co_{50}$ and ~3nm Ag layers the multilayer system remains up to 400 C where higher temperatures cause breakdown of the Ag interlayer. This investigation seeks to improve the thermal stability of the FeCo-Ag multilayer system through varied Ag thickness and understand the mechanism of the nonmagnetic layer breakdown. Transmission Electron Microscopy investigations reveal the Ag layer is coherent up to 77 multilayers (~930 nm) even with increased roughness as the thickness increases resulting in the restricted in-plane magnetization and subsequent lower coercive field.

Nanoscale Science and Technology
Room 320 - Session NS-MoM

Frontiers in Nanoscale Electron, Ion, and Scanning Probes I

Moderators: Dr. Marek Kolmer, Ames National Laboratory, **Dr. Yongtao Liu**, ORNL

10:00am **NS-MoM-1 The Atomic Single-Electron Transistor***,* ***Dahlia Klein****,* University of Chicago **INVITED**

Electrons in solids owe their properties to the periodic potential landscapes they experience. Moiré lattices have given us powerful new ways to engineer such landscapes on nanometer scales, yet directly imaging them remains elusive. In this talk, I introduce the Atomic Single-Electron Transistor (SET), a scanning probe that uses a single atomic defect in a van der Waals material as an ultrasensitive, high-resolution potential sensor. Built upon the quantum twisting microscope (QTM) platform, this probe leverages the QTM's capability to form a pristine, scannable 2D interface between van der Waals heterostructures. Using the Atomic SET, we present the first direct images of the electrostatic potential in graphene aligned to hexagonal boron nitride. This potential exhibits approximate C6 symmetry, minimal dependence on carrier density, and a magnitude of ~60 mV even in the absence of carriers. Notably, this magnitude significantly exceeds theoretical predictions, suggesting that our current understanding may be incomplete. With ~1 nm spatial resolution and sensitivity to potentials generated by only a few millionths of an electron's charge, the Atomic SET opens a path to imaging charge order and thermodynamic properties across a wide range of quantum phenomena.

10:30am **NS-MoM-3 Local Spectroscopy Reveals Quantum Geometry of Magnetic Bloch States and Hyperorbits in Hofstadter Bands***,* ***Dengyu Yang****,* National Institute of Standards and Technology (NIST)/ University of Maryland, College Park*; Lisa Frammolino, Duarte de Sousa,* National Institute of Standards and Technology (NIST)*; Rishav Harsh, Keunhong Min,* National Institute of Standards and Technology (NIST)/ University of Maryland, College Park*; Young Jae Song, Sungmin Kim,* National Institute of Standards and Technology (NIST)*; Ian Mercer,* Penn State University*; Kenji Watanabe, Takashi Taniguchi,* NIMS (National Institute for Materials Science), Japan*; Jon-Paul Maria,* Penn State University*; Paul Haney, Joseph Stroscio,* National Institute of Standards and Technology (NIST)

When a two-dimensional electron system is subjected to both a periodic potential and a magnetic field, its spectrum reorganizes into Hofstadter minibands set by the rational magnetic flux per unit cell. While the resulting subband hierarchy has been widely studied, the semiclassical dynamics of magnetic Bloch states, described as hyperorbits and supporting the higher order fractal spectrum, has remained far less explored experimentally. Here we use ultra-low-temperature STM/STS, supported by band-structure calculations, to study Bernal bilayer graphene in an hBN moiré lattice. We directly resolve Hofstadter minibands across continued fraction fluxes of the form $1/(q_1+1/q_2)$, demonstrate q_1 subbands across moiré filling for $q_2 = 0$, and observe further q_2-fold energy splitting and minigap formation at higher-order fractions. The field evolution of these spectra near commensurate flux show branch connectivity and minigap evolution consistent with hyperorbit quantization of magnetic Bloch bands. Gate-

[1] **Falicov Student Award Finalist**

dependent spectra track Chern-indexed gaps and reveal signatures consistent with interaction-driven flavor symmetry breaking. Theoretical calculations show the importance of the quantum geometry and Berry curvature of the electronic bands in determining the fine features of the energy spectrum. Our measurements show local spectroscopy of the magnetic Bloch states and the direct role of quantum geometry in Hofstadter physics.

10:45am **NS-MoM-4 Cryogenic STM Readout of High-Q MEMS Resonators for Superconducting Casimir-Force Measurements**, ***Robbie Elbertse***, *Minxing Xu, Ata Keşkekler,* Delft University of Technology, Netherlands*; Giuseppe Bimonte,* Università di Napoli Federico II, Italy*; Jinwon Lee, Sander Otte, Richard Norte,* Delft University of Technology, Netherlands

Scanning tunneling microscopy (STM) and micro-electromechanical systems (MEMS) have traditionally operated at vastly different length scales: one resolving atomic-scale structure, the other engineering collective motion in mesoscopic and macroscopic structures. Here we unite these regimes by using an STM junction as a minimally perturbative local actuator and detector for high-aspect-ratio MEMS resonators. Operating at cryogenic temperatures, we resolve acoustic modes of millimeter-scale, high-Q membranes without optical or capacitive readout, while maintaining local sensitivity to displacement and tip–sample interaction forces. The tunneling junction introduces negligible back-action and heating, enabling direct access to the intrinsic dynamics of microgram-scale oscillators. We demonstrate three complementary STM-based measurement modalities and show how they enable precision measurements of displacement, force, and pressure in cryogenic nanomechanical systems. We then apply this platform to the long-standing challenge of measuring changes in Casimir pressure across a superconducting transition, using a highly parallel on-chip membrane geometry. With verified micro-Pascal pressure resolution, this STM–MEMS approach provides a credible route toward studying fluctuation-induced forces in superconducting systems under conditions of alignment, stability, and sensitivity that have been difficult to access with conventional techniques.

11:00am **NS-MoM-5 Andreev Reflection and Electronic Reconstruction in Proximate Contacts to Superconductors**, ***Petro Maksymovych***, Clemson University*; Sang Yong Song,* Daegu Gyeongbuk Institute of Science and Technology, Republic of Korea*; Wonhee Ko,* University of Tennessee Knoxville*; Chengyun Hua, Gabor Halasz, Jiaqiang Yan, Benjamin Lawrie,* Oak Ridge National Laboratory, USA*; Jose Lado,* Aalto University, Finland

The transition from tunneling to contact is a crossover from exponentially decaying wavefunction overlap to coherent electronic hybridization between two conductors, and can be generally expected to produce phenomena distinct from both the tunneling and strong-coupling limits. Using the layered unconventional superconductor FeSe as a model system, we demonstrate that traversing this crossover with a scanning tunneling microscope enables both spectroscopic fingerprinting of the superconducting order parameter and nanoscale manipulation of individual vortex lines.

In the tunneling regime, Tunneling Andreev Reflection (TAR) spectroscopy exploits the exponential sensitivity of the excess decay rate to Andreev reflection, separating Andreev and quasiparticle currents through the additivity of their excess decay rates. Transport simulations show how higher-order scattering processes and the competition between Andreev and quasiparticle channels shape the decay rate spectra as coupling strength increases, distinguishing s-wave, d-wave, and sign-changing order parameters in ways inaccessible to conventional conductance-based methods [1].

At weak physical contact, the STM junction becomes a tunable vortex pinning potential. Tip-induced strain locally suppresses the larger of FeSe's two superconducting gaps while leaving the smaller gap intact, replicating the gap structure observed at twin boundaries and wrinkles. This strain-induced inclusion deflects individual vortex lines with forces of 1–5 pN, orders of magnitude larger than previously achieved in conventional superconductors, and the vortex line deformation grows logarithmically with contact conductance, consistent with an anisotropic inclusion model. Tip geometry further sets the deformation strength, providing a tunable handle even within dense vortex lattices [2].

Together, these results establish the tunneling-to-contact window as a powerful probe of quantum states, opening new pathways for studying exotic superconductors, vortex-bound electronic states, and nanoscale magnetism.

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[1] Maksymovych et al., Fingerprinting superconductors by disentangling Andreev and quasiparticle currents across tunable tunnel junctions, arXiv:2601.20798v1

[2] Song et al. Nanoscale (2026), 10.1039/D5NR04204F.

11:15am **NS-MoM-6 Probing Unconventional Superconductivity by Atomically Resolved Multi-Particle Tunneling Spectroscopy**, ***Wonhee Ko***, University of Tennessee, Knoxville

Unconventional superconductivity is central to emerging quantum technologies, including dissipationless electronics and topological quantum computing. Still, identifying the nature of unconventional superconducting states remains challenging because few experimental techniques can directly probe the superconducting order parameter. Here, we use scanning tunneling microscopy (STM) to perform multi-particle tunneling spectroscopy in atomic resolution and reveal the nature of unconventional superconductivity across a range of material systems. Multi-particle tunneling processes involving Cooper pairs—most notably Andreev reflection and Josephson tunneling—provide direct spectroscopic access to superconductivity [1,2]. With atomic-scale spatial resolution, STM further uncovers local variations in these tunneling spectra, offering insight into the symmetry of the superconducting order parameter. Applying these techniques to Fe-based chalcogenides and epitaxial two-dimensional superconductors, we have identified clear signatures of unconventional superconductivity in both classes of materials [3,4].

[1] W. Ko, E. Dumitrescu, and P. Maksymovych, *Phys. Rev. Res.* **3** 033248 (2021)

[2] W. Ko, J. L. Lado, and P. Maksymovych, *Nano Lett.* **22** 4042 (2022)

[3] W. Ko, S. Y. Song, J. Yan, J. L. Lado, and P. Maksymovych, *Nano Lett.* **23** 8310 (2023)

[4] P. Maksymovych, S. Y. Song, B. Lawrie, W. Ko, and J. L. Lado, *arXiv:2601.20798*

11:30am **NS-MoM-7 Optical Properties of Single Molecules Explored with sub-nm Precision**, ***Anna Roslawska***, Max Planck Institute for Solid State Research, Germany **INVITED**

Light-matter interaction is essential for mechanisms such as luminescence, photosynthesis, and energy harvesting, defining the emission characteristics of molecular systems and governing the conversion of energy between photons and electrons. While these processes are intensively studied and employed, little is known about their dependence on atomic-scale properties since reaching such precision in optics is extremely demanding. This challenge is nowadays overcome thanks to the combination of optical spectroscopy approaches with scanning probe microscopy, which profit from the extreme field enhancement provided by the tip that enables atomic-scale optics. In my talk, I will discuss how this approach can be applied to probe optical properties of individual phthalocyanine [1-3] and chlorophyll molecules.

1. A. Rosławska, T. Neuman, B. Doppagne, A. Borisov, M. Romeo, F. Scheurer, J. Aizpurua, G. Schull, Phys. Rev. X, 12, 011012, 2022.

2. K. Kaiser, S. Jiang, M. Romeo, F. Scheurer, G. Schull, A. Rosławska, Phys. Rev. Lett. 133, 156902, 2024.

3. A. Rosławska, K. Kaiser, M. Romeo, E. Devaux, F. Scheurer, S. Berciaud, T. Neuman, G. Schull, Nat. Nanotechnol., 19, 738-743, 2024.

Plasma Science and Technology
Room 315 - Session PS+AP-MoM

Plasma Processes for Advanced Interconnects

Moderators: Dr. John Arnold, IBM, **Takeshi Ohmori**, Hitachi

10:00am **PS+AP-MoM-1 Interconnect for 7A and Beyond**, ***Scott Allen***, IBM Research Division, Albany, NY **INVITED**

BEOL scaling continues to challenge the limits of plasma etch process capability. Conventional approaches have shown to have limited extendibility for next generation devices. Challenges with the traditional damascene integration and superior resistance scaling with alternate conductors make transition to subtractive patterning more attractive. Capacitance control using new dielectric materials or schemes requires innovation and examination. Additionally, High-NA EUV and other new

patterning techniques provide pathways forward but require significant development. Advances in etch tooling and stack materials are providing options to meet these challenges. Novel use of known techniques can be integrated with these new tools and materials to enable semiconductor technology at 7A and beyond.

10:30am **PS+AP-MoM-3 Epitaxial conductors to replace Cu in advanced interconnect metallization**, ***Jean-Philippe Soulie***, *François Chancerel, Steven Brems, Chen Wu, Johan Swerts, Seongho Park, Christoph Adelmann,* IMEC, Belgium **INVITED**

Cu interconnects face a steep resistance and reliability penalty when line widths approach dimension of 10nm: electron scattering at surfaces and grain boundaries amplifies the resistivity, while diffusion barriers and liners consume an increasing fraction of the available cross–section and are increasingly difficult to scale[1]. In this context, epitaxial conductors offer a fundamentally different route to sustain conductivity at nanoscale dimensions by eliminating large–angle grain boundaries, reducing microstructural variability, and improving pattern–transfer fidelity during direct metal etch. Here, we summarize our recent progress on epitaxial conductors aimed at replacing Cu in advanced BEOL metallization, with a focus on CMOS–compatible epitaxial Ru and metallic delafossite $PtCoO_2$.

For Ru, we demonstrate honeycomb epitaxy on AlN(0001)/Si(111) using standard PVD at a BEOL–relevant thermal budget, scalable to 300–mm wafers[2]. Structural characterization confirms coherent epitaxial alignment and low mosaicity. Electrical transport measurements reveal bulk–like resistivity (7.8μΩcm at 30nm), resulting in a markedly weaker thickness–dependent resistivity increase than polycrystalline Ru and Cu in the ultrathin regime. These findings highlight the advantage of suppressing grain–boundary scattering through epitaxy.

Beyond elemental metals, we show that metallic delafossite $PtCoO_2$ can deliver even lower resistivity at nanoscale thicknesses when epitaxy is stabilized. Using a multilayer PVD approach combined with repeated oxidation anneals, epitaxial $PtCoO_2$ is stabilized down to 4 nm and exhibits an unusual thickness–independent resistivity of 4.8μΩcm over the 8 to17nm range[3]. This behaviour is enabled by solid–phase epitaxial regrowth, film densification, and defect annihilation, underscoring the critical role of interface chemistry and oxygen control in complex oxide conductors.

Looking forward, the integration of epitaxial conductors into realistic interconnect architectures will require scalable strategies compatible with amorphous BEOL dielectrics. Layer–transfer approaches, such as wafer-to-wafer bonding followed by substrate removal, emerge as a universally applicable pathway for epitaxial conductor integration, enabling the decoupling of epitaxial growth from backend processing. Continued progress in epitaxial growth, interface engineering, and transfer integration positions epitaxial Ru and delafossite oxides as strong contenders for future liner–light or linerless interconnect technologies beyond Cu.

[1]J-Ph. Soulié,J. Appl. Phys.136(17)171101(2024).[2]C. Adelmann,2026 ECTC(2026),Orlando(USA).[3]JJ-Ph. Soulié,2026 IEEE IITC(2026),San Jose (USA)

11:00am **PS+AP-MoM-5 Reactive High Power Impulse Magnetron Sputtering with Positive Cathode Reversal Using a Rotary Magnetron**, ***Nicholas Connolly***, *Collin Jeckell,* University of Illinois Urbana-Champaign*; Rajib Paul, Brian Jurczyk,* Starfire Industries, LLC*; David Ruzic,* University of Illinois Urbana-Champaign

This work investigates the novel sputtering technology of HiPIMS with positive cathode reversal (Positive Kick™), herein referred to as HiPIMS+CR, on rotary magnetrons for reactive sputtering. As compared to DC, HiPIMS provides the advantage of higher ion fractions at the target[1] and at the substrate[2]. As compared to standard HiPIMS, positive cathode reversal allows for control of the ion energy at the substrate, allowing for tuning of film properties such as stress as well as increased deposition rate overall[3]. In this work, the deposited film is aluminum nitride (AlN), which has applications in resonator devices, piezoelectric devices, and as a thermal spreader for heat management[4]. Many large-area industrial coating processes utilize rotary magnetrons instead of planar magnetrons, as they offer increased target utilization and higher power throughput due to better heat removal. It has been shown with DC that rotary magnetrons offer some benefits and differing deposition physics when compared to planar targets because of the target shape and rotation[5]. This work characterizes HiPIMS+CR applied to a rotary magnetron with target length of 430mm and target outer diameter of 145mm, identifying where the rotary configuration may offer benefit through a research-scale system.

HiPIMS+CR AlN reactive sputtering in the rotary magnetron configuration is characterized by both plasma diagnostics and film characteristics. To characterize the plasma, a Hiden Analytical PSM probe was used to gather time and energy resolved spectra of each ion species at the substrate location versus various plasma parameters. Whether the target was rotating or not rotating affected both the Al^+ and N^+ ion counts without changing the Ar^+ and N_2^+ counts (see Figures 1 and 2), where the N^+/Al^+ ratio increased by over 50% by simply rotating the target and keeping all other process parameters constant. This indicates target rotation does affect the system and adds another variable to adjust film properties such as stoichiometry. Hysteresis curves were generated at various target rotation speeds to understand how the poisoning point was affected by rotation speed in HiPIMS+CR.

AlN film characterization will be presented across varying HiPIMS+CR process recipe parameters, as well as target rotation speed, for the critical characteristics of the applications of AlN. Characteristics measured include film stoichiometry (including oxygen contamination), crystal structure and orientation measured with X-ray diffraction (XRD), and film density measured with X-ray reflectivity (XRR). Thermal conductivity measurements are also made using time-domain thermoreflectance (TDTR).

11:15am **PS+AP-MoM-6 Two-Step Etching for Suppressing Etch-Depth Variation in Tin Etch-Back**, ***Yudai Mashiko***, *Makoto Satake, Taku Iwase, Naoyuki Kofuji, Yasushi Sonoda,* Hitachi, Ltd., Japan

In the fabrication of advanced semiconductor devices, uniform TiN etch-back—in which TiN is filled into deep trenches—is essential for contact-plug formation. However, seams are unintentionally formed during the filling process. Consequently, the local etching rate increases due to seam widening, resulting in etch-depth variation between the area around the seam and the surrounding region [1].

In our previous study [2, 3], we reported that radical etching was superior to plasma etching because, in the latter, energetic ions accelerated by self-bias voltage exacerbated seam widening. However, even with conventional radical etching, it remains difficult to suppress the direct exposure of radicals to the seam region. Therefore, we propose a two-step etching process that employs a deposition-film formation step prior to etching. In this method, a deposition film is first formed to serve as a mediating layer, after which TiN is etched by radicals while maintaining this film. This approach is designed to prevent the direct exposure of radicals to the seam.

The mechanism underlying seam-widening suppression was investigated using etch-profile simulations. The deposition film on the TiN surface significantly shortens the effective mean free path of the radicals, thereby preventing their direct exposure to the TiN surface. Consequently, the radical flux reaching the seam interior is markedly reduced, shifting the etching process from a reaction-limited to a supply-limited regime. This transition ensures that etching is governed by the arrival rate of radicals rather than their reactivity, which the simulations confirmed effectively suppresses seam widening compared with conventional radical etching.

Based on these findings, the two-step process was experimentally demonstrated. A $SiCl_x$ deposition film was formed using $Cl_2/SiCl_4$-based plasma, followed by TiN etching with Cl_2-based plasma. Cross-sectional observations confirmed that the standard deviation of the etch-depth variation was significantly reduced from 3.8 nm (conventional) to 1.5 nm. These results demonstrate that the proposed two-step etching is an effective approach for achieving uniform TiN etch-back.

[1] G. Vereecke et al., Microelectron Eng. 200 (2018).

[2] Y. Mashiko, et al., DPS 45th international symposium (2024)

[3] T. Iwase, et al., Proc. SPIE PC13429 (2025)

11:30am **PS+AP-MoM-7 Roughness Generation Mechanisms in Ru Etching Using O_2/Cl_2-Based Plasma for Advanced Interconnects**, ***Miyako Matsui***, *Tomoyasu Shohjoh, Taiga Kasai,* Hitachi Ltd., Japan*; Kiyohiko Sato, Makoto Miura,* Hitachi High-Tech Corporation, Japan*; Kenichi Kuwahara,* Hitachi High-Tech Corporation, Jamaica **INVITED**

Continued device miniaturization necessitates further reduction of metal pitch through advanced patterning technologies such as extreme ultraviolet lithography. As metal pitches shrink, alternative metal interconnects are required to replace Cu in order to achieve tighter pitches in the back end of line. Ru is a candidate for alternative interconnects at metal pitches of 20 nm and below, because Ru interconnects are expected to exhibit lower effective resistance than Cu interconnects at such small dimensions. In addition, Ru can be etched directly, enabling new scaling boosters such as semi–damascene patterning. To realize such patterning technologies, Ru

patterns must be etched vertically with high selectivity to hard masks, while roughness and other forms of damage must be suppressed to reduce interconnect resistance.

In this work, we investigated the mechanisms of roughness generation during Ru etching and achieved low–roughness etching of fine Ru patterns using an O_2/Cl_2–based plasma generated by a microwave electron cyclotron resonance etching system. The roughness of Ru line patterns is primarily governed by the transfer of mask pattern roughness, as well as by micromasking effects caused by non–volatile byproducts formed on the sidewalls and by the Ru grain structure.

To analyze the mechanisms of roughness generation in Ru etching, the line edge roughness (LER) of Ru lines and Si_3N_4 masks was evaluated before and after Ru etching using a high–voltage CD–SEM, which simultaneously evaluates Si_3N_4 mask roughness from secondary-electron images and Ru line roughness from backscattered-electron images. Ru etching was performed on 32 nm-pitch Ru patterns with Si_3N_4 mask line widths varied from 23 nm to 10 nm. We found that Ru line roughness is influenced not only by Si_3N_4 mask roughness but also by non–volatile RuO_x and $RuCl_x$ species non–uniformly formed on the Ru sidewalls. In addition, Ru sidewall etching tends to proceed preferentially along grain boundaries. The roughness of Ru sidewalls depends on the balance between ion flux, which generates non–volatile RuO_x and $RuCl_x$ on the sidewalls, and radical flux, which isotropically etches Ru.

To reduce the LER of Ru lines, we proposed adding a passivation gas to the O_2/Cl_2 plasma to form a uniform protective layer on the pattern sidewalls. This uniform protection layer enables stable etching of fine patterns even when the balance between ion flux and radical flux penetrating into the trenches varies to some extent with changes in aspect ratio during Ru etching.

Quantum Science and Technology
Room 304 - Session QS-MoM

Qubit Modalities I — Hybrid Superconducting–Semiconducting Quantum Devices

Moderators: Dr. Aranya Goswami, Nokia Labs, **Dr. Dave Pappas**, Rigetti Computing

10:00am **QS-MoM-1 Quantum Devices based on Sn-InAs Nanowire Josephson Junctions**, ***Sergey Frolov***, University of Pittsburgh **INVITED**

I will discuss superconducting qubits and parametric amplifiers based on hybrid superconductor-semiconductor Josephson junctions. The basic physics of these platforms is fairly understood and non-controversial. The bigger circuits tend to use similar materials, such as aluminum. It is a great superconductor for device applications. But similar qubits can also be made out of different materials which come with larger gaps, stronger spin-orbit interaction, electrical and not magnetic tunability and other nominal advantages. We are working on unexplored materials for those, namely Sn-based InAs nanowire Josephson junctions. Of course new materials are less mature as device platforms, but trying to make them perform can offer valuable lessons and expand our understanding of what works and why. Our InAs-Sn transmonos have reached a T1 relaxation time of 27 microseconds, and T2 dephasing times of 18 microseconds. We also report reduced nonlinearity beyond the short junction limit due to higher-order Josephson harmonics. Our parametric amplifiers operate both in the four-wave mixing mode as well as in the three-wave mixing mode, driven by the unconventional Josephson relation. We also demonstrate Andreev qubits based on nanowires, including the spectroscopy of a perfectly transmitting Majorana-like Andreev bound state.

10:30am **QS-MoM-3 Transport Study of SQUID Devices on Ge Quantum Well for Protected Superconducting Qubit**, ***Shukai Liu***, *Adhilsha Parachikunnumal, Joshua Thompson, Kasra Sardashti,* University of Maryland College Park

Superconductor-semiconductor (super-semi) hybrid Josephson junctions (JJs)emerged as a promising platform for a protected superconducting qubit with a π-periodic potential in phase. The π-periodic potential is achieved by leveraging the non-sinusoidal current-phase relation (CPR) of the super-semi JJs and the phase interference between JJs in a SQUID loop. In this talk, we share our progress toward realizing a moderately-protected superconducting qubit based on super-semi JJs realized on a Ge quantum well(QW), which promises a high baseline coherence from not only the parity protection but also the high- purity Si substrate. We focus on the transport measurement of SQUID devices on Ge QW to extract the current-phase relation at half-integer flux quanta, aiming to optimize the device parameters for qubit protection against both depolarization and dephasing.

10:45am **QS-MoM-4 Characterizing single and double quantum dots with quenched charging energy in semiconductor PbTe nanowires**, ***Seth Byard***, *Maksim Gomanko,* University of Pittsburgh*; Tongxie Zhang, Shixiong Zhang,* Indiana University Bloomington*; Sergey Frolov,* University of Pittsburgh

PbTe is a IV-VI narrow-bandgap semiconductor with potential utility for novel topological or spin qubits. One of PbTe's most notable characteristics is its large static dielectric constant, which exceeds 1000 at cryogenic temperatures and thus results in quenched charging energy in hosted quantum dots (QDs). Here we present our findings from transport measurements of QD systems defined electrostatically in PbTe nanowire devices and examine the implications of these results for our ongoing development of PbTe spin qubits.Our samples display large and highly anisotropic spin-orbit interaction (SOI) strengths and effective Landé g-factors, both of which are generally desirable properties for spin qubits. We characterize these anisotropies through the use of an externally applied magnetic field with variable angle. We discuss our analysis and interpretation of these data, focusing on how they relate to PbTe's rocksalt crystal structure.We additionally report the definition and control of double quantum dots in such systems. We find charge stability diagrams distinguished by the spin degeneracy of all transport resonances at zero magnetic field. We show the fourfold splitting of high-bias triangles in an applied magnetic field to illustrate the lifting of spin degeneracy via the Zeeman effect. We also identify patterns of transport resonances within these high-bias triangles and discuss their possible physical origins.

11:00am **QS-MoM-5 Sn–Inas Nanowire Josephson Parametric Amplifiers as Probes of Hybrid Junction Nonlinearity**, ***Amritesh Sharma***, *Amrita Purkayastha,* University of Pittsburgh, USA*; Param Patel,* Yale University*; Subhayan Sinha, Shreyas Asodekar,* University of Pittsburgh, USA*; An-Hsi Chen,* Grenoble-INP/CNRS, France*; Connor Dempsey,* University of California Santa Barbara*; Kun Zuo,* University of Sydney, Australia*; Chris Palmstrom,* University of California at Santa Barbara*; Moira Hocevar,* Grenoble-INP/CNRS, France*; Michael Hatridge,* Yale University*; Sergey Frolov,* University of Pittsburgh, USA

Hybrid semiconducting Josephson junctions, where proximity-induced superconductivity in a spin–orbit-coupled nanowire can be tuned by gate voltage and magnetic field, offer a rich platform to explore nonlinear quantum dynamics beyond what conventional Josephson tunnel junctions provide. We embed single Sn-InAs nanowire Josephson junctions carrying supercurrents of order 0.5 μA into NbTiN coplanar waveguide resonators to realize Josephson parametric amplifiers (JPAs) and probe the junction's intrinsic nonlinearity in a controlled microwave environment. The intrinsic quartic (Kerr) nonlinearity drives a four-wave mixing process yielding up to 20 dB of parametric gain in reflection, building on our prior demonstration of nanowire-based transmon qubits[1,2] and further establishing Sn-InAs nanowire junctions as effective nonlinear circuit elements at microwave frequencies.

Beyond amplification, we use the parametric response as a sensitive probe of how electrostatic gating, which tunes the resonant frequency by hundreds of MHz, and applied magnetic field modify the junction's nonlinear character. In select devices, we observe signatures of Kerr coefficient suppression and three-wave mixing, pointing to the activation of nonlinear terms beyond the standard quartic nonlinearity. These observations are consistent with higher-order or odd-order contributions expected when strong spin–orbit coupling and time-reversal symmetry breaking lift the constraints that ordinarily confine conventional Al/AlOx junctions to purely four-wave mixing processes [3]. These results establish the Sn-InAs nanowire JPA as both a functional quantum amplifier and a spectroscopic tool for studying field- and gate-tunable nonlinearity in hybrid Josephson systems.

References:

[1] A. Purkayastha et al., *Nano Lett.* 26, 2074 (2026).
[2] A. Purkayastha et al., arXiv:2603.26895 (2026).
[3] T. Reza et al., *SciPost Phys.* 20, 089 (2026).

11:15am **QS-MoM-6 Optimizing Ge/SiGe Quantum Well Interfaces for Low-Noise Spin Qubits via Surface Passivation***, **Iris Boateng**, Rebika Makaju, Giovanni Franco-Rivera, Kasra Sardashti,* Quantum Collaborative Research Corps & Department of Physics, University of Maryland, College Park MD, USA

Silicon-Germanium (SiGe) heterostructures are one of the leading platforms for semiconductor-based spin qubits. In silicon-based heterostructures, quantum dots (QDs) are defined electrostatically by lithographically patterned surface gates, allowing the confinement of a few electrons or holes and the manipulation of their spin degree of freedom for quantum information processing. However, a critical challenge in fabricating low-noise Ge/SiGe quantum dots is controlling the interface between the semiconductor and the high-κ gate dielectric, such as Al_2O_3. Imperfections at this boundary, primarily driven by the formation of unstable Ge-O bonds, lead to a high density of interface traps (D_{it}) [1]. These charge traps act as prominent sources of electrical noise, degrading device tune-up reliability and coherence [2]. In this work, we explore a systematic series of pre-deposition surface passivation methods designed to mitigate these interfacial defects and minimize D_{it}. We investigate a range of in-situ and ex-situ chemical treatments applied prior to atomic layer deposition (ALD). These protocols are specifically targeted at suppressing the formation of deleterious Germanium suboxides and promoting stable, stoichiometric bonding across the semiconductor-dielectric boundary. To evaluate the physical and chemical efficacy of these varying passivation techniques, X-ray photoelectron spectroscopy (XPS) is utilized to meticulously characterize the Silicon and Germanium chemical specie concentrations after each processing step. By correlating these chemical depth profiles with frequency dependent capacitance-voltage (C-V) measurements performed on Metal-Oxide-Semiconductor Capacitor (MOSCAP) devices, our aim is to establish a deterministic link between the targeted interface chemistry and the resulting electrical trap density. Ultimately, this comparative analysis aims to identify optimal interface engineering protocols, providing a clear pathway for the fabrication of highly stable, low-noise quantum dot devices for semiconducting based quantum computing architectures.

References:

[1] Duygu, K. et al. Microelectronic Engineering 88, 3428-3431 (2011).

[2] Leonardo, M. et al. Commun. Mater. 5, 151 (2024).

11:30am **QS-MoM-7 A Rapidly Iterable, Materials-Agnostic Platform for Correlating Loss in Superconducting Qubits***, **Mihir Pendharkar**,* Stanford University **INVITED**

Most superconducting qubits use Josephson junctions made by angled evaporation, which ties the device to a narrow set of materials and processes. I will share our group's work on a junction approach that loosens these constraints. By decoupling junction synthesis from device geometry — the essence of a trilayer architecture — the junction becomes a designer element whose materials, barrier, and layering are chosen deliberately and iterated rapidly. The approach is, in a useful sense, materials-agnostic, since it accommodates many material systems; yet that same freedom makes it deeply materials-focused, turning the junction stack into a controlled experimental variable. It also extends naturally across qubit geometries, from transmons to mergemons and beyond, and supports industry-scalable practices such as lift-off-free junction fabrication.

I will delve into the novel junction materials this approach makes accessible and how they push qubit operation toward higher frequencies and temperatures than conventional devices reach. From there I will turn to what synchrotron x-ray techniques uncover about a working junction — the buried interfaces, disorder, and composition that define its true nature within the qubit and that electrical measurements leave hidden. Threading these together is a fast loop — design a junction, build it, measure it, resolve its structure — through which we aim to draw direct, microscopic correlations between materials and the sources of loss in superconducting qubits.

Surface Science
Room 305 - Session SS-MoM
Precision On-Surface Synthesis

Moderators: Dr. Nathan Guisinger, Argonne National Laboratory, USA, **Pavel Jelinek**, Institute of Physics of the Czech Academy of Sciences

10:00am **SS-MoM-1 Porous Graphene Nanoribbons and Nanomeshes***, **Alexander Sinitskii**,* University of Nebraska-Lincoln **INVITED**

Atomically precise porous graphene nanostructures provide a versatile platform for tailoring electronic properties through controlled structural design. Here, we present a bottom-up synthetic strategy that provides access to a family of nanoporous graphene nanomaterials, including porous nanographenes, porous graphene nanoribbons (pGNRs), and extended nanoporous graphene (NPG) networks, all derived from closely related triphenylene-based molecular precursors [1]. By varying the synthetic environment, the same molecular building blocks can be directed toward distinct carbon architectures: solution-phase coupling yields cyclotrimeric porous nanographenes, whereas on-surface synthesis on Au(111) promotes linear polymerization and cyclodehydrogenation into atomically precise pGNRs. At high surface coverage and elevated annealing temperatures, these ribbons laterally fuse into extended nanoporous graphene sheets, establishing a modular and broadly tunable synthetic framework for porous carbon nanomaterials.

This platform further enables systematic investigation of how nanopore incorporation influences GNR properties [2]. By comparing a pristine N = 15 armchair GNR (15-AGNR), its periodically perforated analogue containing [18]annulene pores (15-pGNR), and the more extensively carved chevron GNR (cGNR), we track the evolution of the electronic structure with progressive pore opening. STS and ARPES measurements, as well as theoretical calculations, reveal that introducing periodic nanopores into the 15-AGNR produces a greater-than-twofold increase in bandgap, while further evolution toward the cGNR architecture results in comparatively smaller changes. These findings provide direct insight into the combined roles of geometric confinement and periodic lattice perforation in tuning GNR electronic structure.

We further expand the structural complexity of these systems by laterally fusing pGNRs into NPG networks containing periodically spaced biphenylene units, representing a novel 2D carbon allotrope [3]. STM, nc-AFM, and DFT calculations demonstrate that incorporation of biphenylene motifs into a porous graphene framework gives rise to distinct electronic behavior, including reduced and indirect bandgaps. Collectively, these studies establish a unified molecular design strategy for structurally related porous graphene nanomaterials with tunable topology and electronic functionality, spanning 0D, 1D, and 2D carbon architectures.

[1] M. Sarker, *et al*., *J. Am. Chem. Soc.*, **2024**, *146*, 14453.

[2] J.D. Teeter, *et al*., *ACS Nano*, **2026**, *20*, 8372.

[3] P. Angulo-Portugal, *et al*., *Adv. Mater.*, **2026**, e11706.

10:30am **SS-MoM-3 On-surface Synthesis of Porphyrin-Based MONs: a Model System for -Artificial Spin Lattices***, Eidsa Brenda Costa Ferreira,* University of Campinas (UNICAMP), Brazil*; Rafael Reis Barreto,* university of campinas (UNICAMP), Brazil*; Otavio Rodrigues de Oliveira, Iago Aedon Silva Prior, Isabela Costa Tonon,* University of Campinas (UNICAMP), Brazil*; Vanessa Carrenõ-Diaz, Breno Santimaria Sertori,* university of Campinas (UNICAMP), Brazil*; Igor Stein Weiler, **Abner de Siervo**,* University of Campinas (UNICAMP), Brazil

Over the past decade, significant advances have been achieved in the on-surface synthesis of atomically precise one-dimensional (1D) and two-dimensional (2D) metal–organic networks (MONs) using selected molecular precursors as modular building blocks in a "molecular LEGO" approach. This strategy exploits substrate properties, precursor molecular geometry, functional groups, diffusion behavior, and thermal activation energies to steer hierarchical reactions and the formation of novel nanostructures [1]. Porphyrins have well-defined geometry, rich electronic properties, and the ability to accommodate a central metal atom within their mycrocycles, making them particularly promising building blocks. When their molecular periphery is terminated with cyano, pyridyl, carboxylic, or halogen groups, deposited or substrate-derived adatoms can be trapped to form metal–organic coordination nodes. This leads to MONs with linear, square, rectangular, hexagonal, or kagome lattices, with geometries dictated by the molecular structure and substrate registry. Such architectures serve as important model systems for two-dimensional artificial spin lattices, among other phenomena. In this work, we present recent examples of MON

formation using two types of free-base porphyrins: 5,10,15,20-tetra(4-pyridyl)porphyrin (2H-TPyP) on Ag(100) [2] and 5,10,15,20-tetrakis[4'-(4-pyridyl)phenyl]porphyrin (2H-TPyPP) on Ag(111)[3]. In both cases, the introduction of Fe promotes de formation of different MONs with well-ordered and extended spin lattices. These different structures can be selectively realized by controlling the annealing protocol and the Fe deposition sequence [2,3]. These studies combine scanning tunneling microscopy (STM) and X-ray photoelectron spectroscopy (XPS) experiments, supported by density functional theory (DFT) calculations.

Acknowledgements

This work was financially supported by FAPESP (2022/12929-3; 2024/07409-6; 2025/02160-2), CNPq, and CAPES from Brazil.

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[1] J. Barth, G. Costantini, K. Kern, *Nature* **437,** 671–679 (2005).

[2] Rafael Reis Barreto, et al., Surface Science 766, 122897 (2026).

[3] Eidsa Brenda da Costa Ferreira, et al., "Engineering Two-Dimensional Artificial Spin Lattice Based on Porphyrins Metal-Organic Networks" (under preparation).

10:45am **SS-MoM-4 Deciphering Atomic Layer Deposition in Materials Processing: A Surface Science Perspective***, **Joerg Libuda**,* Friedrich-Alexander-University Erlangen-Nürnberg (FAU), Germany

Atomic Layer Deposition (ALD) enables controlled growth of ultrathin films with sub-nanometer precision, making it a key technique for nanoelectronics, catalysis, and energy applications. However, its success critically depends on the early stages of nucleation, which determine film continuity, uniformity, and defect density. Achieving uniform nucleation and atomic-level control remains challenging. Among the emerging materials accessible by ALD, transition-metal dichalcogenides (TMDCs) are of particular interest due to their tunable band gaps. Besides the extensively studied MoS_2, HfS_2 is a promising candidate, offering higher carrier mobility and a suitable band gap for electronic applications.

Here, we present our work on elucidating ALD nucleation mechanisms using a surface-science approach under ultrahigh vacuum (UHV). Atomically defined films and nanoislands of transition metal oxides (CoO(100), Co_3O_4(111)) on metal single crystals (Ir(100), Au(111)) serve as model substrates. HfS_2 growth is achieved via self-limiting reactions of tetrakis(dimethylamido)hafnium (TDMAH) with H_2S (or D_2S). The nucleation and growth processes are investigated in situ by combining scanning tunneling microscopy (STM) with time-resolved and temperature-programmed infrared reflection absorption spectroscopy (TR-IRAS, TP-IRAS).

Our results reveal that initial ALD nucleation is highly complex, involving multiple mechanisms and surface species. In the presence of surface OH/H_2O, mobile OH species induce full TDMAH hydrolysis (Brønsted acid–base mechanism). With increasing exposure, nuclei evolve dynamically through reactions of partially hydrolyzed species. While OH-functionalized self-assembled monolayers reduce OH mobility, substantial stoichiometric changes persist during early growth. Notably, nucleation also occurs on oxide surfaces in the complete absence of OH groups, indicating a Lewis acid–base mechanism with ligands bound to surface Co^{2+} sites. On CoO nanoislands, STM identifies initial intermediates, providing direct evidence for the Lewis acid–base mechanism. At elevated temperatures, dehydrogenation sets in as an additional reaction channel and generates OH groups that subsequently react via the Brønsted acid–base mechanism.

Overall, nucleation involves a highly complex interplay of Brønsted and Lewis acid–base pathways and dehydrogenation processes. These findings highlight that precise control over process parameters, surface structure, OH/H_2O chemistry, and reactant purity is essential for achieving controlled ALD nucleation.

11:00am **SS-MoM-5 Iterative Organic Modification of Pt Nanoparticles for Site-Selective Surface Engineering***, **Yongju Yun**, Minji Yun,* Pohang University of Science and Technology (POSTECH), Republic of Korea

The controlled modification of surface chemical environments is important for understanding structure-sensitive reactions on metal nanoparticles. However, conventional single-step surface modification methods often lead to non-selective coverage of surface sites, limiting precise control over local surface environments. In this study, we present an iterative organic modification strategy using ethylenediamine (EDA) as a molecular modifier to tune the electronic and geometric properties of Pt/Al_2O_3 surfaces. Successive cycles of molecular adsorption and mild thermal annealing progressively introduced N-containing surface species. X-ray photoelectron spectroscopy (XPS) showed an increase in the fraction of electron-deficient $Pt^{\delta+}$ species through Pt–N interfacial interactions. In parallel, CO diffuse reflectance infrared Fourier transform spectroscopy (CO-DRIFTS) suggested preferential modification of under-coordinated (UC) sites, leading to a relative increase in the exposure of well-coordinated (WC) terrace sites. Compared with conventional single-step modification, the iterative approach resulted in a higher WC/UC ratio, indicating improved site selectivity. The modified catalysts exhibited enhanced enantioselective hydrogenation performance for α-keto esters, achieving an enantiomeric excess (ee) of up to 96.5%. These results demonstrate that iterative organic modification can provide an effective approach for tuning interfacial surface environments and surface-site distributions on heterogeneous catalysts.

11:15am **SS-MoM-6 Probing the Role of Anodization Leading to Improved Sn Uptake for the Creation of High-Performance Nb_3Sn SRF Cavities***, **Jasper Brown**, Van Do,* University of Chicago*; Liana Shpani,* Cornell University*; Helena Lew-Kiedrowski,* University of Chicago*; Matthias Liepe,* Cornell University*; Steven Sibener,* University of Chicago

One of the primary obstacles to implementing Nb_3Sn in the creation of high performance superconductnction radio frequency cavities (SRF) for use with high gradient particle accelerators is the presence of film-growth inhomogeneities, which promote vortex pinning and generate localized surface hot spots that degrade cavity performance. Studies have shown that pre-anodizing Nb enhances Sn nucleation, leading to the formation of more stoichiometric and uniform Nb_3Sn coatings. Although anodized Nb surfaces have been widely investigated, there remains limited understanding of the chemical and structural evolution of these surfaces under Sn nucleation conditions. In this work, we employ in-situ X-ray photoelectron spectroscopy (XPS) and atomic force microscopy (AFM) to examine the thermal evolution of anodized polycrystalline Nb samples annealed to 773 K at heating rates of 3 K/min and 7 K/min in the absence of Sn. We find that compared to the control sample, the anodized Nb surface exhibits an RMS roughness an order of magnitude greater and displays an isotropically rough and porous morphology that persisted throughout the annealing process. Additionally, XPS measurements revealed persistent surface contamination associated with the anodizing electrolyte both prior to and following annealing. Through this study, we quantified surface roughness, chemical composition, and the oxide dissolution activation energy for both anodized and native Nb surfaces. These findings provide important insight into the role of anodization in influencing Sn nucleation behavior and the subsequent Nb_3Sn alloying process.

11:30am **SS-MoM-7 Methods and Mechanisms to Engineer Monodispersed Noble Metal Single Atoms, Dimers, Trimers, and Bi-atomic Metal–Oxygen Dimers on TiO_2(110)-(1×1) Surface for Catalysis***, **Xiao Tong**,* BNL

Monodispersion of size-selected nanoclusters supported on metal oxide is critical for catalytic activity, selectivity, and stability, but small clusters often diffuse and aggregate into 3D structures after adsorption, losing their size specificity. This study examines how oxygen vacancy density, cluster landing energy, and environmental water influence the adsorption of Au_1, Ag_n (n = 1–3), and VO clusters on TiO_2(110)-(1×1). High landing energies of clusters or elevated substrate temperatures promote monodispersion of monomers, dimers, trimers, and 2D sheet growth by creating transient defects that pin clusters while thermal dissipation heals surrounding damage, or by preserving oxygen vacancies from passivation by environmental water. Water can displace Au_1 from oxygen vacancies to nearby 5-fold Ti sites and passivate the vacancies through hydroxyl formation. VO clusters stabilize water dimer strings that act as barriers and spacers, preventing aggregation of incoming clusters and enabling control over monodispersion density by modulating string length. These findings demonstrate how tuning physical and chemical parameters can stabilize the monodispersion of size- and composition-selected clusters, advancing novel catalytic design.

11:45am **SS-MoM-8 Ni Porphyrin as a Model Single Atom Catalyst for CO_2 Adsorption***, J. Sanchez,* The University of Texas at San Antonio*; J. Martinez, P. Sharma, H. Wang,* University of North Texas*; **Fang Xu**,* The University of Texas at San Antonio

Metalloporphyrin is an ideal model for fundamental studies of single atom catalysis (SAC), becaues the electronic structure of the central metal atom is tunable by electron donating or withdrawing substituents.In this work, we investigate the self-assembly and electronic structure of Ni-tetraisopropylporphyrin (Ni-TIPP) and its substituent Ni-tetrabromoisopropylporphyrin (Ni-TBTIPP) for CO_2 activation on Au(111) surface. Scanning tunneling microscopy and spectroscopy (STM/STS) were

employed to qualitatively probe changes in local density of states associated with variations in the porphyrin substituents and central metal environment. STS detects a large band gap associated with the strong insulating porphyrin molecules. The STM results show that Ni-TIPP forms a 2D network of porphyrin islands with an upward tilted phenyl in each molecule due to possible tension, while molecules at the edge of the islands appear relaxed and more planar to the surface. The tilt was not observed in the case of Ni-TBTIPP which self-assembles planarly and flatly to the Au(111) substrate. The assembled Ni-TIPP was subsequentially exposed to CO_2 through a direct dosing tube with enhanced pressure effect. Control experiments of STM and temperature desorption indicate the formation of formate as the intermediate of CO_2 activation. This work visualizes CO_2 activation to formate over Ni metalated porphyrins for the first time, and the fundamental understanding provides key insight toward catalytic designs of CO_2 conversions.

Biomaterial Interfaces
Room 321 - Session BI-MoA

The Future of Biointerface Science

Moderator: Prof. Dr. Tobias Weidner, Aarhus University, Denmark

4:00pm **BI-MoA-11 Interactions Between Marinobacter atlanticus and Heavy Metals**, ***Sara Tuck,*** Naval Medical Research Command*; Maryssa Beasley, Rebecca Mickol,* U.S. Naval Research Laboratory*; Katherine Franz,* Duke University*; Kenan Fears,* U.S. Naval Research Laboratory

Marine bacteria have evolved mechanisms for the regulation of essential heavy metal ions (e.g., copper, zinc, cobalt). Understanding the interplay between these ions and marine bacteria is relevant to a variety of applications, including the development of antifouling coatings and materials and the capture and sensing of metal ions in seawater. Here we investigate the interactions between *Marinobacter atlanticus* and heavy metals commonly found in natural environments at trace levels. Further, *M. atlanticus* can produce small amounts of electricity and this ability is affected by labile metal ion concentration and can influence mineral cycling. We hypothesized that *M. atlanticus* may be a promising candidate for applications in heavy metal remediation or as a biosensor for heavy metal contamination. We utilized broth microdilution assays to expose *M. atlanticus* to a concentration range of essential and non-essential metal ions. *M. atlanticus* demonstrated a profound ability to grow in the presence of metal concentrations that significantly exceed those found in native environments. In metal depletion assays, where the ability of *M. atlanticus* to remove metal ions from solution was assessed, we found that this bacterium exhibited a marginal ability to reduce metal concentrations, with cadmium being the only heavy metal whose uptake significantly increased throughout a 72-hour evaluation period. Our results suggest *M. atlanticus* has limited use for bioremediation but could be used for biosensing.

4:15pm **BI-MoA-12 Addressing Agricultural Challenges Through Biomimetic Surfaces: Reframing Foliar Fungal Disease as a Biointerface Problem**, ***River Pachulicz,*** *Bryan Coad,* Adelaide University, Australia

Food security and agricultural economies depend on the continued production of grain crops, including barley, wheat and oats. Foliar fungal diseases pose a major threat to grains production worldwide, and solutions to reduce their incidence heavily rely on broadacre fungicide applications after disease occurs. This can be costly, environmentally harmful and eventually promote the emergence of chemically resistant pathogens. Prophylactic strategies to prevent fungal disease occurrence are scarce, but a shared bottleneck to fungal disease progression may a key target for intervention: the fungal pathogen must detect and successfully recognise the host's surface. This initial point of contact in plant-fungi interactions can hence be reframed as a biointerfaces problem that materials science can address.

The cuticle is a waxy bio-composite that coats the surface of leaves and is comprised of a cutin matrix that is embedded and/or coated with cuticular waxes, long chain aliphatic compounds that display an extensive range of carbon chain lengths and functional groups. Physiologically, the cuticle plays vital roles in water retention and physical defence against disease, however; increasing evidence has demonstrated that some cuticular waxes can signal recognition to pathogenic fungi to promote infection. The complexity of these plant-fungi interactions hence make them challenging to study and require model systems that can assess the effect of individual surface variables on fungal development.

To address this, we propose the development of a biomimetic model system using fabricated wax films to replicate native leaf chemistries on inert substrates. Using fabrication techniques including spin-coating to generate thin films that can be characterised using a suite of analytical techniques to assess their hydrophobicity, thickness, uniformity and morphology, precise tuning of surface physicochemical properties can be achieved. Individual surface parameters can then be disentangled and systematically assessed in the context of fungal development to identify key virulence traits at the leaf surface.

4:30pm **BI-MoA-13 Scaling Biomaterials Manufacturing: Lessons from the Paper Industry**, ***Sandro Zier,*** University of Maine

Biomaterials are increasingly being explored as sustainable alternatives to petroleum-derived materials, but many systems that perform well at laboratory scale remain difficult to manufacture reliably at industrial scale. One reason for this disconnect is that biomaterial structure and function are strongly influenced by the physical conditions present during assembly, including flow, transport, dewatering, and drying conditions that differ substantially between laboratory and industrial environments. This talk presents a framework for designing biomaterials with formation conditions and manufacturing environments considered from the outset instead of introducing process constraints only after laboratory optimization. Using papermaking and related large-scale bio-based manufacturing systems as examples, the presentation examines how process-dependent assembly governs interfacial structure development across systems including microfibrillated cellulose, protein-based materials, biofilms, and mycelium composites. Differences between benchtop and industrial processing are discussed in terms of flow behavior, transport limitations, shear history, and consolidation dynamics, demonstrating that scale-dependent physical regimes can produce fundamentally different structures and functional behavior. The talk further outlines a process-integrated framework in which material selection, structure formation, and manufacturing constraints are treated as interconnected design variables. Finally, future needs in process-relevant characterization, multiscale modeling, and experimental tools capable of probing biomaterial formation under realistic manufacturing conditions are discussed. Incorporating formation pathways into biomaterials research may improve reproducibility and help bridge the gap between laboratory discovery and industrial implementation.

4:45pm **BI-MoA-14 Extreme Copper Tolerance and Genomic Adaptation in Early-Stage Marine Biofilms**, ***Kailey Richard,*** U.S. Naval Research Laboratory*; Sara Tuck,* Naval Medical Research Command*; Sophie Colston, Marryssa Beasley, William Hervey,* U.S. Naval Research Laboratory*; Kevin Le,* NOVA Research, Inc.*; Sean Brown,* U.S. Naval Research Laboratory*; Katherine Franz,* Duke University*; Kenan Fears,* U.S. Naval Research Laboratory

Biofouling, the accumulation of unwanted organisms on submerged assets, presents an ongoing challenge within the maritime industry. Conventional methods to inhibit growth rely heavily on the application of copper-laden (≤75% copper compounds) antifouling coatings. However, the efficacy of these coatings is declining due to the broad emergence of copper-tolerant species. Here we investigated the mechanisms underlying this decline in antifouling performance. Polyvinyl chloride (PVC) panels coated with a commercial copper ablative paint were deployed in the Chesapeake Bay to collect early-stage biofilms; uncoated PVC panels were deployed as an inert control group. Community profiles of the harvested biofilms were obtained via 16S amplicon sequencing of the V4-V5 region. To elucidate genomics information about specific bacteria, primary bacterial colonizers were isolated on marine agar plates and identified through 16S amplicon sequencing and whole genome sequencing (WGS). The isolates were subsequently assessed for copper tolerance using copper sulfate ($CuSO_4$) in both marine agar and broth assays. While bacterial tolerance declined with increasing $CuSO_4$ concentrations on agar, tolerance was significantly greater in liquid media. We observed all isolates survived extreme concentrations, with minimum inhibitory concentrations (MIC) equal to or above 5 mM $CuSO_4$. Genomic annotation confirmed that this high phenotypic tolerance was driven by active genetic resistance mechanisms. Every isolate harbored at least three copper-related genes (e.g., *copA, cueO, copZ*), with highly adaptable species carrying a full spectrum of resistant genes. Ultimately, these findings highlight how the accumulation of metal resistance genes allows bacteria to colonize metal-rich surfaces, paving the way for subsequent macrofouling and coating failure.

Advances in EUV Lithography
Room 316 - Session EUV-MoA

Advances in EUV Lithography II

Moderators: Prof. Alain Diebold, University at Albany-SUNY, **Mr. Lior Huli**, TEL, **Dr. Dustin Janes**, TEL, **Dr. Lovejeet Singh**, JSR Micro, **Dr. Kandabara Tapily**, TEL

1:30pm **EUV-MoA-1 EUV Resists: Chemistry, Mechanisms and Challenges**, ***Robert Brainard,*** University at Albany **INVITED**

The lithography community has studied EUV photoresists for nearly thirty years. Yet, some of the most basic details of the interaction of EUV photons with photoresists remain poorly understood.In a typical photochemical reaction using longer-wavelength light (l = 157-1000 nm), photons create excited states in photoactive compounds, thereby creating known quantities of intermediates and photoproducts at measurable rates.The photochemical reactions occurring during EUV exposure are much more complex and, as yet, not fully explored.

This presentation will start with a quick introduction to photoresists and EUV lithography.It then will describe how 92 eV EUV photons ionize molecules in resists, creating holes and free electrons, and identify and discuss the individual interactions that occur with atoms (Figure 1).However, the number of electrons created, their reaction mechanisms, their lifetimes and their reaction cross-sections are not well known. The presentation will discuss experimental results and provide insight into these poorly understood aspects of EUV exposure mechanisms.

2:00pm **EUV-MoA-3 The Effect of Molecular Weight and Polydispersity Index on the Ultimate Roughness of EUV Photoresists***, Greg Denbeaux,* University at Albany

In EUV lithography, one of the critical challenges is the line edge roughness (LER) or line width roughness (LWR) of the resist pattern. There are many contributing sources to the roughness in the resist including photon stochastics. In this paper, we correlate molecular weight and the distribution of the molecular weight of the photoresist on the roughness of the exposed pattern using top-down low energy electron exposures and atomic force microscopy. Most of the results will be based on PMMA as a simple model system for exploration.

2:15pm **EUV-MoA-4 XPS Analysis of Inpria Metal-oxide Photoresists after Post-EUV Exposure to Oxygen and Water***, Mark Johnson,* Inpria Corporation*; Sonia Castellanos Ortega,* Inpria Corporation, Belgium*; Lauren McQuade, Kirsten Louthan, Michael Greer, Brian Cardineau,* Inpria Corporation

The field of Metal Oxide Resists (MOR) for EUV lithography has been pioneered by Inpria Corporation. The reactions that occur in Inpria materials following exposure to EUV photons (13.5 nm wavelength) are critical to their functioning. EUV radiolysis of these resists in UHV produces active sites that react with both oxygen and water, resulting in the differing solubility that is necessary for pattern formation during development. Previous work has shown the importance of both oxygen and humidity for photolithographic performance of similar resists [1]. It is hypothesized that both oxygen and water affect the condensation of the metal-oxo clusters and thus, their photolithographic performance [2,3]. In this study, compositional changes that occur post-EUV radiolysis, upon gas exposure to oxygen and humidity, are investigated by XPS. The post-exposure atmosphere and temperature were controlled, including the inert transfer of samples into the XPS. Some aspects and technical challenges associated with studying radiation-sensitive materials by XPS will be discussed, including the sensitivity to X-ray damage and strategies to minimize this effect. Results will be presented of Inpria MORs following EUV exposure and controlled post-treatment atmospheres with different thermal treatments in varying nitrogen, oxygen, and humidity concentrations, along with the resulting changes in composition, carbon chemistry, oxygen chemistry, and tin chemistry. A mechanistic interpretation of post-EUV chemical interactions will be proposed.

1. Ivan Pollentier, Fabian Holzmeier, Hyo Seon Suh, Kevin Dorney, Proceedings Volume 13983, Advances in Patterning Materials and Processes XLIII; 139831G (2026)
2. Sonia Castellanos, Peter De Schepper, Maireyee Bhattacharya, Jan Doise, Joren Wouters, Amrit K. Narasimhan, Brian Cardineau, Lauren McQuade, Craig Needham, Michael Kocsis, Kazuki Kasahara, and Stephen Meyers "EUV metal oxide resists: impact of the environment composition on CD during post-exposure delay", Proc. SPIE 12957, Advances in Patterning Materials and Processes XLI, 1295707 (10 April 2024); https://doi.org/10.1117/12.3010921
3. Yu Zhang, Jarich Haitjema, Xiaomeng Liu, Fredrik Johansson, Andreas Lindblad, Sonia Castellanos, Niklas Ottosson, and Albert M. Brouwer "Photochemical conversion of tin-oxo cage compounds studied using hard x-ray photoelectron spectroscopy", Proc. SPIE 10146, Advances in Patterning Materials and Processes XXXIV, 1014606 (27 March 2017); https://doi.org/10.1117/12.2257893

2:30pm **EUV-MoA-5 Closing the Stochastics Resolution Gap***, Chris Mack,* FRACTILIA **INVITED**

Background: Since the birth of the integrated circuit, electronics industry growth and innovation have relied on semiconductor manufacturers putting ever smaller features (described by their critical dimensions or CDs) into production. Yet today, stochastics, the randomness inherent to chip making near the atomic scale, is threatening the continued ability to manufacture the smallest possible features in volume production. Aim: To understand the impact of stochastics on semiconductor manufacturing today, the Stochastics Resolution Gap is defined and used as a framework assessing the value of reducing stochastics variability. Approach: This paper provides an introduction to stochastics, their emerging limitations on lithography resolution, technology solutions for improving resolution and yield, and the importance of accurate measurement technology for bridging the stochastics resolution gap. Results: Using one stochastics-aware design rule example, a method for determining the optimum via size in a specific 28-nm pitch process is presented in order to minimize the detrimental role of stochastics. Conclusions: The Stochastics Resolution Gap is a real limitation, but it is not fixed. Further efforts are needed to continue to close this gap.

3:00pm **EUV-MoA-7 The Role of Environmental Humidity During Processing on the Properties of Indium Nitrate Sol-Gel EUV Resists***, Cody Allen, Mohsen Moayedi, Raphael Nam, Kevin Brenner, Julia Hsu,* The University of Texas at Dallas

As EUV lithography moves to higher numerical aperture patterning, appropriate photoresists must simultaneously meet increasingly stringent requirements for reduced resist thickness, high sensitivity, and low stochastic variability. Metal-containing resists offer improved EUV absorption compared with conventional light-element organic resists, with organotin (Sn-oxo) materials being a prominent example. Our group has investigated indium nitrate-based sol-gel photoresists as an alternative metal-oxide resist platform, as indium has an EUV absorption cross-section similar to that of tin. In this work, we examine how film formation and dose response of indium nitrate resist are influenced by ambient moisture during resist processing.[1]

Because access to EUV exposure tools remains limited for academic research, we primarily evaluate resist contrast using 100-eV electron-beam exposure as a practical alternative. The energy of the electrons is similar to that of EUV photons, 92.5 eV. The indium nitrate resists demonstrate sensitivity comparable to that of the Sn-oxo resist and can be patterned by electron-beam lithography (EBL) into 50 nm half-pitch line/space features.[2,3] EUV flood-gun dose curves further indicate sensitivities as low as 10 – 20 mJ/cm^2.[2,3] However, processing under elevated relative humidity produces nanoscale bump-like crystalline defects that degrade pattern fidelity by increasing line-edge roughness (LER).[2] Controlled-humidity processing suppresses these defects, enabling defect-free films made at relative humidities up to 35% RH.[4] At 25% RH, defect-free line/space patterns were achieved with an LER of 2 nm and a linewidth of 19 nm.[4]

These preliminary results motivate a systematic controlled-humidity EBL study in which indium nitrate films will be processed across defined relative humidity conditions and evaluated by dose response, retained film thickness, linewidth, LER, and nanoscale defect density. Correlating these lithographic metrics with film morphology measured by atomic force microscopy and chemical characterization using Fourier transform infrared (FTIR) spectroscopy will clarify how water uptake alters hydrolysis/condensation chemistry, defect formation, and resist sensitivity. More broadly, this work can help identify the mechanism through which ambient moisture acts as a critical processing variable for solution-processed metal-oxide resists.

3:15pm **EUV-MoA-8 Incorporating Bismuth into Hybrid Inorganic-Organic Films using Molecular Layer Deposition for Advanced Lithography Applications***, Jane Keth, Duncan Reece, David Bergsman,* University of Washington

To address the exponential rise in memory demand and improve energy efficiency per transistor, continued scaling of semiconductor feature sizes will be essential. The semiconductor industry has converged on the idea that achieving high-resolution patterning at sub-10 nm critical dimensions needed for next-generation devices will require extreme ultraviolet (EUV) lithography. Enabling this technology will further require photoresists compatible with EUV, often through incorporating high-Z elements that enhance radiation absorption. Several high-Z elements, such as tin, zirconium, hafnium, zinc, titanium, and indium have been investigated for use in metal-oxide or hybrid metal-organic photoresists for EUV/e-beam (EB) applications. However, many of the methods used to deposit these resists rely on wet chemical processing methods, such as spin-coating or sol-gel synthesis, which can complicate uniform ultrathin film formation and increase susceptibility to defects. One alternative approach for testing and manufacturing these resists is molecular layer deposition (MLD), which provides a compelling dry, solvent-free approach for photoresist fabrication. In MLD, vapor precursors are sequentially pulsed into a reactor, where they undergo self-limiting surface reactions to deposit molecular layers with precise thickness control. MLD is also amenable to area-

selective patterning and high aspect ratio deposition, which could be used in processes inaccessible to chemical vapor deposition.

In this work, we examine a relatively underexplored hybrid MLD chemistry for use as a photoresist for EUV lithography: a Bismuth-based hybrid. Bi photoresists offer a promising photoresist candidate for EUV/EB lithography, due to its high EUV absorption and low toxicity comparatively to other high-Z metals. Here, we demonstrate the successful deposition of Bi-based hybrid MLD films. We describe the ambient and chemical stability of the biscone films, as verified by XPS and FTIR. We further expose the film to EB lithography to create a dose matrix and quantify the film's potential EUV-sensitivity. Through this work, we hope to expand the library of MLD chemistries and further demonstrate the potential for MLD as an approach for creating next-generation photoresist materials.

3:30pm **EUV-MoA-9 X-ray Spectroscopy of EUV Exposed SnOx Nanocluster Thin Films Yields Insights Towards Radiolytic Mechanism***, **Trey Diulus,*** NIST-Gaithersburg*; Priyanka Ketkar,* NIST*; Matthew A. Wade,* NIST-Gaithersburg*; Conan Weiland, Cherno Jaye,* NIST*; Daniel Sunday, R. Joseph Kline,* NIST-Gaithersburg

The semiconductor industry is focused on optimizing extreme ultra-violet (EUV) lithography to fabricate leading edge microchips with smaller device features. Metal-oxide (MOx) nanoclusters are being developed as EUV photoresists due to high photon absorption cross sections at the EUV wavelength (13.5 nm) and smaller component size relative to chemically amplified photoresists. Thin films of organo-tin clusters can be made with precise control using solution-based methods, utilizing precursor fragments that link together to form a wide range of structures and compositions, but the radiolytic mechanism that induces a solubility change in these films is still elusive. To identify EUV induced chemistry, we have prepared organotin dodecamer resist films with varying EUV dose exposures and utilized a suite of several synchrotron-based x-ray spectroscopy measurements, specifically synchrotron source hard x-ray photoelectron spectroscopy (HAXPES) to interrogate changes in composition, x-ray absorption spectroscopy (XAS) to examine the electronic structure of the film components, resonant soft x-ray reflectivity (RSoXR) to identify changes in optical constants, and standard x-ray reflectivity (XRR) to track film density. With XAS, we are getting bond-specific information that complements the oxidation state information from the HAXPES. RSoXR provides nanoscale resolved optical constant depth profiles, which complement the surface sensitive XAS. HAXPES shows a decrease in C 1s intensity along with an increase in the O 1s corresponding to the metal oxide, a result expected due to removal of ligands and cross-linking that was previously mentioned. Comparing the Sn L-edge in the TEY XAS for the unexposed versus exposed regions display a clear increase in absorption intensity, as the cross-linked nanocluster forms more of a metal-oxo lattice. This increase in intensity suggests an increase in film density, which was explicitly seen in XRR as the unexposed density increases upon exposure. Further XAS images of the C and K-edges provide spatial information with a chemical contrast corresponding to the resonant absorption energy for the elements present in the film. Evidence of a carbonyl species formed upon EUV exposure can be seen, which may play a role in the polymerization of the clusters. Overall, we highlight the importance of a comprehensive and multi-modal metrology approach that is necessary for providing improved resist designs for optimal performance. Identifying this chemistry will ideally lead to design of more efficient EUV photoresists that can help advance next generation EUV lithography.

4:00pm **EUV-MoA-11 CD-RSoXS: Latent Image Metrology for Source–Mask–Resist Co-Optimization in High-NA EUV Lithography***, **Cheng Wang,*** Lawrence Berkeley National Laboratory **INVITED**

As critical dimensions in extreme ultraviolet (EUV) lithography shrink below 10 nm, particularly for high-NA and hyper-NA systems with reduced depth of focus, three-dimensional effects and absorption gradients within photoresists become increasingly important. In this regime, latent image metrology is essential for co-optimization of the lithography stack, where the source and mask define the aerial image, and the heterogeneous photoresist chemistry governs subsequent reaction and development processes. We introduce critical-dimension resonant soft X-ray scattering (CD-RSoXS), a non-destructive metrology approach combining near-edge X-ray absorption spectroscopy, resonant scattering, and multiphysics modeling to probe 3D morphology and chemical profiles in photoresists. CD-RSoXS enables chemically sensitive characterization across lithographic stages, including latent image formation, post-exposure bake (PEB), and development, revealing nanoscale chemical gradients and structural evolution that drive stochastic variability. By directly mapping resist chemical heterogeneity and its evolution, CD-RSoXS provides critical input for co-optimization frameworks, linking aerial image design with material response. Complementary RSoXR measurements further quantify underlayer properties and their influence on EUV absorption and resist performance. Machine-learning-assisted reconstruction accelerates interpretation of complex scattering data. Together, this work establishes CD-RSoXS as a powerful platform for latent image metrology and integrated materials–process co-optimization in next-generation EUV lithography.

4:30pm **EUV-MoA-13 Outlook for Future EUV Patterning Opportunities and Challenges***, **Eric Liu**, Steven Grzeskowiak, Alexandra Krawicz, Katie Lukter-Lee, HungYu Chang, Surya Padinjarekutt, Yen-Tien Lu, Christopher Cole, Julian Michaels, Amrit Kaphle,* Tokyo Electron America, Inc.*; Akiteru Ko,* Tokyo Electron America, Inc., Japan **INVITED**

EUV (extreme ultraviolet) lithography has been the major driving force behind extending device density scaling. In both logic and memory devices, EUV improves imaging resolution and enables single-print patterning to replace the complex multi-patterning method. This technology simplifies the process and reduces design complexity, promoting manufacturability and cost control for high-volume production. One of the fundamental challenges that we observed is the slowing down of pattern variation scaling. By leveraging advancements in lithography technology, such as the transition from Low NA (numerical aperture) to High NA EUV, and process integration solutions, such as self-aligned multiple patterning (SAMP), the minimum pattern scaling is theoretically achievable to meet the requirements of area scaling going forward. However, the pattern variation has not improved with the reduction of designed pattern feature, which has a significant impact on device reliability and a narrow process window across technology nodes.

Controlling pattern variation, reducing dose-to-size, and maintaining the imaging resolution are the classic patterning trade-off relationships. The challenges and opportunities are aimed for improvement in pattern variation and dose-to-size without the penalty in imaging resolution. In this presentation, we examine several technology options and innovations to realize the formation of minimum metal pitch at the advanced node. These technologies include:

1. Advancements in EUV lithography single patterning and self-aligned multi-patterning.
2. Patterning challenges and plasma interaction in MOR (metalorganic resist) system.
3. Innovative patterning and process integration solution to improve pattern variation.

5:00pm **EUV-MoA-15 Edge Placement Error Reduction using Directional Etching for Via Resistance Improvement***, **Jennifer Oakley,*** *Takumi Nishinobo, Yen-Tien Lu, Jeffrey Smith, Reo Kosaka, Rintaro Yamamoto, Sheldon Meyers, Lior Huli, Eric Liu, Hirokazu Aizawa, Angelique Raley, Luis Fernandez,* TEL US

Back End of Line (BEOL) metal pitches are projected to scale to ~18 nm by 2029–2030 and ~12 nm by 2035–2036 driving an increased need for precise Edge Placement Error (EPE) control.This work reports simulation and experimental demonstrations of post-lithography EPE correction using a Gas Cluster Beam (GCB) system.The GCB system performs nanometer-scale, location-specific film etching integrated with a wafer scanner. This system generates gas clusters from a fixed nozzle and uses scanner tilt and controlled wafer motion to deliver spatially selective etching in either X or Y directions. Chemistries were developed to enable etching of both organic and inorganic materials, permitting small, targeted adjustments to feature edges after lithography.

Simulations for a representative M0/M1 stack (16 nm M0 pitch, 28 nm M1 pitch, and 7 × 13 nm V0 slot via) indicate that correcting EPE by ~2 nm can reduce via resistance by over 20% for an M1 subtractive integration scheme, implying measurable device performance benefits. Experimentally, post-via-lithography GCB etching was applied to a two-level dual damascene Cu process (36p lower-level lines, 28–36p upper-level features) using a chemically reactive gas cluster to trim positive-tone chemically amplified resist. Controlled unidirectional etches showed predictable increases in via opening in the intended direction (CD growth consistent with programmed shifts) while preserving orthogonal CD. Measured overlay shifts matched expectations, demonstrating precise directional control.

To assess electrical impact, wafers were intentionally exposed with a 4 nm via misalignment; one set was corrected using GCB while a control set was left uncorrected. GCB-treated wafers reduced misalignment to under 1 nm and exhibited a ~17% decrease in via resistance at M2. TEM imaging

confirmed restoration of via centering after GCB correction. These results validate GCB's capability to perform nanoscale, location-specific EPE corrections that improve critical BEOL electrical parameters. Future work will integrate measured overlay data into a Location Specific Processing (LSP) workflow to perform localized, data-driven corrections. The demonstrated GCB approach is extensible beyond BEOL to potential FEOL and other applications where sub-nanometer edge control can enhance device performance and yield.

5:15pm **EUV-MoA-16 Measurement of H* Radicals and SnHx Vapor Species in a Simultaneous Deposition and Etch Experiment***, Jameson Crouse, Nathan Bartlett, Emily Greene,* University of Illinois at Urbana-Champaign*; Shiva Rajavalu, Sergio Ferraris, Niels Braaksma,* ASML*; Andrew Herschberg, David Ruzic,* University of Illinois at Urbana-Champaign

Extreme ultraviolet (EUV) lithography sources use Sn in the process of generating 13.5nm wavelength light. This Sn expands out and coats plasma facing devices around the source. H2 buffer gas is added to mitigate transport to important surfaces such as the collector mirrors. Sn that has deposited on surfaces can only be removed in situ through etching by H*, which produces SnHx in the gas phase. The EUV light generates a background hydrogen plasma, which includes varying densities of H* radicals. Knowledge of the local H* radical density is important for understanding the etch rate on wall segments throughout the device, and errors propagate, leading to incorrect predictions of Sn accumulation. This work seeks to validate diagnostics for radical measurement in EUV sources, along with validation of predicted etch rates through the lowering of error bars in a Sn etching experiment being conducted at UIUC. This presentation covers initial results from spatial OES measurement of hydrogen radicals in the presence of an ICP generated hydrogen plasma at pressures between 10-100mTorr, and powers between 1-200W. The presentation also will cover the development of a TALIF based H* radical diagnostic at UIUC for the measurement of H* radicals. The spatial OES data will be benchmarked using the TALIF system, with actinometry used to measure trends in H* radicals and approximate absolute radical densities. Development of a unique collisional radiative model for the H2 plasma will be discussed with effects on local Sn gas species. Future work looking into Sn and SnH gas species will be addressed.

5:30pm **EUV-MoA-17 Enabling an Accelerated Pathway Within the Us for Learning on Lowna Euv, Hina Euv and What'S Next***, Erin Lavigne,* NY CREATES

Within the Albany Nanotech Complex, a deeply integrated ecosystem of state–of–the–art semiconductor fabrication tools, advanced materials laboratories, and data–driven infrastructure is already accelerating breakthroughs across device, process, and systems research. The introduction of HiNA further amplifies this capability by providing a tightly coupled, pre–competitive environment optimized for high–velocity collaboration across academia, industry, and government. Researchers gain direct access to advanced lithography, deposition, etch, metrology, and integration platforms—co–located and orchestrated to support rapid learning cycles at leading–edge and beyond–CMOS nodes.

The impact is immediate and tangible: rapid screening, design–of–experiments, and prototyping workflows enable accelerated exploration of novel materials systems, heterogeneous integration strategies, and next–generation device architectures. From custom optical and electronic materials to advanced interconnect, memory, and logic concepts, iteration cycles are shortened through shared process modules, standardized interfaces, and real–time characterization. High–throughput experimentation, coupled with advanced modeling and data analytics, enables faster convergence on viable process windows while dramatically reducing cost and risk relative to traditional development paths.

By lowering barriers to access—whether capital, tooling, or organizational silos—HiNA enables ambitious, cross–disciplinary ideas to transition from theoretical concepts to validated hardware with unprecedented speed. The platform supports seamless scaling from early material feasibility through device demonstration and system–level integration, creating a continuous pipeline from discovery to manufacturable solutions.

This talk will examine the technical drivers and roadmaps underpinning this acceleration, including next–generation light sources for advanced patterning and metrology, emerging process integration schemes, and co–optimization strategies spanning materials, devices, and architecture. Equally important, it will detail the engagement and partnership models that make this ecosystem uniquely effective—highlighting how shared infrastructure, aligned incentives, and collaborative governance enable participants to innovate faster together than any organization could alone.

From Ionic Crystals to Ionic Conductivity: An Iconic Celebration of Gary W. Rubloff's 50+ Years in Science
Room 317 - Session GWR-MoA

From Ionic Crystals to Ionic Conductivity: A Special Celebration of Gary W. Rubloffs 50+ Years in Science II

Moderators: Prof. Parag Banerjee, University of Central Florida, **Prof. Alexander Kozen**, University of Vermont

1:30pm **GWR-MoA-1 Pyridine-Catalyzed Molecular Layer Deposition of Silicon Oxycarbide***, Gregory Parsons,* Department of Chemical & Biomolecular Engineering*; Man Hou Vong, Seoyeon Kim, Michael Dickey,* North Carolina State University

Hydrogenated silicon oxycarbide (SiOC-H) is a common low-permittivity dielectric material in integrated circuits. As integrated circuits continue to downsize, SiOC-H deposition processes, such as molecular layer deposition (MLD) that offer precise thickness control and high conformity are increasingly vital. MLD of SiOC-H using bis(trichlorosilyl)methane and water satisfies these demands via self-limiting surface reactions. Herein, we introduce the use of pyridine in the precursor dosing step to catalyze SiOC-H MLD, resulting in a growth per cycle (GPC) of 0.31 nm/cycle, 2x larger than previously reported, and ten times larger than observed under identical conditions without catalyst present. Upon annealing at 250 – 550 °C, the Si–CH_2–Si and Si–OH groups in SiOC-H undergo intramolecular reactions to form terminal Si–CH_3 groups. These Si–CH_3 groups decreases the density and dielectric permittivity (from ~8 to 3.55). Annealing induces a transition in the SiOC-H which enhances its etch resistance against diluted hydrofluoric acid solution. We compare the etch selectivity of as-deposited and annealed SiOC-H with that of silicon dioxide during CHF_3/Ar reactive ion etching. Overall, our findings advance the practicality of SiOC-H MLD for fabrication of nanoelectronics.

1:45pm **GWR-MoA-2 From Micro-Batteries to Nano-Ionics: a Two-Decade Journey with Ionic Thin Films***, Keith Gregorczyk,* University of Maryland College Park

Keith Gregorczyk completed his PhD under Gary Rubloff in 2013, followed by a postdoctoral fellowship with Mato Knez at CIC nanoGUNE in San Sebastián, Spain. He returned to the University of Maryland as a Research Scientist, where he spent over 15 years — and more than two decades in total working alongside Prof. Gary Rubloff — developing new scientific directions, designing experimental research programs, and mentoring the next generation of graduate students and post docs.

This talk reflects on the scientific journey that emerged from that collaboration: the integration of thin-film ionic materials into semiconductor device architectures using vapor-phase synthesis techniques, particularly atomic layer deposition (ALD). Materials such as $LiPO_3$, LiPON, lithium titanium phosphate (NASICON), and zirconium phosphate introduce new electrochemical functionality — including Faradaic energy storage, electrochromic switching, and non-volatile tunable electronic and ionic conductivities — into platforms traditionally defined by semiconductor design rules. Critically, many of these functional states are low-energy and non-decaying, making them highly attractive for next-generation device integration.

The talk will trace the arc of this work from foundational studies validating the power-energy relationships predicted by Rolison, Dunn, White, and Long in thin-film lithium solid-state batteries, through the development of solid-state sodium-ion systems, to the emergence of a broader framework for advanced nano-ionics: adding electrochemical functionality to solid-state, semiconductor-manufactured devices. This body of work exemplifies the cross-disciplinary spirit that has defined Prof. Rubloff's career — bridging surface science, thin-film synthesis, and electrochemistry to open new frontiers in functional device design.

Light Source Enabled Science
Room 319 - Session LS-MoA

Light Source Enabled Science

Moderators: Prof. Alexander Gray, Temple University, **Prof. Juanita Hidalgo**, NYU

1:30pm **LS-MoA-1 Advancing the Sample Space to Elevate the Power of Resonant X-ray Scattering**, ***Philip Ryan,*** Argonne National Laboratory, USA **INVITED**

Deploying *in-situ* strain withelectrical *multi-modal* x-ray scattering measurements has allowed for powerful experimental configurations deepening our understanding of complex quantum phenomena. Touching upon a few recent topics e.g., nematic behavior in Fe superconductors (1-4) and quantum paraelectric behavior in $SrTO_3$ membranes (5) I'll demonstrate the value-added power of investing in the sample space and overview our plans to explore dopant-vacancy color center qubit behavior with symmetry and strain combining photoluminescent spectroscopy and x-ray scattering.

The ability to measure and control structure, symmetry or domain population of a twinned system, like an orthorhombic crystal or magnetic orientated domains can be a critical sample control parameter to study intricate quantum behaviors. In the iron-based superconductor, electronic nematicity is coupled to both the lattice and the conducting electrons leading to both structural and transport measurements sensitive to nematic fluctuations. While spin driven nematicity is prevalent in Fe pnictides, the role of spin versus orbit in the chalcogenide nematic behavior has been under investigation. The consortium of electrical and x-ray scattering measurements keenly addresses the relationship of lattice, spin and orbital order in the nematic phase space. $SrTO_3$ is a ubiquitous prototype material but is itself an intriguing enigmatic host of quantum behaviors, using strain as a tuning parameter we investigate the transition from classical to quantum behaviors and consider the unbounded potential studies deploying this combination of strained single crystal membranes with resonant x-ray scattering.

1.Strain-Switchable Field-Induced Superconductivity, Joshua J. Sanchez [https://arxiv.org/search/cond-mat?searchtype=author&query=Sanchez%2C+J+J], et al., Science Advances 9, eadj5200(2023). DOI:10.1126/sciadv.adj5200 [https://doi.org/10.1126/sciadv.adj5200] 2.Suppression of superconductivity by anisotropic strain near a nematic quantum critical point, P. Malinowski, et al., Nature Physics, 1-5, (2020)3.Spontaneous orbital polarization in the nematic phase of FeSe. Connor A. Occhialini, et al., Nature Materials 22, 985 (2023). doi:10.1038/s41563-023-01585-2 4. The transport–structural correspondence across the nematic phase transition probed by elasto X-ray diffraction. J.J. Sanchez, Nat. Mater. (2021) 5.Li J., et al. The classical-to-quantum crossover in the strain-induced ferroelectric transition in SrTiO3 membranes. Nat Commun 16, 4445 (2025

2:00pm **LS-MoA-3 Monolithic 2D Multilayer Laue Lens Optics for Hard X-ray Nanoimaging**, ***Wei Xu,*** *Zirui Gao, Weihe Xu, Nathalie Bouet, Juan Zhou, Hanfei Yan, Xiaojing Huang, Ming Lu, Mingyuan Ge, Yong Chu, Evgeny Nazaretski,* Brookhaven National Laboratory

Multilayer Laue lenses (MLLs) are promising X-ray optics for nanometer-scale, high-efficiency focusing in the hard X-ray regime. Achieving high-performance two-dimensional (2D) focusing requires precise angular and translational alignment of two sets of linear MLLs, involving eight degrees of freedom of motion. For nanoimaging with sub-10 nm resolution, the tolerance for the relative angular alignment between the lenses is approximately 0.01°. Such stringent requirements pose significant challenges for microscopy systems and have hindered the application of MLLs in synchrotron light sources. In this work, we present the development of an advanced generation of monolithic 2DMLLs that address these challenges through a microfabrication-enabled assembly approach.

The monolithic optics were assembled using a silicon-based micro-electro-mechanical systems (MEMS) template. The template incorporates microfabricated alignment and holding structures that enable precise control of the angular and lateral positions of the MLLs mounted on the template. By engineering the alignment microstructures, an angular alignment resolution on the order of a few millidegrees was achieved, which was characterized by white-light interferometry and validated by synchrotron X-ray measurements.

The performance of the monolithic 2D MLLs was demonstrated at the Hard X-ray Nanoprobe (HXN) beamline at NSLS-II using ptychographic imaging. High-resolution 2D imaging achieved sub-10 nm spatial resolution, as verified by Siemens star test patterns. Furthermore, the optics were used to perform nanoscale X-ray tomography, revealing internal interfacial grain boundary structures in a $CoFe_2O_4$-$Ce_{0.8}Gd_{0.2}O_2$-based mixed ionic-electronic conductors (MIECs) system with nanoscale resolution.

This work demonstrates an effective and robust approach to simplifying alignment while advancing the performance of 2D MLL optics. The new optics with high alignment accuracy represent an important step toward the development of monolithic 2D MLL optics for hard X-ray nanoimaging.

2:15pm **LS-MoA-4 Development of Advanced High-Speed Fly-Scan Technology for sub-10 nm Hard X-Ray Imaging at NSLS-II**, ***Weihe Xu,*** *Takenori Shimamura,* Brookhaven National Laboratory*; Dmitri Gavrilov,* brookhaven National Laboratory*; Huijuan Xu,* Brookhaven National Laboratory*; Wei Xu, Hanfei Yan,* brookhaven National Laboratory*; Nathalie Bouet, Juan Zhou, Randy Smith, Jun Ma, Xiaojing Huang, Yong S. Chu, Evgeny Nazaretski,* Brookhaven National Laboratory

Multilayer Laue lenses (MLLs) offer significant advantages over traditional diffractive focusing optics, such as zone plates (ZPs), particularly in terms of efficiency when focusing hard X-rays to 10 nm and below. The resulting increase in photon flux density drives the need for faster fly-scan capabilities to minimize radiation damage and improve data acquisition rates.

To answer this challenge, we developed a next-generation scanning X-ray microscopy testbed designed for high-speed data acquisition. The system demonstrated sub 10-nm ptychographic imaging, and achieved data acquisition rates exceeding 1 kPPS (kilo-points-per-second) while being fully compatibility with the Experimental Physics and Industrial Control System (EPICS) environment used at NSLS-II.

This system, called RASMI (RApid Scanning Microscopy Instrument) [1], is a stand–alone microscope that uses a modular design to accommodate either two orthogonally arranged 1D multilayer Laue lenses (MLLs) or a single 2D optic—such as a zone plate or a monolithically assembled 2D MLL—for point focusing. RASMI supports both sample–scanning and 2D–optics–scanning modes of operation through the use of interchangeable modules. In the sample–scanning mode, the sample is moved during imaging experiments while the focusing optics remain stationary. This approach is insensitive to the structural variations in the incoming X–ray wavefront, ensuring consistent illumination across the entire sample. In the 2D–optics–scanning mode, the 2D optic is moved while the sample remains stationary. This approach can achieve higher scanning speeds, particularly when working with heavy or bulky samples, such as large environmental or in-situ/in-operando experimental cells. Both scanning modes use a laser interferometer as the fast-axis encoder for position data acquisition. The entire RASMI control system is EPICS compatible. The developed microscope can be operated in both time- or position-triggering modes with the maximum photon flux- and detector-limited rate of 1.25 kPPS. The 2D X-ray image results show ~6 nm resolution at sample scanning and ~8 nm resolutions at 2D optics scanning [2]. The developed fly–scan technology has already been implemented in the user instrument at the Hard X–ray Nanoprobe (HXN) beamline at NSLS–II. In this presentation, we also highlight preliminary work aimed at further increasing position–triggered data acquisition speeds.

REFERENCE:

1. Weihe Xu, et al., *Rev. Sci. Instrum.* 95, 113705, Nov 2024
2. Weihe Xu, et al., *Optics Continuum*, 5, 3 937-943, Mar 2026

2:30pm **LS-MoA-5 A Beamline for Probing Morphology and Dynamics of Thin Film Materials at the Advanced Photon Source**, ***Joseph Strzalka,*** Argonne National Laboratory

Feature beamline 9-ID at the recently upgraded Advanced Photon Source hosts the program in nanoscale structure, kinetics and dynamics, focusing on surfaces and interfaces of soft materials. The beamline is tunable over the range 6-25 keV, with highly coherent x-rays provided by a revolver undulator with a double crystal monochromator. Two transfocators focus the beam to about a 5 um spot size at the sample. A robust diffractometer allows for alignment of thin film samples in a variety of sample environments for operando studies in a horizontal grazing-incidence geometry. An in-air area detector captures wide-angle scattering (GIWAXS) while a large vacuum flight path with an in-vacuum pixel array detector accommodates sample-detector distances from 3- 20 m for GISAXS and also grazing-incidence x-ray photon correlation spectroscopy (GI-XPCS) probing dynamics over time scales from 10^{-3} to 10^3 s. Early experiments at 9-ID make use of these capabilities to study the structure and dynamics of

organic mixed ionic electronic conducting materials, organic semiconductors, block copolymers for separation science and perovskite-based materials for energy applications.

Acknowledgments: This work would not be possible without contributions from the 9-ID CSSI beamline development team: Ray Ziegler, Jayson Anton, Sunil Chitra, Miaoqi Chu, Peco Myint,Jonathan Knopp, Luca Rebuffi, Xianbo Shi, Deming Shu, Sunil Bean, Ashish Tripathi, Chasen Wolford, Luis Diaz, Steven Kearney, Kevin Wakefield, Altaf Khan, Dana Capatina, Miaoqi Chu, Peco Myint, Hannah Parraga, Scientific Co-Leads Zhang Jiang and Jin Wang, and Dynamics and Structure group leader Suresh Narayanan and team member Hongrui He. We are grateful for collaborations with the groups of Prof. Jonathan Rivnay (Northwestern University) and Prof. Alamgir Karim (University of Houston), Prof. Po-Chun Hsu (University of Chicago) and Prof. Wanyi Nie and Prof. Hsinhan Tsai (SUNY Buffalo). This research was performed on APS beam time award(s) (DOI: https://doi.org/10.46936/APS-189194/60013707, https://doi.org/10.46936/APS-190153/60014220 , https://doi.org/10.46936/APS-190281/60014340 , https://doi.org/10.46936/APS-191475/60015201) from the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science user facility at Argonne National Laboratory, and is based on research supported by the U.S. DOE Office of Science-Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

2:45pm **LS-MoA-6 The Role of Artificial Intelligence and Spectral Databases in Minimizing Analysis Errors, Illustrated with EXAFS, XES, and Core Level Photoemission***, **Jeff Terry,*** Illinois Institute of Technology

We have developed artificial intelligence-based methodologies that can be used to reliably analyze experimental results from Extended X-ray Absorption Fine Structure (EXAFS), X-ray Emission Spectroscopy (XES), and core level X-ray Photoelectron Spectroscopy (XPS). These efforts address persistent reproducibility problems that slow research progress and inhibit effective technology transfer and manufacturing innovation in materials science and related disciplines.

Our initial work focused on the analysis of EXAFS spectra collected at synchrotron radiation facilities. A machine learning approach, based on a genetic algorithm, was developed to fit measured spectra and extract relevant structural parameters. In the current approach, a set of possible chemical compounds, represented by feff.inp input files, that may be present in the sample. The algorithm then identifies the structural scattering paths from these candidate compounds that best reproduce the experimental measurement. The automated analysis searches for the primary EXAFS path contributors, calculates a goodness-of-fit value, and uses that metric to help identify the chemical moieties present in the material.

The resulting analysis package, EXAFS Neo, is an open-source Python code that uses Larch and FEFF to calculate and fit EXAFS paths. More recently, we have expanded this artificial intelligence framework beyond EXAFS to include XES and XPS analysis. These extensions make use of curated spectral databases for X-ray emission and core level photoemission, providing reference data that can be compared systematically with experimental spectra. By combining machine learning methods with database-driven spectral comparison, the analysis can reduce operator bias, improve consistency across users and laboratories, and provide more reproducible identification of chemical states, local bonding environments, and electronic structure signatures.

Together, these developments demonstrate how artificial intelligence, physics-based modeling, and experimentally grounded spectral databases can be integrated to minimize analysis errors in X-ray spectroscopies. The EXAFS Neo package and related information are available at: https://plutonium.phys.iit.edu/~jeff_terry/exafsneo.html or by contacting the speaker.

3:00pm **LS-MoA-7 Reliable Quantification of Oxygen Vacancies in Ferroelectric Hafnia Using Synchrotron-Based X-Ray Photoelectron Spectroscopy***, **Lucía Pérez Ramírez,*** *Tom Iung, Vineeta Yadav, Christophe Lubin,* CEA Saclay, France*; Uwe Schroeder, Florian Wunderwald,* Namlab, Germany*; Luis Azevedo Antunes, Alfred Kersch,* Munich University of Applied Sciences, Germany*; Tyson C. Back,* Air Force Research Laboratory, Materials and Manufacturing Directorate, USA*; Conan Weiland,* NIST*; Mickael Gros-Jean,* ST Microelectronics, France*; Nicholas Barrett,* CEA Saclay, France **INVITED**

Oxygen vacancy (V_O) is the most common anion defect observed in metal oxides. Its presence can effectively alter the electronic and physico-chemical properties of oxides thin films, thus determining the overall performances of entire devices built on these materials. This is the case of ultra-thin ferroelectric hafnium oxide (HfO_2) films used for emergent non-volatile memory and logic devices. As it has been demonstrated that V_O have a significant impact on the stabilization of the polar orthorhombic phase, responsible for hafnia's ferroelectric character [1,2], determining their global concentration in hafnia layers is crucial for optimal device engineering. Moreover, their migration during electrical field cycling can modify the internal field of the device, affecting the coercive voltage (E_C) and remnant polarization (P_R) values [3]. It is thus of major importance to have an insight on the V_O distribution profile along the hafnia ferroelectric film.

So far, X-ray photoelectron spectroscopy (XPS) combined with Ar^+ ion sputtering has been the preferred method for V_O quantification and depth-profiling, but this is an ill-chosen approach given its destructive character. Here, we show that the use of non-destructive, hard X-ray photoemission (HAXPES) using synchrotron radiation ought to be favored [4], in order to avoid the artifacts introduced by the sputtering process. The particular example of V_O quantification in hafnia appears as a good occasion to review the basics of core-level spectral analysis, focusing on the Hf 4*f* doublet, as widespread mistakes in literature with wrong fitting procedures unfortunately hinder the reliability of quantitative analysis. Finally, we disprove the erroneous assignation of one of the O 1s core-level peak components to the presence of V_O. We demonstrate that there is no concrete evidence to support the theory that associates this component to a charge transfer to second nearest neighbor oxygen anions upon a V_O creation. It is more judicious to assign the O 1s high-binding energy components to physisorbed or chemisorbed species. Our conclusions are supported by careful comparison between XPS/HAXPES experimental results and first-principles calculations [5]. We provide clear indications for reliable analysis and interpretation of the photoemission data, which should allow progress in materials engineering of ferroelectric devices.

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3:30pm **LS-MoA-9 A Proposal for Fully Coherent nanoARPES: Probing Electronic Phase at the 10 nm Scale***, **Aaron Bostwick,*** *Chris Jozwiak, Eli Rotenberg,* Advanced Light Source, Lawrence Berkeley National Laboratory*; Simon Moser,* Ruhr-University Bochum, Germany

Current nanofocused ARPES experiments have achieved ~100 nm spatial resolution, bringing the power of ARPES to microscopic samples and device geometries. Here we propose a new experiment— "Fully Coherent ARPES" — targeting spatial resolutions of 10 nm, where fundamentally new physics becomes accessible. At this length scale, true low-dimensional systems become directly accessible, including 1D edge states, quantum Hall states, and isolated nanotubes, as well as potentially 0D quantum dots and materials with nanoscale electronic phase segregation such as high-Tc_cc superconductors.

Achieving this resolution requires a move to higher photon energies (~200 eV) and a transmission rather than reflection geometry, with the increased coherent flux of the 4th generation synchrotrons offsetting reduced cross sections. When the beam spot approaches or falls below the electron coherence length, the photoemission process enters a fully coherent regime. In analogy with Fourier ptychography, interference effects can then be exploited to extract electronic phase variations induced by defects, strain, and structural inhomogeneities at sub-beam-size length scales — a capability with no current equivalent in electronic structure measurements.

4:00pm **LS-MoA-11 Probing Magnetic Interactions with Coherent Soft X-ray Scattering***, **Andi Barbour,*** Brookhaven National Laboratory **INVITED**

The Coherent Soft X-ray (CSX) beamline at the National Synchrotron Light Source II (NSLS-II) welcomed its first facility users just over a decade ago, providing world–leading coherent X-ray flux in the soft X-ray regime. This capability has enabled fresh perspectives on a wide range of materials and has driven new insights, including the development and application of computational techniques that accelerate discovery—for example, deep-learning denoising models for X-ray Photon Correlation Spectroscopy (XPCS) data and Coherent Correlation Imaging (CCI). In this talk, I will highlight impactful results, along with the computational methods behind

them, that reveal the spatiotemporal dynamics of magnetic systems, ranging from domain-wall motion to coherent rotational control of skyrmion lattices.

4:30pm **LS-MoA-13 Alloy Oxidation for Corrosion Mitigation: Synchrotron Based X-Ray-Photoemission Electron Microscope (XPEEM) Studies from NiCr to High Entropy Alloys**, *Keithen Orson,* University of Virginia*; Jurek Sadowski,* Brookhaven National Laboratory*; Yuran Niu, Alexei Zakharov,* Max IV Laboratory, Sweden*;* ***Petra Reinke****,* University of Virginia

Oxide layers are critical to protect alloys but design prioritizes bulk properties which leads to a narrow compositional and microstructural range to optimize environmental resilience. We study the initial reaction steps during the transformation of alloy to oxide in a kinetically limited regime (T < 800 ° C). We used XPEEM in the study of oxidation for binary (NiCr), ternary (NiCr with Mo or W), and septenary dual phase compositionally complex alloys (CCA).

XPEEM captures chemical, structural, and temporal evolution of the oxide for several grains or phases at the same time. The multi-mode capabilities access work functions, surface structure (m-LEED), and chemistry via XAS/ XPS and nanoscale resolution. The video rate time resolution allows operando studies with chemical sensitivity. The XPEEM studies are combined with (i) laboratory XPS, (ii) synchrotron based ambient pressure XPS, and, in the future, (iii) ToF-SIMS to access sub-surface alloy composition.

We will show oxidation as a function of crystallographic orientation for NiCr, and discuss the role of Mo/ W in moving the oxidation reactions to a preference for chromia over NiO. Several surface orientations were observed simultaneously and confirmed with EBSD analysis. The distribution of chromia islands was extracted from single-energy, time resolved images (operando mode) and hyperspectral XAS images. The analysis of the image stacks required alignments, distortion and brightness correction, linear combination analysis and cosine similarity to yield the composition Cr/Cr_2O_3 for each pixel as a function of oxidation time. The corresponding workflow and code are published. Significant differences are observed as a function of surface orientation but the endpoint for chromia island growth is controlled by Cr supply from the alloy (Figure 1). In contrast, for the ternary alloy (NiCr with Mo/W) the initial adsorption kinetics differ with orientation but chromia always grows in a layer-by-layer mode along [0001]. An atomic scale mechanism which favors specific O-adsorption sites contributes to this development.

For the two-phase septenary alloy $Al_{0.3}Cr_{0.5}Fe_2Mn_{0.25}Mo_{0.15}Ni_{1.5}Ti_{0.3}$ (Figure 2) we are interested in the speciation of elements in the two phases FCC and $L2_1$, their oxides, and the sharpness of the interface. We focus on hyperspectral XAS images for 6 out of the 7 elements for native oxide, clean and oxidized alloy. The alloy design achieved identical work function for both phases but the sharp interface at the boundary remains a breaking point. We will compare the element speciation between the phases in alloy and oxide and discuss the challenges of oxide identification with XAS.

4:45pm **LS-MoA-14 Bragg-Enhanced XAS for Monitoring Real-Time Reactions at Interfaces**, ***Karthika Madathil,*** Lawrence Berkeley National Laboratory (LBNL)*; Alisson Thill,* Universidade Federal do Rio Grande do Sul, Brazil*; Cheng Wang,* Lawrence Berkeley National Laboratory (LBNL)*; Baran Eren,* Weizmann Institute of Science, Israel*; Slavomir Nemsak,* Lawrence Berkeley National Laboratory (LBNL)

Heterogeneous catalysis is central to addressing global energy and environmental challenges. Detailed understanding of Interfacial phenomena during catalysis is limited via traditional X-ray absorption spectroscopy (XAS) due to low temporal resolution arising from the small volume of the interfacial region and the low signal to noise ratio. With Bragg-enhanced XAS (BEXAS) we incorporate diffraction optics into the material of interest using customized periodic nanopattern design enabling coherent addition of scattered intensity. Combining the element specific sensitivity of soft x-rays and intensity amplification from constructive scattering, we capture transient signals arising from chemical changes at thin interfaces. In this work we demonstrate BEXAS for monitoring real time interfacial dynamics in model cerium oxide samples. The evolution of XAS was monitored during heating and gas phase annealing of the sample. The experimental scattering data is compared with simulation results to connect the observed changes in scattered intensity to changes in interfacial chemical composition and structure during the reactions. BEXAS allows the expansion of XAS to the time domain, which is critical for understanding interfacial reactions and investigating transient states which are crucial for developing new catalysts.

5:00pm **LS-MoA-15 Novel Lattice-Matched Substrates for Scalable III-N Power Electronics**, ***Amitayush Jha Thakur,*** Argonne National Laboratory, India

Next-generation power conversion technologies will be central to a highly electrified energy system, motivating new materials and manufacturing approaches for power electronics built for speed, scale, and resilience. This work focuses on crystalline, electrically conductive substrates for III-nitride power electronics and the co-design of commensurate heterostructure interfaces for AlGaN growth. Lattice-matched substrates such as ScB_2 and $Ta_{1-x}Hf_xC$/TaC offer new opportunities for AlGaN heteroepitaxy by reducing interfacial strain while providing higher thermal and electrical conductivity than conventional substrates such as Al_2O_3 or SiC. ScB_2 is lattice matched to approximately $Al_{0.6}Ga_{0.4}N$, while $Ta_{1-x}Hf_xC$/TaC provides tunable lattice matching around $Al_{0.5}Ga_{0.5}N$. Preliminary X-ray characterization, including XRD, XPS, and XAS, probes crystallinity, orientation, chemical composition, charge state, and local electronic structure across multiple length scales, establishing an initial foundation for understanding structure–function relationships in novel AlGaN/substrate interfaces.

5:15pm **LS-MoA-16 Studying Energy Materials with Bragg Coherent Diffractive Imaging**, ***Luxi Li,*** Argonne National Laboratory

Coherent X-ray diffraction methods provide unique opportunities to probe nanoscale structural heterogeneity in energy materials. With the recent upgrade of the Advanced Photon Source, the coherent X-ray flux has increased by up to two orders of magnitude, significantly expanding the capabilities of coherence-based imaging techniques. Among these methods, Bragg coherent diffractive imaging (BCDI) enables three-dimensional imaging of morphology, crystal structure, and internal strain fields in individual crystalline grains without the need for imaging optics.

In this presentation, I will highlight recent applications of BCDI to energy storage and conversion materials, with emphasis on how nanoscale strain, defect evolution, and morphological changes can be directly visualized under relevant conditions. These measurements provide insight into how local structural evolution influences materials performance, degradation, and functionality. I will also discuss how the upgraded APS enables new opportunities for operando and statistically meaningful BCDI studies, including faster measurements, improved sensitivity to weakly scattering systems, and the possibility of tracking dynamic structural processes in complex energy materials.

Multifunctional and Hybrid Microsystems
Room 321 - Session MC-MoA

Multifunctional and Hybrid Microsystems: Optomechanics and Quantum Transduction

Moderators: Dr. Matthew Jordan, Sandia National Laboratory, **Prof. Dr. Yanan Wang**, University of Nebraska-Lincoln

1:30pm **MC-MoA-1 All-Dielectric Cavity Electro-Optic Systems for Quantum Sensing and Transduction**, *Mihir Khanna,* ***Thomas Purdy,*** University of Pittsburgh **INVITED**

Currently, the best methods to manipulate microwave signals at the quantum level require complex, millikelvin temperature, superconducting electronics.Many platforms are being explored to couple microwave and optical systems, leveraging the quantum coherence inherent in room-temperature optical fields to enable quantum-limited readout and control of microwave devices.We are investigating how it is be possible to turn an electro-optic modulator, a workhorse of modern classical telecommunications systems for encoding microwave signals on laser light, into a transducer capable of efficiently moving quantum information between the optical and microwave domains.We have recently demonstrated bulk resonant electro-optic devices with photon-number transduction efficiency approaching unity, surpassing classical telecom modulators by more than six orders of magnitude. We are currently exploring how laser light in this room-temperature system can be used to manipulate and measure microwave devices in analogy to laser cooling in atomic and optomechanical systems, and via electro-optic parametric amplification.

2:00pm **MC-MoA-3 A Quantum Microwave-Optical Interface via Silicon Nanomechanics**, ***Han Zhao,*** University of Central Florida **INVITED**

Optically interconnected networks of heterogeneous quantum hardware are milestones of future quantum information infrastructure. Integrating superconducting qubits as the prominent quantum processors in such a

network requires microwave-optical interfaces with high conversion rate and low input-referred added noise. Here, we meet these requirements in an integrated electro-optomechanical device that utilizes electrostatic coupling between high-impedance microwave resonators and crystalline silicon nanomechanical oscillators [1]. Leveraging the small acoustic loss and low optical absorption heating of silicon, we demonstrate continuous quantum-enabled microwave-to-optical conversion with an external efficiency of 2.20 ± 0.06%, bandwidth of 88.9 ± 2.1 kHz, and a sub-photon input-referred added noise at 0.94 ± 0.03 [2]. Our device provides a realistic path towards optically heralded high-rate entanglement of superconducting quantum processors over long distances.

[1] A. Bozkurt, H. Zhao, C. Joshi, H. LeDuc, P. Day, M. Mirhosseini. A quantum electromechanical interface for long-lived phonons. Nat. Phys. 19, 1326-1332 (2023)[2] H. Zhao, W. D. Chen, A. Kejriwal, M. Mirhosseini. Quantum-enabled microwave-to-optical transduction via silicon nanomechanics. Nat. Nanotech. 20, 602-608 (2025).

2:30pm **MC-MoA-5 High-Performance 4H-SiC Optomechanical Resonators in the Sideband-Resolved Regime***, **Xirui Gou**, Qing Li,* Carnegie Mellon University

4H-silicon carbide (4H-SiC) has emerged as an exceptional material for integrated optomechanics, combining outstanding nonlinear optical properties with low acoustic dissipation. This work presents recent advances in the design, fabrication, and characterization of ultracompact, undercut 4H-SiC microdisk resonators operating in the sideband-resolved regime. These microdisks, with radii ranging from 2.1 to 2.7 microns, are fabricated through a combination of electron-beam lithography and fluorine-based dry etching to define the photonic structures. This is followed by a precisely timed isotropic buffered oxide wet etch to selectively remove the underlying silicon dioxide layer and achieve the targeted undercut ratios.

Optically, these microdisk resonators support both TE and TM modes with measured loaded optical quality factors consistently exceeding one million in the telecom band. Mechanically, the dominant mode is the fundamental radial breathing mode (RBM) at frequencies ranging from 1.5 to 2 GHz. At room temperature, the acoustic frequency is approximately eight times the optical cavity linewidth (~0.2 GHz), placing our system deep into the sideband-resolved regime. This is a critical prerequisite for resolving mechanical sidebands, enabling coherent optomechanical interactions, and advancing toward ground-state cooling.

A key focus of our investigation has been understanding and mitigating mechanical anchor loss. Using finite-element method (FEM) simulations alongside experimental validation, we analyzed the impact of the pedestal undercut ratio on the mechanical quality factor. Our simulations revealed a distinct local resonance where the anchor-loss-limited Q-factor exhibits a sharp maximum at specific pedestal widths. By tracking the mechanical Q-factor across consecutive undercutting rounds, we experimentally confirmed an optimal undercut ratio regime between 55% and 65%. This regime offers a critical balance between minimizing anchor loss and maintaining high fabrication yield. Engineering this balance allowed us to demonstrate mechanical Q-factors exceeding 15,000 at 1.58 GHz in ambient conditions. Leveraging these high-Q resonators, we observed strong nonlinear dynamics, including phonon lasing and the generation of a coherent harmonic frequency comb extending up to 70 GHz with only 1 mW of dropped optical power. These results highlight the vast potential of 4H-SiC microdisks as an integrated platform for low-noise microwave photonics and quantum interfaces.

2:45pm **MC-MoA-6 Parametrically Coupled Nanomechanical and Macroscopic Mechanical Resonators***, **Chris Ligato**, Thomas Purdy, Youssef Tawfik,* University of Pittsburgh

We develop a novel hybrid mechanical system that leverages an acoustic intermediary for high-precision optomechanical sensing. The motion of a macroscopic silicon tuning fork resonator is measured and manipulated by coupling to a nanomechanical high-stress silicon nitride (SiN) string. We fabricate these devices from a high-stress, SiN-coated silicon wafer by using double-sided photolithography and reactive-ion etching to pattern the SiN, followed by through-wafer KOH wet etching to define the tuning fork and release the string. This process yields centimeter-scale, milligram-mass tuning forks with kHz-frequency modes, bridged by an MHz-frequency, nanogram-mass string stretched across the tines. Vibrations of the tuning fork stretch the string, modulating its mode frequencies. This interaction is similar to cavity optomechanics, where mechanical motion modulates the modes of an electromagnetic resonator. Following this analogy, we demonstrate cooling of the tuning fork, sensitive detection of its motion, and phonon swapping between the tuning fork and string. We drive the system with a piezoelectric shaker. When the drive is red-detuned from the string frequency by the tuning-fork frequency, phonons transfer from the tuning fork into the string and dissipate into the environment, cooling the tuning fork. By reading out the string using an optical interferometer, we can detect the motion of the tuning fork imprinted on the string with high sensitivity. Driving the string harder allows us to enter the strong-coupling regime, where the string and tuning-fork modes hybridize. We aim to explore this system's potential for high-precision accelerometry and measurements at quantum limits.

3:00pm **MC-MoA-7 Magnetic Nanostructures for Coupling and Control of Defect Spin Qubits***, **Jesse Berezovsky**,* Case Western Reserve University **INVITED**

Defect spin qubits, such as the nitrogen-vacancy (NV) defect in diamond, perform splendidly as single qubits. With a coherence time that can exceed 1 s at room temperature, defect spins provide an excellent basis for single qubit devices, such as nanoscale magnetometers. But to go beyond single qubits, we require an efficient scalable platform for controlling defect spin qubit registers, and controllably coupling qubits to engineer entanglement. In this talk, I will describe recent advances in our understanding of how magnetic materials and structures couple to defect spin qubits, and how this opens an avenue towards engineering the magnetic environment of the spins for control and coupling. Magnetic nanostructures such as nanoisland arrays and nanoscale magnetization textures such as magnetic vortices provide strong, local magnetic field gradients that can be controlled dynamically for addressable control of qubits [1]. Coupling between qubits may be enabled by a magnon-mediated process. On the other hand, spin-magnon interactions can lead to enhanced spin relaxation or decoherence (e.g. [2]). I will review recent work exploring the interactions of defect spins with magnons in adjacent magnetic structures and discuss the implications for proposed technologies incorporating coherent spins with proximal magnetic elements.We acknowledge support from NSF awards No. 2326528 and 2403743[1] Wolf, M. S., Badea, R., and Berezovsky, J. “Fast, Nanoscale Addressability of Nitrogen-Vacancy Spins via Coupling to a Dynamic Ferromagnetic Vortex” Nature Communications 7, (2016): 5.[2] Trimble, J., Gould, B., Heremans, F. J., Zhang, S. S.-L., Awschalom, D. D., amd Berezovsky, J. “Relaxation of a single defect spin by the low-frequency gyrotropic mode of a magnetic vortex” J. Appl. Phys. 130, (2021).

3:30pm **MC-MoA-9 Robust Topological Phonon Transport in Suspended Hexagonal Boron Nitride Waveguides***, **Sanchaya Pandit**,* University of Nebraska - Lincoln*; Jaesung Lee,* University of Central Florida*; Yanan (Laura) Wang,* University of Nebraska-Lincoln

Topological concepts, originally developed in electronic condensed-matter systems, have recently been extended to bosonic platforms such as photons and phonons, enabling new approaches for robust wave transport in engineered media. These concepts have opened pathways toward designing waveguides that suppress backscattering and maintain stable propagation even in the presence of structural disorder, which is essential for scalable integrated phononic circuits. In this work, we demonstrate a quasi-one-dimensional Su-Schrieffer-Heeger (SSH) topological phononic waveguide based on suspended hexagonal boron nitride (h-BN), a mechanically robust two-dimensional material suitable for high-frequency phonon propagation. By engineering the unit-cell geometry, we construct two distinct phononic lattices representing trivial and nontrivial topological phases with matched band structures. At the interface between these two phases, a confined phononic state emerges within the bandgap, analogous to topologically protected edge states in electronic systems. Furthermore, geometric optimization of the unit cells—including variations in hole shape (circular and oval) and feature size (diameter)—is used to tune the phononic bandgap and control the spectral position of the interfacial mode. The robustness of this mode is systematically evaluated under variations in strain and membrane thickness, and it remains stable, confirming its topological origin rather than defect-induced localization. Overall, the proposed h-BN-based platform provides a promising route toward robust and low-loss phononic transport and may enable future hybrid optomechanical systems through integration with defect-based quantum emitters.

Magnetic Interfaces and Nanostructures
Room 318 - Session MI1-MoA

Advanced Magnetic Materials in Low Dimensional Structures II

Moderators: Prof. Dr. Markus Donath, Muenster University, Germany, **Dr. Valeria Lauter**, Oak Ridge National Laboratory

1:30pm **MI1-MoA-1 Observation of Mirror-Odd and Mirror-Even Spin Texture in Ultra-Thin Epitaxially-Strained RuO_2 Films**, *Ming Yi,* Rice University*; **Yichen Zhang,*** Caltech **INVITED**

Recently, rutile RuO_2 has attracted renewed interest due to expectations of prominent altermagnetic spin-splitting. However, accumulating experimental evidence suggests that in its bulk and thick-film forms, RuO_2 does not display any form of magnetic ordering. Despite this, the spin structure of RuO_2 remains largely unexplored in the ultra-thin limit, where substrate-imposed epitaxial strain can be substantial. Here, we employ spin-resolved angle-resolved photoemission spectroscopy, supported by ab-initio calculations, to reveal the electronic structure of 2.7~nm-thick epitaxial RuO_2 heterostructures. We observe an unconventional spin texture characterized by the coexistence of mirror-even and mirror-odd momentum-dependent components. A comprehensive symmetry analysis rules out nonmagnetic origins of this spin texture. These findings suggest an emergent non-relativistic spin structure enabled by epitaxial strain in the ultra-thin limit, marking a distinct departure from the behavior of relaxed or bulk RuO_2. Our work opens new perspectives for exploring symmetry-breaking mechanisms and spin textures in oxide heterostructures.

2:00pm **MI1-MoA-3 On the Sign of the Rashba Parameter in Image-Potential States**, ***Markus Donath**, Fabian Schöttke,* University of Münster, Germany*; Kaishu Kawaguchi,* University of Tokyo, Japan*; Kenta Kuroda,* Hiroshima University, Japan*; Peter Krüger, Thorsten Deilmann,* University of Münster, Germany*; Ayumi Harasawa, Shuntaro Tani, Yohei Kobayashi, Takeshi Kondo,* University of Tokyo, Japan

For spintronic devices, spin manipulation without external magnetic fields is highly desirable. At surfaces and two-dimensional materials, the spin degeneracy of electronic states can be lifted by the Rashba effect. The Rashba effect in surface states at high-*Z* materials is related to both the strong spin-orbit interaction in heavy atoms and the orbital angular momentum arising from the inversion-symmetry breaking at the surface. Image-potential surface states are simple model systems, where spin-dependent effects can be studied in view of spintronic applications. Our study on Bi_2Se_3 and Bi_2Te_3 showcases that the orbital angular momentum causes an intrinsically reversed Rashba parameter $\alpha_R \approx -100$ meV Å, i.e., a reversed spin splitting compared with the prototypical Rashba-split Au(111) crystal-induced surface state [1] or the image-potential state at Re(0001) [2]. The sign of α_R is decisive for controlling the absolute spin directions in view of spintronic devices. We present a consistent picture of spin-resolved experimental data from inverse photoemission and three-photon photoemission together with calculations from density-functional theory and many-body perturbation theory.

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[2] F. Schöttke *et al.*, Phys. Rev. B **105**, 155419 (2022).

2:15pm **MI1-MoA-4 High Magnetocrystalline Anisotropy-Driven Fuel Cell Electrocatalysis in PtPdFe Intermetallic Alloys**, *Muhammad Irfansyah Maulana, **Jong-Sung Yu,*** DGIST, Republic of Korea

Ordered Pt-based intermetallic alloys are emerging as efficient oxygen reduction reaction (ORR) electrocatalysts in hydrogen fuel cells, outperforming their disordered counterparts. However, the intrinsic role of atomic ordering in governing ORR catalytic performance remains unclear. In this work, we report ferromagnetic PtPdFe ternary intermetallics with structurally ordered tetragonal $L1_0$ and cubic $L1_2$ phases (Figure 1a), each featuring distinct crystal structures and atomic arrangements. Our study highlights magnetocrystalline anisotropy as a key structure-dependent descriptor that governs ORR activity in these alloys. Electrochemical half- and single-cell tests reveal that $L1_0$-PtPdFe magnetic intermetallic catalysts (MICs) deliver higher ORR activity than their $L1_2$ counterparts (Figure 1b). Combined experimental and theoretical analyses attribute this enhancement to the unique tetragonal $L1_0$ structure, where strong 5d–3d orbital interactions along the c-axis induce ferromagnetic ordering and elevate magnetocrystalline anisotropy energy, thereby accelerating ORR kinetics. Furthermore, membrane electrode assemblies fabricated by $L1_0$-PtPdFe cathode MICs sustain fuel cell performance beyond the 2025 US Department of Energy stability targets under H_2–O_2, H_2–air, and H_2–N_2 conditions. These findings establish a new design principle for Pt-based intermetallic catalysts, demonstrating that magnetic anisotropy arising from ferromagnetic ordering can be strategically harnessed to optimize fuel cell performance.

Magnetic Interfaces and Nanostructures
Room 318 - Session MI2-MoA

Emergent Magnetism at Molecular Interfaces, Chirality Induced Spin Selectivity, Molecular Magnetoresistance

Moderators: Prof. Oliver Monti, University of Arizona, **Prof. Yonatan Dubi**, Ben Gurion University of the Negev

2:30pm **MI2-MoA-5 THz Light Emission via Inverse Chiral Induced Spin Selectivity in Chiral Perovskite**, ***Matthew Beard,*** The National Laboratory of the Rockies. **INVITED**

Understanding and the interconversion between spin and charge current under chirality induced spin selectivity (CISS) is critical in leverage chiral semiconductors for developing room-temperature control over spin, charge and light. CISS phenomena arise from an interplay among structural chirality, electron spin orientation, and charge current. Steady-state observations such as magnetoresistance (MR) offer little insight into the timescales that govern the spin-charge interconversion. In contrast, inverse CISS involves the conversion of spin to a charge current. Terahertz (THz) emission spectroscopy (TES) offers a non-contact probe of the induced charge current that maps the charge current direction in three dimensions. We show how the THz emission can map the spin-to-charge conversion and study THz emission in FM/chiral perovskite heterostructures. We contrast with room temperature magnetoresistance in similar films. We show that both CISS and ICISS exhibit similar symmetry, i.e., for ICISS the current direction reverses either for changing the chirality or magnetization direction. These observations directly demonstrate the inherent coupling between spin and charge currents in chiral systems. These observations suggest constraints on the CISS mechanism. For a chiral/FM interface there is spin accumulation at the interface: injection of either charge (CISS) or spin (ICISS) drives the spin configuration out of equilibrium and movement of spin (CISS) or charge (ICISS) must compensate, thus driving the spin-to-charge interconversion.

3:00pm **MI2-MoA-7 Toward Spin Selectivity in Solids - Efficient Charge-to-Spin Conversion and Long Spin Lifetimes in Chiral Crystals**, ***Jagoda Slawinska,*** University of Groningen, Netherlands

Chiral crystals, which lack inversion and mirror symmetries, offer unique ways for controlling electron spin using purely electrical means. In these systems, chirality gives rise to charge-to-spin conversion in which spin accumulation aligns parallel or antiparallel to the applied current, resembling the chirality-induced spin selectivity (CISS) observed in molecular systems.

Our recent studies have shown that in semiconducting tellurium, chirality leads to remarkably efficient charge-to-spin conversion accompanied by long-range spin transport. These two properties, traditionally viewed as mutually exclusive, are reconciled through the emergence of slow collective relaxation modes (“slow relaxons”), which suppress spin dephasing despite strong spin-orbit coupling.

Building on these results, we explore how chirality impacts spin accumulation across a broader class of chiral materials. In both semiconducting and metallic chiral systems, including Te, $TaSi_2$, OsSi, and $NiTa_3S_6$, symmetry-enforced persistent spin textures remain robust over large regions of the Brillouin zone, enabling efficient spin generation and enhanced spin lifetimes.

These findings establish chiral crystals as a solid-state platform for CISS-like spin physics and highlight chirality as a powerful approach for achieving efficient spin generation and robust spin transport in quantum materials.

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3:15pm **MI2-MoA-8 Vibrationally-Mediated Dzyaloshinskii-Moriya Interaction as the Origin of Chirality-Induced Spin Selectivity in Donor-Acceptor Molecules***, **Leonardo Celada**, Alessandro Chiesa, D. K. Andrea Phan Huu, Arianna Cantarella,* Università degli Studi di Parma, Italy*; Michael R. Wasielewski,* Northwestern University*; Paolo Santini, Stefano Carretta,* Università degli Studi di Parma, Italy

Chirality-induced spin selectivity (CISS) in photoinduced electron transfer poses a fundamental challenge: how can sizable spin polarization emerge in molecular systems with weak spin-orbit coupling and large electronic energy gaps [1]. Here we show that low-energy torsional vibrations provide a solution to this energy-scale paradox by generating a Dzyaloshinskii-Moriya interaction between the transferred electron and the donor spin during electron transfer [2].

Starting from a microscopic vibronic model for donor–chiral bridge–acceptor molecules, we derive an effective low-energy spin Hamiltonian where vibrational modulation of hopping and spin-orbit coupling produces Dzyaloshinskii-Moriya interactions comparable to isotropic exchange. This interaction mixes singlet and triplet radical-pair states and yields large spin polarization for realistic parameters, while naturally introducing the low-energy scale required to explain the magnetic-field dependence observed in time-resolved EPR experiments [3].

Numerical simulations of the electron-transfer dynamics show that this mechanism produces sizable CISS efficiencies, predicts a non-trivial temperature dependence, and explains avoided-level-crossing features controlling the field response. In contrast to purely electronic mechanisms, the effect is amplified by low-energy vibrations and remains robust under realistic thermal conditions.

These results identify vibrationally mediated spin interactions as a microscopic origin of CISS in electron transfer, reconcile apparently conflicting experimental observations, and provide experimentally testable signatures for molecular spintronics and quantum technologies [4].

This project is supported by the Horizon Europe program through the ERC-Synergy CASTLE project (proj. n.101071533).

References

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3:30pm **MI2-MoA-9 Unconventional Spintronics from Chiral Perovskites to Altermagnets***, **Igor Zutic,*** University at Buffalo

With the growing class of materials that support spin-polarized carriers, current, and excitations, it is possible to envision emerging spintronic applications that are not limited to net magnetization and magnetoresistance. Here we focus on chiral perovskites with no net magnetization where the space-inversion and mirror symmetries are broken to induce chiral structure. The known importance of these perovskites is further expanded by the demonstration of the chiral-induced spin selectivity (CISS). However, the generation of the spin-polarized carriers across the interface with these chiral perovskites remains to be fully understood. Our first-principles studies for two-dimensional PbBr4-based chiral perovskites provide their electronic structure and an orbital-based symmetry analysis, which allows us to establish an effective Hamiltonian to elucidate the underlying origin of their chirality [1]. The resulting chiral proximity effect can be viewed as an equilibrium precursor to CISS and an element in materials design through proximity effects [2]. We also use this analysis for electrical generation of the nonequilibrium spin polarization in many materials, which in chiral perovskites could be a mechanism contributing to CISS. To accurately obtain optical properties and excitonic energies in these materials, we combine quasi-particle self-consistent Green function framework for calculating the self-energy of the many-body from first principles together with the Bethe-Salpeter equations [1,3]. Furthermore, by examining optical properties of chiral perovskites and the opportunity to use them to realize tunable altermagnets [4], another class of zero-magnetization spintronic materials, we put forth a versatile materials platform for unconventional spintronics and proximity effects [5].

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3:45pm **MI2-MoA-10 Chiral Nanoparticles as a Platform for Probing the CISS Effect***, **Elizabeth Shiby**, Brian Bloom,* University of Pittsburgh, USA

The chiral-induced spin selectivity (CISS) effect, which links molecular chirality and electron spin, holds considerable promise for next-generation room-temperature spintronic devices, quantum computing, and beyond. Despite significant progress, the factors governing this phenomenon and its full range of applications remain incompletely understood. Using chiral nanoparticles as a versatile material platform, we present two studies that, together, identify key factors controlling the CISS response. In the first study, we employ chiral CdSe quantum dots to show that the chiral strength of a material is a critical determinant of the CISS response, which we experimentally validate using a combination of spin-polarized charge current measurements via magnetic conductive atomic force microscopy (mcAFM) and pure spin current measurements via ferromagnetic resonance (FMR). Building on this, the second study demonstrates that dopants can further modulate the CISS response beyond the effect of chirality alone, using lanthanide-doped CdS quantum dots as a model system; crucially, this modulation is strongly governed by the nature of the electronic and magnetic coupling between the dopant and the host lattice.

Collectively, these studies advance our understanding of the structural and chemical factors that govern the CISS effect and highlight its potential to enable new classes of functional nanomaterials.

4:00pm **MI2-MoA-11 Spin-dependent Charge Transport in Single-Molecule Junctions of a-helical Peptide Sequences***, **Ismael Diez Perez**,* King's college london, UK*; Vladimiro Mujica,* Arizona State University*; Wenzhu Kuang,* King's College Lonodon, UK*; Qiankun Wang,* King's College London, UK*; Mario Galante,* Arizona State University*; Albert Cortijos,* University of Barcelona, Spain **INVITED**

In this contribution, we will present our latest experimental results on spin-dependence charge transport through single-molecule electrical contacts made with chiral alpha-helical peptide backbones. We synthesize a series of a-helical peptides sequences of varying lengths, *i.e.*, from 6 to 22 amino acids and their two corresponding D- and L-optical isomer, all bearing the repeating pattern (H_2N-Cys(Acm)-**(**Glu-Ala-Ala-Ala-Lys**)$_n$**-NH-CH_2-CH_2-SH). The peptide is flanked by two axial thiol groups; an Acm (acetamidomethyl)-protected *Cys*(-SH) residue and a alkanethiol terminal group. The chosen specific sequence presents an a-helix favored conformation in the working polar mixture water : TFE (trifluoroethanol). We use a magnetic STM break-junction approach we have previously exploited to measure magnetoresistance in a single-molecule contact[1,2]. This approach allows us to trap individual a-helical peptide between two metal beads (namely, a Au and a ferromagnetic Ni electrode) oriented along the main helix axis though the two side thiol groups specifically binding to the two metal electrodes. We are then able to inject spin-polarized electrons from the ferromagnetic Ni to individual a-helical chiral structures and measure the conductance as a function of the Ni magnetization direction. The analysis of the single-peptide charge transport results provides an intuitive picture combining both CISS and spinterface effects that has enough flexibility to accommodate the description of the observed differences in magnetoresistance as a function of the peptide chirality[3]. The latter picture is then studied as a function of well-known structural drivers of the CISS/Spinterface manifestation such as the electric dipole direction of the helical structure[4], the molecular length and the

secondary structure[5]. We hope our work demonstrates the feasibility of our single-molecule platform to study fundamental mechanisms of spin-dependent transport in chiral biomolecular motifs, and proposes to expand the studies to more complex metalloproteins with redox-dependent functions where the electron spin might play a key quantum biological role.

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[4] A.C. Aragonès*et al. JACS* **2025***,* 147, 36453

[5] W. Kuang *et al.* **2026***in preparation.*

4:30pm **MI2-MoA-13 The Role of Electron Correlations in Chirality-Induced Spin Selectivity of Molecular Junctions***, **Aadi Konidena,*** King's College London, UK

Chirality-induced spin selectivity is an exciting phenomenon where the geometry of helicoid molecules evidently determines the resulting electron spin when a current is driven through the molecule. Despite experimental backing, the details of the primary mechanism that drives spin selection is still not understood. In fact, theoretical simulations based on spin-orbit coupling alone still disagree substantially with experimental data, prompting the investigation into alternate rationales for the observed spin-polarised current. To assess the possible role of the electron-electron correlation effects in current spin polarisation, we study the quantum transport through a molecular junction with Hubbard interactions added on each site of a helical molecule alongside the spin-orbit coupling. We employ the Non-Equilibrium Green's Function formalism and Feynman diagram technique to account for the Hubbard interactions within the Second Born approximation. To calculate the spin current as a function of the temperature and the applied bias, our treatment goes beyond the simple Landauer approach and incorporates the Hubbard self-energies in the equation for the full current.

4:45pm **MI2-MoA-14 Strong Paramagnetic Correlation in Spin Crossover Molecular Complex in a Matrix of Polyaniline***, **Wai Kiat Chin***[1], University of Nebraska-Lincoln, Malaysia*; Mohammad Zaid Zaz,* University of Nebraska-Lincoln, India*; Sartaz Sarkib,* University of Nebraska-Lincoln, Bangladesh*; Faruk Soso,* Tuskegee University, Nigeria*; Ignatius Ebo-Quansah,* Tuskegee University, Ghana*; Peace Ikeoluwa Adegbite,* University of Nebraska-Lincoln, Nigeria*; Gauthami Viswan,* University of Nebraska-Lincoln, India*; Arjun Subedi,* University of Nebraska-Lincoln, USA, Nepal*; Alpha T. N'Diaye,* Lawrence Berkeley National Lab*; Vijay Rangari,* Tuskegee University*; Rebecca Lai, Peter Dowben,* University of Nebraska-Lincoln, USA

To investigate the paramagnetic correlation length of a spin crossover complex, a tri-composite system of Fe(Phen)2(NCS)2 plus polyaniline plus NiCo2O4 magnetic nanoparticles were fabricated. Owing to its anti-ferromagnetic coupling nature between the Fe(Phen)2(NCS)2 and NiCo2O4, the paramagnetic correlation length can be evaluated, which is estimated to be 20.1nm. Such a long paramagnetic correlation length, in a disordered molecular system which has no free electron density to mediate the exchange, is extraordinary.

5:00pm **MI2-MoA-15 Electron Spin, Chiral Symmetry Breaking, and Life's Homochirality***, **Furkan Ozturk,*** Caltech **INVITED**

Electron spin couples strongly to molecular chirality through the recently discovered phenomenon of chiral-induced spin selectivity. As such, spin-polarized magnetic surfaces can function as robust chiral reagents and facilitate asymmetric processes. I will discuss recent experiments that exploit the strong coupling between electron spin, molecular chirality, and chiral phonons, as well as explain their relation to life's homochirality—one of the grandest challenges in origin-of-life research since Pasteur's discovery of molecular chirality more than 175 years ago.

5:30pm **MI2-MoA-17 A Theoretical Model for Surface Chirality Sensors***, **Vladimiro Mujica,*** Arizona State University

We present a theoretical approach to the design of surface chirality sensors, based on a model of spin-dependent van der Waals interactions between chiral molecules, and the physics of spinterface effects. This combination of theoretical approaches allow us to describe both the physisorption and the chemisorption regimes, and the possibility of comparing with experiments designed to achieve chiral recognition, both through measurements of absorption energies and magnetic interactions.

Nanoscale Science and Technology
Room 320 - Session NS-MoA

Frontiers in Nanoscale Electron, Ion, and Scanning Probes II

Moderators: Dr. Alex Belianinov, Sandia National Laboratory, **Prof. Dr. Nancy Burnham**, Worcester Polytechnic Institute

1:30pm **NS-MoA-1 Medard Welch Award Talk: Mimicking Nature: Controlling Charge, Heat, and Spin at Interfaces***, **Paul S. Weiss**[2]**,* University of California, Los Angeles **INVITED**

Many interactions and processes in nature operate at low energy and with critical energy balance, enabling repeated cycling and highly efficient transport. Inspired by these processes, we try to understand them, and to replicate them in synthetic systems. The energies involved are well below those of visible photon energies; thus, we predominantly use tunneling spectroscopies and imaging to probe them. If we could replicate such systems in our devices, we could save most of the energy required to run them. If we could mimic biochemical cycling, we could develop efficient recycling at large scales rather than the extremely labor- and energy-intensive processes of today. We look for underlying principles and what we are currently missing in our understanding. Two of the areas we are exploring are spin conservation in chiral molecules and the roles of polarizability in biological, and now synthetic, systems. Taking this perspective has already led to novel discoveries and inventions, including thermal control with orders of magnitude improvements, in scale, speed, and effect. One of the key advances in nanoscience and nanotechnology has been our increasing ability to reach the limits of atomically precise structures. By having developed the "eyes" to see, to record spectra, and to measure function at the nanoscale, we have been able to fabricate structures with precision as well as to understand the important and intrinsic heterogeneity of function found in these assemblies. The physical, electronic, mechanical, thermal, and chemical connections that materials make to one another and to the outside world are critical. Just as the properties and applications of conventional semiconductor devices depend on these contacts, so do nanomaterials, many nanoscale measurements, and devices of the future.

2:00pm **NS-MoA-3 Probing Surface Phonon Polariton-Mediated Radiative Heat Transfer at the Nanoscale: Influence of Thickness and Temperature***, **Rohith Mittapally,*** North Carolina State University

Surface phonon polaritons (SPhPs) are hybrid electromagnetic modes that arise at dielectric-vacuum interfaces from the coupling of mid-infrared electromagnetic radiation with optical phonons in polar dielectric materials. Because thermal radiation near room temperature is predominantly in the mid-infrared, SPhPs play a significant role in radiative heat transfer (RHT), particularly at the nanoscale. Indeed, theoretical predictions made several decades ago showed that RHT can exceed the blackbody limit by several orders of magnitude when two surfaces are separated by nanometric gaps, a phenomenon known as near-field radiative heat transfer (NFRHT). Experimental demonstrations over the past decade have further increased interest in understanding and controlling NFRHT.

In this work, I will describe how state-of-the-art experiments have revealed new insights into SPhP-mediated NFRHT and its dependence on thickness and temperature. In the first part, I will present our measurements of thickness-dependent NFRHT between planar magnesium fluoride nanofilms, performed using microfabricated devices and a custom-developed nanopositioner [1]. Our results show an 800-fold enhancement in RHT above the blackbody limit and demonstrate that nanofilms can be as effective as bulk materials when the gap between the two surfaces is smaller than the film thickness.

In the second part, I will briefly discuss our work on NFRHT between a silica sphere and a planar silica surface from 77 to 300 K [2]. Our results reveal that cryogenic NFRHT has strong contributions from SPhPs and does not follow the temperature dependence expected from far-field radiative thermal conductance. The microfabricated devices and techniques developed in this work enable advances in nanoscale RHT, with relevance to applications in thermal management, energy conversion, and photonic cooling technologies.

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2. S. Yan, Y. Luan, J. W. Lim, R. Mittapally, A. Reihani, Z. Wang, Y. Tsurimaki, S. Fan, P. Reddy, E. Meyhofer. Surface phonon polariton-

[1] **Falicov Student Award Finalist**

[2] **Medard W. Welch Award Winner**

mediated near-field radiative heat transfer at cryogenic temperatures. *Physical Review Letters*, 131 (19), 196302 (2023)

2:15pm **NS-MoA-4 Incommensurately Tiled Superlattices of Free-Standing $SrTiO_3$ Membranes***, **Jay Shah**, Shivasheesh Varshney, Rishi Raj, Sooho Choo, Bharat Jalan, Andre Mkhoyan,* University of Minnesota Twin Cities

Twisting and stacking two-dimensional materials provides an innovative method for designing materials with novel properties. Moiré superlattices of 2D van der Waals (vdW) materials can host strong correlations that lead to unconventional and emergent phenomena, such as superconductivity and magnetism. Recently, 3D free-standing perovskite oxide membranes have been prepared by employing a sacrificial layer. Their moiré superlattices are shown to host topological polar vortices and new electronic states. In this study, we investigate using analytical transmission electron microscopy two free-standing $SrTiO_3$ membranes stacked at a 45° twist angle. The STO membranes are synthesized by epitaxial growth on a SrO sacrificial layer, utilizing a hybrid MBE method, followed by dissolution of the SrO layer. The 45° twist angle between the top and bottom membranes produces an 8-fold rotational symmetry at the interface, when viewed using HAADF-STEM along the plan-view orientation. This symmetry, forbidden in periodic crystals, demonstrates the ordered but incommensurate quasi-periodic structure at the interface. Ti-$L_{2,3}$ and O-*K* EELS mapping are also performed along the twisted interface stack. Significant changes are observed in the Ti-$L_{2,3}$ edge fine structure at the interface as compared to that of the bulk STO spectra. The O-*K* EELS edge at the interface is also dissimilar to that of the bulk. The changes in the Ti-$L_{2,3}$ and O-*K* EELS spectra at the twisted membrane interface arise from novel electronic states present due to the quasi-periodic moiré structure of the interface.

2:30pm **NS-MoA-5 Propagating Phase Boundaries as Deterministic Drivers of Supported Nanoparticle Organization***, Cheng-Yu Chen,* University of Pennsylvania*; Duncan M. Burns, Peter Voorhees,* Northwestern University*; **Eric Stach**,* University of Pennsylvania **INVITED**

Supported metal nanoparticles are central to heterogeneous catalysis, yet their evolution is traditionally modeled assuming static, inert supports. In situ TEM observations show that dynamic substrate transformations reshape nanoparticle behavior through interfacial energy landscapes. However, the mechanisms by which propagating phase boundaries couple to particle motion remain unexplored. Quantifying such coupled dynamics requires extracting quantitative information from high-resolution time-series microscopy data, a technically demanding task that until now has limited our ability to build predictive models at the nanoscale.

We developed an unsupervised convolutional neural network framework for automated segmentation and real-time tracking of individual nanoparticles in high-resolution in situ TEM image sequences. The framework extracts size, position, and trajectory data for hundreds of particles simultaneously with minimal human intervention. By pairing automated image analysis with time-resolved diffraction, we establish direct temporal correlations between substrate transformation and particle motion.

Applying this framework to Pt nanoparticles on crystallizing AlO_x demonstrates that propagating amorphous-to-crystalline transformation fronts actively drag supported particles over long distances through interfacial energy gradients. Temporal correlation between SAED-detected crystallization onset and rapid particle migration, combined with 4D-STEM virtual crystallinity maps, directly links substrate dynamics to particle transport. Phase-field simulations confirm that asymmetric particle-substrate interfacial energy at the advancing front acts through curvature gradients to redistribute atomic mass and sustain long-range drag.

The results establish a general principle: any propagating solid-state phase boundary generating surface-energy contrast can deterministically drive nanoparticle organization. These mechanistic insights enable rational design of catalyst supports through deliberate engineering of substrate crystallization sequences or separated crystalline regions, offering pathways to suppress unwanted sintering or direct particle assembly for enhanced catalytic performance.

3:00pm **NS-MoA-7 Disorder and Domains in Novel Ferroelectric Thin Films: Insights from Electron Microscopy***, **Elizabeth Dickey**, Sebastian Calderon, Ece Gunay,* Carnegie Mellon University, USA **INVITED**

New materials exhibiting robust polarization reversal and CMOS-compatible processing (e.g. alloys based on AlN, ZnO, and HfO_2) provide new opportunities for integrated ferroelectrics. To understand the mechanisms that control and induce switchable states in these materials, including the influence of microstructure and electrode interfaces, we employ a variety of transmission electron microscopy (TEM) and spectroscopy techniques to study and quantify structure from micrometer to sub-ångstrom length scales. In particular, scanning TEM (STEM) imaging is used to determine local atomic structure that is subsequently utilized to calculate partial pair distribution functions and local spontaneous polarization. The atomic- to meso-scale structural and chemical insights obtained through STEM-based microscopy, including those associated with interfaces, grain boundaries, domain boundaries, and their interactions, are invaluable for understanding polarization phenomena in these emerging classes of ferroelectrics. Furthermore, in situ biasing experiments provide insight into domain nucleation and domain wall propagation, both of which remain topics of active investigation and exhibit behavior distinct from that of more traditional perovskite ferroelectrics.

3:30pm **NS-MoA-9 Venturing Off-the-Rails: Localized Reconstruction of the Partial Density of States of Complex Oxide Heterostructures***, Hayden Barry, **Kory Burns**,* University of Virginia, USA

Perovskite oxide heterostructures provide a versatile platform for engineering emergent electronic and magnetic phenomena through atomic-scale control of interfaces. In particular, $SrTiO_3$/$LaMnO_3$ (STO/LMO) systems exhibit enhanced interfacial magnetism arising from structural disorder; however, the influence of local termination chemistry and defect-driven heterogeneity on electronic structure remains poorly understood. This is because studying these interfaces across a few unit cells is challenging with conventional methods, as optical probes tend to be around 1 µm in diameter. This makes it's impossible to study an individual interface of a vertically stacked transition metal oxide from a cross-sectional sample as the optical probe collects an averaged signal from each layer. In this talk, electron probes are used to overcome the diffraction-limit set by optical probes. This is done by converging electrons to a focused beam to collect spectroscopic signal from an oxide-interface with electron energy loss spectroscopy (EELS). A monochromated aberration corrected scanning transmission electron microscopy (MAC-STEM) is used to couple unprecedented energy resolution and spatial resolution to do optical and vibrational spectroscopy at atomic resolution. When the EELS aperture is in conventional settings, where the bright field disc is perfectly aligned with the entrance aperture, the EELS signal is delocalized and dominated by optical selection rules. Accordingly, the bright field disc is electrostatically shifted by the projector lens so that the dark field disc is highlighted, which describes a technique known as off-axis EELS. We use this to create a localized signal dominated by impact scattering so that the long-range contributions are suppressed, and band edges can be resolved without plasmon interference. Ultimately, we aim to introduce a novel technique to determine the structure-property relationship of complex oxides to bring oxide-electronics to new heights.

4:00pm **NS-MoA-11 Novelty-Aware Multimodal Machine Learning in Autonomous Microscopy for Nanoscale Discovery***, **Yongtao Liu**,* Oak Ridge Natinal Laboratory **INVITED**

Self-driving lab or autonomous experimentation is transforming scientific research by integrating artificial intelligence with automated experimental platforms, enabling adaptive exploration of complex material systems. However, most current autonomous experimentation frameworks focus on optimizing predefined targets, which can restrict dataset diversity and limit the discovery of unexpected physical phenomena. Here, I will talk about an integrated framework for autonomous microscopy that combines novelty-driven exploration with representation learning to enhance scientific discovery at the nanoscale. The novelty-driven exploration quantifies the uniqueness of experimental observations that actively guides microscopy measurements toward structurally and spectroscopically novel regions. This significantly increases the diversity of sampled phenomena compared with conventional optimization-based routines. The representation learning embeds local structural features and spectroscopic responses into a shared latent manifold that serves as a structure-property relationship map. This framework integrates self-driving microscopy and multimodal machine learning to accelerate the discovery and characterization of functional materials beyond conventional scalar objective driven experimentation.Acknowledgments: This research was supported by the Center for Nanophase Materials Sciences (CNMS), which is a US Department of Energy, Office of Science User Facility at Oak Ridge National Laboratory.

4:30pm **NS-MoA-13 Low-Resolution and Noisy Scanning Probe Microscopy Images Enhanced by Deep Learning**, ***Nir Kampf***, *Samuel Gelman, Irit Rosenhek-Goldian, Marek Patočka, Maricarmen Rios,* Weizmann Institute of Science, Israel*; Marcos Penedo, Georg fantner,* EPFL, Switzerland*; Amir Beker, Sidney Cohen,* Weizmann Institute of Science, Israel

High quality AFM imaging is time-consuming process.With the current emerging deep learning concept, can low-resolution AFM images be improved by such technique? In this study (1) a model sample was imaged under standard ambient scanning conditions. Both traditional image enhancement methods and deep learning models were applied to improve image resolution and were benchmarked in terms of fidelity, quality, and expert evaluation by AFM experts. The deep learning models outperform the traditional methods, yielding superior results. Furthermore, common AFM artifacts such as streaking, present in the high-resolution ground truth images, were only partially attenuated by traditional methods but were eliminated by the deep learning models. This work demonstrates that deep learning models are superior for super-resolution tasks and enable a significant reduction in AFM measurement time, as low-pixel-resolution AFM images can be enhanced in both resolution and fidelity through deep learning.

(1) Beilstein J. Nanotechnol. 2025, 16, 1129–1140.

4:45pm **NS-MoA-14 Structural and Functional Characterization of Single Mitochondria Using Atomic Force Microscopy**, ***Irit Rosenhek-Goldian***, *Ekaterina O. Zorikova, Sabita Chourasia, Sidney R. Cohen,* Weizmann Institute of Science, Israel*; Semen V. Nesterov,* NRC "Kurchatov Institute", Russian Federation*; Atan Gross,* Weizmann Institute of Science, Israel

Mitochondria govern energy conversion and cell fate, yet label-free methods to assess their functional and physical states at the single-organelle level do not currently exist. We address this need by combining the imaging capabilities of atomic force microscopy (AFM) with functional phenotyping by quantifying nanomechanics and noise spectrum of height signal of isolated mitochondria. Under various respiratory manipulations, a simple scalar of low-frequency height fluctuations closely paralleled changes in mitochondrial membrane potential (ΔΨm). This confirms that the AFM can be used to monitor functional changes at the level of a single mitochondria. In liver mitochondria lacking mitochondrial carrier homolog 2 (MTCH2), AFM revealed a compact, mechanically stiff, fluctuation-elevated state consistent with hyperpolarization and distinct from inhibitor/uncoupler signatures. Extending to mitochondria isolated from mouse embryonic fibroblasts, AFM data can distinguish between genotypes: loss of mitofusin 1 or 2 (MFN1 or MFN2) produced a stiff, low-fluctuation, low-ΔΨm phenotype, whereas loss of MTCH2 yielded a stiff, high-fluctuation, high-ΔΨm profile. By bridging nanomechanics and mitochondrial bioenergetics, this approach provides an orthogonal, dye-free platform for single-organelle functional phenotyping across tissues, energetic state, and disease models.

5:00pm **NS-MoA-15 Measuring Electron Charge Transfer and Reorganization Energies on a Single Metalloenzyme**, ***Catherine Boisvert***, *Peter Grutter,* McGill University, Canada

Metalloenzymes, enzymes containing a metal co-factor, are of great interest in green energy production. Although their structure is well known, their high efficiencies remain poorly understood, as calculating reorganization energies, i.e. the coupling of electronic and vibronic degrees of freedom, is challenging for large systems. As a result, modelling requires multiple approximations that need to be validated by experiments.

We use electrostatic force microscopy (*e*-EFM) to measure energy levels, single-electron tunneling rates, reorganization energies, and transitions between vibronic states with single molecule resolution. In *e*-EFM, single electron charge transfer between a back electrode and the sample lead to a change in cantilever frequency shift and dissipation. These are measured at cryogenic temperatures with well-established frequency modulated atomic force microscopy techniques. By changing the bias between the tip and the back electrode the electron energy levels of the system can directly be quantified. The ratio of the dissipation rate and frequency shift is proportional to the charge transfer rate; the energy dependence of this rate allows the degeneracy of the state to be determined. Importantly, we have shown that force detected Franck-Condon blockade can be used to directly measure molecular vibrations and reorganization energies at the single molecule level.

We have adapted a system developed by Abad et al., where the metal center of a metalloenzyme is electrically connected to a gold back electrode via a functionalized 1.6 nm gold nanoparticle (AuNP), which is covalently bound to a conductive self-assembled monolayer (SAM). This sample architecture ensures an electrical contact between the gold back electrode and the metalloenzyme. Preliminary *e*-EFM measurements of the AuNP–SAM system alone confirm high SAM conductance. Bias spectroscopy reveals highly localized sharp Coulomb blockade features in both frequency shift and dissipation. We extract tunneling rates consistent with electrochemical measurements from these sites. This shows that the SAM-AuNP is not the charge transfer rate-limiting step, thus validating the enzyme-AuNP-SAM-electrode system. On-going single-electron spectroscopy on metalloenzyme-functionalized AuNP-SAM-electrode devices will enable direct measurements of enzymatic electron transfer. This will allow spatial variations of the redox as well as reorganization energy to be measured and will provide experimental validation of theoretical electrochemical models.

5:15pm **NS-MoA-16 Atomically Precise Additive and Subtractive Mechanosynthesis**, ***Brandon Blue***, *Zehra Ahmed, Damian Allis, Adam Bottomley, Doreen Cheng, Rosemary Cranston, Christian Imperiale, Cameron Mackie, Terry McCallum, Mathieu Morin, Adam Powell, Sam Rohe, Luis Sandoval,* CBN Nano Technologies, Inc., Canada

We have recently explored molecular tools for atomically-precise chemical reactions with 3D, sub-Å manipulation of individual reactants (positionally-controlled mechanosynthesis)[1,2]. Enabled by inverted-mode scanning tunneling microscopy (IM-STM) and our Silicon Probe Chips (SPCs)[3], we demonstrate the mechanosynthetic addition (donation) and subtraction (abstraction) of individual Si atoms and C_2 moieties at 4 and 77 K via custom-synthesized molecular tools[2]. Atomically clean and crystalline Si(100)-2x1 is used as the build site under ultra-high vacuum (UHV) conditions in this work, though other materials are also feasible. Preliminary explorations of the mechanosynthetic parameter space will also be highlighted. The structures resulting from the use of these molecular tools represent the first demonstrations of an emerging field of positionally-controlled chemical interactions not achievable by any other known method. References:

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3. E. Barrera et. al., "Inverted-mode scanning tunneling microscopy for atomically precise fabrication," arXiv:2512.24431 [cond-mat.mes-hall] (2025), https://doi.org/10.48550/arxiv.2512.24431 (submitted for peer review).

5:30pm **NS-MoA-17 Real-Space Manifestation of Frustrated Hopping of Flat Band Electrons in Molecular Kagome Lattice**, ***Wooin Yang***, *Connor Vernachio2, Chris Howard,* University of Tennessee Knoxville*; Panchapakesan Ganesh,* Oak Ridge Natinal Laboratory*; Wonhee Ko,* University of Tennessee Knoxville*; An-Ping Li,* Oak Ridge Natinal Laboratory

Control of destructive interference between neighboring electrons in frustrated hopping systems results in highly tunable electronic properties stemming from real-space topology. The kagome lattice has been a representative example of frustrated hopping system that hosts flat band accompanied by spatially localized electronic states. In real kagome materials, however, it is difficult to tune hopping energies independently, making it challenging to separate destructive-interference effects frommaterial-dependent structural and orbital effects. Here, we use atomic manipulation with a scanning tunneling microscope to build molecular kagome lattices. Carbon monoxide (CO) molecules are individually positioned on Cu(111) to confine surface states at the kagome lattice sites. By varying the lattice constant, we tuned the hopping energies and measured local density of states associated with flat band using scanning tunneling spectroscopy over various hopping ratio t_{NN}/t_{NNN}. A defect was introduced to probe the real-space response of the flat band states, which confirms the frustrated hopping model in molecular kagome lattices.

Plasma Science and Technology
Room 315 - Session PS1-MoA

Plasma Diagnostics

Moderators: Prof. Dr. Sumit Agarwal, Colorado School of Mines, USA, **Dr. John Arnold**, IBM

1:30pm **PS1-MoA-1 Plasma Diagnostics for Industry: Restrictions, Reluctance, and Reward**, ***James Ellis***, *Ben Harris, Montu Bhuva, Jordyn Polito, Geoffrey Hassall,* Oxford Instruments Plasma Technology, UK **INVITED**

The compound semiconductor industry continues to push the boundaries of device performance across markets such as power electronics and data communications; however, this success has increased the emphasis on precision in plasma processing. For a capital equipment manufacturer, it is imperative that a pragmatic approach is taken when using plasma diagnostics to bridge the gap between plasma physics and high-volume manufacturing. This presentation will explore the restrictions, reluctance, and rewards of deploying plasma diagnostics within this sector.

There are significant restrictions when using plasma diagnostics within an industrial setting. For example, commercial systems are often limited by their optical access for complex diagnostics. Furthermore, any integrated diagnostic (or sensor) must meet rigorous standards for robustness, cost, and usability to ensure they remain relevant for industrial applications. This presentation will give an overview of these restrictions in contrast to academic constraints.

The semiconductor sector takes a conservative stance against risk due to the high costs involved with change; this understandably gives a 'process-first' mentality that must be considered when using diagnostics. Any diagnostic that risks contaminating the chamber or may cause drift in an already qualified process is a liability. This presentation will discuss how diagnostics need to be tested to ensure that they do not impact the process, with a specific case study on the curling probe.

Whilst the complexities of using diagnostics in industrial settings are apparent, the reward certainly justifies the effort. Integrating diagnostics enables the acceleration of hardware development and provides the ground truth necessary to validate complex plasma models. This can narrow the process optimisation envelope, enabling a faster transition from process development to the satisfaction of a performance specification. Finally, we highlight the role of external academic partnerships in this journey. For example, by utilising more complex laser-based diagnostics we can build greater confidence in the simplified diagnostic approaches used internally and the complex chemistry models that they validate.

2:00pm **PS1-MoA-3 Use of the OES Signal as an Indicator of Si Etch-Rate Uniformity During Fluorocarbon Plasma Etching**, ***Nobuyuki Kuboi***, *Takashi Yagisawa, Yasufumi Miyoshi, Akiko Kawamoto, Shoji Kobayashi, Yoshiya Hagimoto,* Sony Semiconductor Solutions Corporation, Japan*; Hiroshi Akatsuka,* Institute of Science Tokyo, Japan

During the plasma etching of complex structures with high aspect ratios such as advanced CMOS devices and image sensors, the quantitative prediction and accurate control of the etch rate and uniformity is essential to realize process stability and high yield in mass production. However, variations in these properties are almost impossible to detect during plasma etching in mass production, and their real-time monitoring has been limited to optical emission spectroscopy (OES) analysis. Therefore, the OES signal must be used to address this issue.

The authors previously investigated SiN etch-rate variations during $CF_4/Ar/H_2$ plasma etching using the OES signal of the H Balmer line and found that this variation could be tracked[1]. In this work, to better understand the relationship between Si etch-rate uniformity and the OES signal, the authors experimentally measured variations in Si etch-rate uniformities for 75 process conditions using an ICP reactor with $C_4F_8/SF_6/Ar$ plasma. Analysis of the results using PCA and PLS regression suggests that variations in Si etch-rates at the wafer center and in edge regions depend on variations in the OES signals originating from de-excitation on F with a wavelength of 780 nm and de-excitation on CF (240 nm) and CF_2 (246 nm), respectively. This result indicates that these OES signals can be used as indicators of Si etch-rate uniformity.

To confirm the validity of the analysis, we used a collisional-radiative model to model the emissions of F (780 nm), CF (240 nm), and CF_2 (246 nm) considering gas diffusion and wall sticking as loss processes with electron density (N_e), electron temperature (T_e), and ground-state gas density as input parameters. The simulation results showed that the F (780 nm) intensity is large when N_e and T_e are large, which corresponds to the wafer center region in the ICP reactor, whereas the CF (240 nm) and CF_2 (246 nm) intensities have inverse trends in the F intensity. Therefore, these OES signals can be indicators of Si etch-rate uniformity during fluorocarbon plasma etching.

Combining an inverse analysis of the experimental OES signals [2] with our emission models, distributions of N_e, T_e, and ion/radical densities can be quantitatively derived. Using these values as inputs for our voxel-slab model [3], the uniformities of feature profiles and plasma-induced damage can be predicted, reflecting real-time chamber conditions. This future work will be introduced in our presentation.

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2:15pm **PS1-MoA-4 Non-Invasive Viewport Plasma Resonance Sensor for in-Situ Monitoring of Plasma Etching via Electron Density Measurement**, ***InYong Park***, *GeonWoong Eom, SangHo Lee, Min Hur, WooSeok Kang, Dae-Woong Kim,* Korea Institute of Machinery and Materials, Korea (Democratic People's Republic of)

In semiconductor plasma etching, process reproducibility is a critical requirement. However, the nonlinear nature of plasma can produce different outcomes under nominally identical recipes. Small variations at the etch endpoint can damage the wafer and the underlying interconnect layers, requiring precise in-situ monitoring. Optical emission spectroscopy (OES) is widely used for end-point detection (EPD), owing to its non-invasive nature and its sensitivity to changes in the plasma emission spectrum at the etch endpoint. However, the OES emission intensity depends on multiple coupled parameters: electron density, electron temperature, and emitting-species concentration. As a result, a single emission line cannot uniquely identify the plasma state. As the critical dimensions of semiconductor devices shrink, the open area exposed to the etchant decreases, reducing the flux of reaction byproducts and degrading the signal-to-noise ratio of EPD. Moreover, OES alone, without supplementary calibration, does not directly yield quantitative plasma parameters, which limits its ability to resolve subtle variations in plasma state.

A microwave probe directly measures the electron density by detecting microwave resonances of the plasma. The electron density, in turn, tracks the etch rate through the ion flux at the wafer surface under controlled plasma chemistry, pressure, and bias. However, conventional microwave probes must be inserted into the chamber, which is an invasive configuration that perturbs the plasma and restricts their use in production-grade equipment.

To overcome this limitation, we developed a viewport plasma resonance (VPR) sensor that measures the electron density non-invasively through a dielectric viewport, with the sensor positioned outside the chamber. To our best knowledge, this is the first viewport-coupled microwave resonance diagnostic for in-situ electron-density measurement during plasma etching. Electron densities measured by the VPR sensor were benchmarked against a conventional invasive microwave probe, and the correlations among etch rate, electron density, and OES intensity were quantitatively analyzed through simultaneous measurement. The resulting multi-sensor framework separates density-driven plasma variations from chemistry-driven emission changes, providing a route to non-invasive, quantitative monitoring of plasma etching for improved process reproducibility.

2:30pm **PS1-MoA-5 Non-Invasive Detection of RF Plasma Arcing by View-Port-Type Radio Emission Spectrometry**, ***Geon Woong Eom***, *SangHo Lee, In Yong Park, Woo Seok Kang, Min Hur, Dae-Woong Kim,* Korea Institute of Machinery and Materials, Republic of Korea

Arcing in radio-frequency (RF) plasma is a transient, localized discharge that can be triggered by field enhancement near cracks, protrusions, particles, or locally heated surfaces. Because such events can damage the process chamber, generate particles, and degrade wafer yield, real-time detection of arcing is essential for plasma process monitoring. In this work, we propose a non-invasive arcing detection method based on view-port-type radio emission spectrometry (VP-RES), which senses RF electromagnetic emission from the plasma through an optical/electrical access port without direct insertion into the discharge region.

Artificial arcing was generated in a capacitively coupled plasma reactor using an arcing-inducing metal structure. The VP-RES response was compared with voltage and current waveforms measured by a conventional voltage–current probe. To resolve transient RF signatures, the measured signals were analyzed in the time–frequency domain using wavelet

transform analysis, allowing normal plasma operation and arcing events to be distinguished by their spectral and temporal features. In parallel, three-dimensional electromagnetic simulations of the field distribution inside the reactor were used to guide the sensor geometry and viewport location, with the design goal of maximizing signal coupling to arc-induced emission and spatial sensitivity within the discharge volume.

The results suggest that VP-RES can provide a practical, non-invasive diagnostic route for real-time arcing detection in RF plasma systems. By combining view-port-based RF emission sensing with time–frequency analysis, the proposed method offers a potential alternative or complementary approach to conventional electrical monitoring, particularly where direct probe installation is constrained or where localized transient detection is required.

2:45pm **PS1-MoA-6 High Sensitivity Detection of Subtle Electron Density Variations Using a Cutoff Probe***, **Jang Jinhyeok,*** Applied Physics lab for Plasma Engineering (APPLE), Department of Physics, Chungnam National University, Korea (Democratic People's Republic of)*; Cho Chulhee,* Institute of Quantum Systems (IQS), Chungnam National University, Korea (Democratic People's Republic of)*; Seong Inho, Jeong Wonnyoung, Choi Byeongyeop, Seo Seonghyun, Lee Isak,* Applied Physics lab for Plasma Engineering (APPLE), Department of Physics, Chungnam National University, Korea (Democratic People's Republic of)*; You Shinjae,* Applied Physics lab for Plasma Engineering (APPLE), Department of Physics & Institute of Quantum Systems (IQS), Chungnam National University, Republic of Korea

The electron density is one of the key plasma parameters that affect process reproducibility in plasma processing, and even small variations in the electron density can influence the process outcome. Accurately detecting such subtle variations critically depends on the sensitivity of the diagnostic instrument employed, and therefore a comparative evaluation of different diagnostic methods is required.

In this study, we demonstrate the high sensitivity of a cutoff probe for detecting subtle electron density variations. Small variations in the electron density were introduced by slightly varying the RF power, and the resulting changes were simultaneously measured by a cutoff probe and a Langmuir probe to compare their detection performance.

The results showed that the cutoff probe clearly resolved the subtle electron density variations in a stepwise manner, whereas the Langmuir probe could not distinguish the same variations because they were comparable to its measurement scatter.

In conclusion, the cutoff probe was confirmed to detect subtle electron density variations more effectively than the Langmuir probe. These findings can contribute to the selection of appropriate diagnostic methods in environments where the detection of small electron density variations is required

3:00pm **PS1-MoA-7 Young Investigator Awardee Talk: Spatially Resolved Probes for the Measurement of Hydrogen, Oxygen, Nitrogen, Chlorine, and Fluorine Radicals***, **Dren Qerimi,*** University of Illinois **INVITED**

Accurate measurement of reactive radical species in low-temperature plasmas is critical for understanding plasma chemistry, plasma-surface interactions, and semiconductor processing. Conventional optical diagnostics generally provide line-of-sight or volume-averaged measurements and often lack the spatial resolution necessary to resolve localized plasma behavior. In this work, we present spatially resolved catalytic radical probes capable of measuring H, O, N, and F radicals in plasma sources, with ongoing efforts extending the technique to chlorine-containing plasmas. The diagnostic platform utilizes catalytic probe surfaces that convert radical recombination or reactive loss into a measurable thermal response. Arrays of probes with different catalytic materials enable discrimination between multiple reactive species while maintaining sub-centimeter spatial resolution. Measurements of H, O, and N radicals were performed in a helicon plasma source over powers from 300–1100 W and pressures from 10–100 mTorr. Radical densities on the order of 10^{12}–10^{14}cm^{-3} were measured, while electron densities ranged from 10^{10}–10^{12}cm^{-3} and electron temperatures from ~2–8 eV. Radical densities increased with both pressure and power and followed trends consistent with independently measured plasma parameters. The probe framework was further extended to fluorine radical measurements relevant to plasma etching applications. Because fluorine plasmas present chemically aggressive environments, a non-equilibrium radical probe technique was developed in which radical-induced tungsten etching serves as the sensing mechanism. Experiments in NF_3 and SF_6 plasmas demonstrated a linear correlation between probe response and fluorine density up to 10^{21}m^{-3}. Calibration in a research-scale etcher enabled quantitative spatial fluorine density measurements and comparison with actinometry. Spatially resolved measurements revealed substantial radial nonuniformities in fluorine density above the wafer surface that are not captured by conventional optical diagnostics, improving interpretation of silicon etch kinetics and etch probability measurements. Current work focuses on extending these diagnostics to chlorine radical measurements for halogen-based plasma processing chemistries. These results demonstrate that catalytic radical probes provide a versatile diagnostic platform for spatially resolved measurements of reactive species in plasma environments relevant to both fundamental plasma studies and advanced semiconductor manufacturing.

3:30pm **PS1-MoA-9 Operando Plasma-XPS: Platform Development, Capabilities, and Metrology Challenges***, **Andrei Kolmakov,*** NIST

Plasma-driven processes are central to technologies spanning semiconductor manufacturing, advanced materials synthesis, energy systems, aerospace engineering, catalysis, environmental remediation, and biomedicine. Although conventional ultra-high vacuum (UHV) X-ray photoelectron spectroscopy (XPS) is a powerful tool for surface chemical analysis, its inability to operate at plasma-processing pressures has created a major metrological gap for operando measurements. Recent advances in ambient-pressure XPS (AP-XPS) instrumentation open new opportunities for direct studies of plasma-solid, plasma-liquid, and plasma-gas interactions. Here, we report on the hardware development and pilot testing of a plasma-compatible AP-XPS (plasma-XPS) platform for operando characterization of plasma-assisted processes and reactive environments [1]. We demonstrate conditions under which XPS spectra can be collected directly during plasma operation, enabling simultaneous monitoring of transient surface chemistry, gas-phase species, and mass- and optical spectra. We observed plasma-induced oxidation/reduction reactions, metastable surface species, and the importance of plasma-chamber wall reactions on local plasma chemistry [2]. Wealso observed RF/AC plasma-induced shifts in binding energy, XPS peak broadening, and splitting associated with surface charging and neutralization, particularly in poorly conducting materials. Gas-phase XPS spectra acquired during these plasma conditions also exhibit plasma-dependent binding-energy shifts and satellite structures, offering additional opportunities for real-time plasma diagnostics [3]. Overall, plasma-XPS emerges as a potentially versatile operando metrology platform for real-time diagnostics, process monitoring, and mechanistic studies across a broad spectrum of plasma-enabled technologies.

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Plasma Science and Technology
Room 315 - Session PS2-MoA
Plasma Catalysis and Synthesis

Moderators: Prof. François Reniers, Université Libre de Bruxelles, **Prof. Dr. Mohan Sankaran**, University of Illinois at Urbana-Champaign

4:00pm **PS2-MoA-11 Electrifying C1 Chemistry via Nonthermal Plasma Catalysis***, **Tomohiro Nozaki,*** Institute of Science Tokyo, Japan **INVITED**

The growing demand for both reducing anthropogenic CO_2 emissions and utilizing CO_2 as a renewable carbon resource has accelerated global interest in circular carbon technologies. In this context, extensive efforts are being devoted to the development of next-generation chemical conversion processes capable of transforming CO_2 into value-added chemicals. Because such chemical transformations inevitably require external energy input, the integration of low-carbon energy sources, particularly renewable electricity, has become indispensable for realizing sustainable CO_2 conversion systems. Among these technologies, Plasma Catalysis - a combination of nonthermal plasma and heterogeneous catalysts - has attracted tremendous interest as a promising low-carbon technology where renewable electricity is readily coupled into chemical conversion processes [1]. In the meantime, significant challenges remain in establishing a fundamental understanding of plasma–surface interactions, reaction pathways under non-equilibrium

conditions, and catalyst functions specific to plasma environments. Further advances, therefore, require not only reactor engineering and process optimization, but also the development of plasma-adapted catalytic materials and scientifically grounded reaction design methodologies. This invited lecture presents recent progress in plasma-catalytic CO_2 conversion, with particular emphasis on CO_2 methanation, as one of the most extensively studied in modern C1 chemistry for carbon recycling and mechanistically understood plasma-catalytic reactions. First, in situ FTIR and XAFS spectroscopy of CO_2 hydrogenation over Pd_2Ga/SiO_2 are discussed, which emphasizes the key role of vibrationally excited CO_2 [2]. Moreover, an Eley-Rideal-type reaction, induced by atomic hydrogen, is explained as necessary to overcome the rate-determining step (decomposition of formates) [3]. Second, a large-scale methanation is introduced, where exothermic reaction heat also promotes the methanation reaction: the bifunctional contribution of plasma catalysis, cooperative interaction between reaction heat and activated species, is clarified [4,5]. These findings are not limited to the methanation reaction but are applicable to various types of CO_2 conversion in the scope of C1 chemistry. Finally, a future perspective is presented.[1] D-Y Kim, et al., *ACS Catalysis*, **15**, 19424, 2025.[2] D-Y Kim, et al., *J Am Chem Soc*, **144**, 14140, 2022.[3] D-Y Kim, et al., *JACS Au*, **5**, 169, 2025.[4] W Zhang, et al., *Chem Eng J*, **512**, 162520, 2025.[5] W Zhang, et al., *J Ener Chem*, **115**, 858, 2026.

4:30pm **PS2-MoA-13 Methane Reforming in Nanosecond-to-Millisecond Pulsed Plasmas***, Norleakvisoth Lim,* ***Michael Gordon****,* University of California Santa Barbara

Plasma-assisted methane reforming provides an electrified pathway for producing hydrogen and value-added hydrocarbons without direct CO_2 emissions while potentially enabling co-production of solid carbon. Here, we systematically investigate how the timescale of energy deposition governs methane plasma chemistry by examining atmospheric-pressure pulsed CH_4 discharges spanning six orders of magnitude in pulse duration, from nanoseconds to milliseconds, while maintaining comparable pulse energies of 10–50 mJ/pulse. Experiments were conducted in a coaxial flow reactor operated at low repetition frequencies (50–300 Hz) to specifically minimize pulse-to-pulse interactions. Plasma characteristics (gas temperature, electron density, presence of radicals, etc.) were quantified using electrical diagnostics and high-resolution OES, and reaction products were analyzed via online mass spectrometry.

Substantial changes in discharge physics and reaction products were observed across the ns-to-ms pulse-width range. Electron density varied from ~10^{14}–10^{18} cm^{-3} and gas temperature ranged from ~2500–5200 K, depending on pulse duration and discharge current. Short-pulse discharges (<1 µs) generated high electron densities (10^{17}–10^{18} cm^{-3}) and highly non-equilibrium conditions, where methane conversion proceeded through both electron-impact and thermal dissociation pathways. In contrast, longer pulses (>10 µs) operated at lower electron densities (10^{14}–10^{17} cm^{-3}) and were dominated primarily by thermal chemistry. Nanosecond discharges exhibited the highest total C_2 selectivity (>70%), producing approximately 17% C_2H_6, 18–20% C_2H_4, and 35% C_2H_2. Increasing pulse duration shifted product distributions toward sequential dehydrogenation pathways consistent with Kassel-type chemistry, promoting acetylene formation at the expense of ethylene and ethane.

Energy deposition timescale produced a distinct tradeoff between selectivity and conversion. Rapid energy deposition and quenching in short-pulse plasmas favored partially dehydrogenated intermediates, whereas longer pulses improved methane conversion and process efficiency through increased reaction volume and residence time. The best overall performance was achieved near 100 µs pulse duration, yielding methane conversion energy cost as low as ~370 kJ/mol CH_4 and specific energy requirements of ~15 kWh/kg for C_2H_2 and ~40 kWh/kg for H_2, comparable to thermal plasma processes. These results demonstrate that pulse duration serves as a powerful control parameter for tuning plasma reaction pathways and optimizing selective methane conversion to hydrogen and value-added hydrocarbons.

4:45pm **PS2-MoA-14 Asymmetric Plasma-Electrocatalyst Process for Tunable Nitrogen Fixation***, Mohammad Ali Eslamisaray,* Department of Nuclear, Plasma, and Radiological Engineering, University of Illinois Urbana-Champaign, Champaign, IL, USA*; Hee-Eun Kim, Xiao Su,* Department of Chemical and Biomolecular Engineering, University of Illinois Urbana-Champaign, Urbana, IL, USA*; R. Mohan Sankaran,* Department of Nuclear, Plasma, and Radiological Engineering, University of Illinois Urbana-Champaign, Champaign, IL, USA

Nitrogen-containing compounds, such as ammonia and nitrate, are critical to applications in agriculture, polymer synthesis, and biomanufacturing. Industrially, ammonia is primarily produced by the Haber-Bosch process, in which nitrogen reacts with fossil-fuel-derived hydrogen over a catalyst bed, and nitrate or nitric acid is produced by subsequent oxidation of ammonia via the Ostwald process. Both the Haber-Bosch and Ostwald processes are carried out in large, centralized manufacturing facilities with substantial capital expenditure and supporting infrastructure. Such production schemes create significant logistic and economic challenges, including transportation, safety and handling, and supply chain vulnerabilities. In addition, both processes require elevated temperatures and pressures making them incompatible with intermittent renewable energy. Recently, there has been a growing interest in sustainable and decentralized alternatives for nitrogen fixation. Electrochemical approaches have been challenged by the activation of molecular nitrogen but can efficiently reduce nitrate to ammonia. In comparison, nonthermal plasmas can react air to efficiently produce nitrate. These complementary features have been exploited in combined strategies, but only as separate reactors.

In this work, we investigated an asymmetric plasma-electrocatalyst process that directly converts air and water into tunable nitrogen products within a single reactor. Specifically, the plasma and electrocatalytic electrodes share the same electrical circuit and electrolyte, with a plasma serving as the anode and a cobalt oxide-based electrocatalyst acting as the cathode. We first evaluated the performance of the system in a single-supply configuration, in which the plasma and electrocatalyst operating conditions are coupled. We then introduced an independent cathodic bias to decouple the plasma and electrocatalyst operating conditions. With the latter configuration, we were able to demonstrate significant control over product selectivity, with final compositions ranging from nitrate-dominant to ammonia-dominant and solution pH ranging from acidic to alkaline.

5:00pm **PS2-MoA-15 Operando Spectroscopic Insights into Plasma-Driven Ammonia Synthesis via Isocyanate Intermediates***, Casey O'Brien,* Texas Tech University

Coupling nonthermal N_2 plasmas with heterogeneous catalysts offers a promising route to sustainable ammonia synthesis under mild conditions. Here, we demonstrate a plasma-catalytic pathway that utilizes H_2O as a carbon-free hydrogen source and leverages trace CO_2/CO_x impurities as catalytic promoters rather than undesirable contaminants. Using a multi-modal operando spectroscopy platform capable of simultaneously probing plasma-phase species and surface-bound intermediates, we identify a distinct vibrational feature at ~2200 cm^{-1}. Isotopic labeling confirms this band arises from surface-bound isocyanate (NCO) species formed via reactions between plasma-activated nitrogen and trace CO_x present at ppm levels in commercial N_2 feeds.

We show that these NCO intermediates react readily with water vapor to produce ammonia at ambient temperature and pressure. Notably, NCO formation is observed across a broad range of metal catalysts, including Pd, Ni, Ag, Au, and Cu, with metal-dependent vibrational signatures, binding energetics, and reaction kinetics for NCO + H_2O conversion. These results indicate that ammonia synthesis via NCO intermediates is a generalizable pathway and that both catalyst identity and gas composition can be tuned to control activity and selectivity. This work highlights the potential of plasma-catalyst coupling to access new reaction mechanisms enabled by trace species and metastable intermediates under non-equilibrium conditions.

5:15pm **PS2-MoA-16 Structural Changes of Plasma Modified Polymers for Applications in Catalytic Deconstruction***, Aunic Goodin,* North Carolina State University*; Sujoy Bepari,* North Carolina A&T State University*; Tridip Das,* California Institute of Technology*; Duncan Trosan,* North Carolina State University*; Zahidul Islam,* North Carolina A&T State University*; William Goddard III,* California Institute of Technology*; Debasish Kuila,* North Carolina A&T State University*; Steven Shannon,* North Carolina State University

1. **Introduction**

The disposal of plastic waste has become an increasing global challenge as single use consumer plastics continues to grow. Catalytic deconstruction is a potential method for upcycling this plastic waste, with plasma being added at different steps to improve the yields or vary/modify the products.

This work investigates the effects of a plasma pre-treatment using atmospheric pressure air plasma to pre-treat polymers prior to catalytic deconstruction. The structural changes of the polymers and the effect on the product distribution under different plasma conditions is investigated.

2. **Methods**

Plasma treatment is performed in a sealed vial with a rubber septum cap. A steel hypodermic needle is used to both deliver synthetic air and apply a high voltage in a pin-to-cup configuration. The grounding cup is made up of a copper pipe soldered to a copper plate. The vial is placed the copper "cup" with the whole assembly surrounded with a 3D printed holder to prevent arcing from the high voltage to ground. The treatment voltage, frequency, flow rate, and power are varied and the modification of polypropylene and polyethylene are investigated using XPS, FTIR, NMR, and MALDI-TOF measurements.

3. **Results and Discussion**

Plasma pre-treatment has been shown to improve yields and modify product distribution depending on the plasma parameters. Previous work has shown this trend with polypropylene and ZSM-5/SBA-15 composite catalyst [1]. The method has been shown to apply with polyethylene and a FeRu-HM catalyst to improve the yield of jet fuel (C_8-C_{16}) products. Further investigation of the structural changes of the plasma treated polymers is therefore necessary to better understand this process.

4. **Conclusion**

Through variations in plasma pre-treatment, catalytic deconstruction can be tuned to produce different product distributions. This method can be applied to other polymer based catalytic deconstruction applications but requires more understanding of the changes in the pr-treatment step.

Acknowledgement

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5:30pm **PS2-MoA-17 Dynamics of Intermediates Formed from Ionizing Radiation of Aqueous Salt Solutions: A Transient Absorption Study**, ***William Maza,*** US Naval Research Laboratory*; Sara Gebre,* us naval Research Laboratory*; Adam Dunkelberger,* US NAval Research Laboratory

The ionization products of laser-induced plasmas generated in water are of great interest; in particular, as they relate to plasmas generated in marine waters. However, despite the complexities involving the ionization of neat water we have endeavored to study ionization of aqueous solutions that mimic the conditions found in seawater. To simplify the strong ionization power of intense pulsed-laser interactions with seawater leading to the formation of undersea plasmas, and to provide a baseline for the study of undersea plasmas, we have begun investigating the softer ionization of aqueous salt solutions by two-photon absorption. We find that the spectra and dynamics observed from two-photon absorption of simulated seawater solutions are complex and indicate the formation of multiple meta-stable intermediates that can be temporally resolved. These include the very short lived (< 50 ns) hydroxyl radical, longer-lived hydrated electron (up to ~ 1 µs), and even longer-lived products of anion ionization like Cl_2^- and CO_2^- (> 10 µs). The presence of humic acids, meant to model dissolved organic matter typically found in seawater, further complicates our analysis. We will discuss these results and their potential significance to underwater plasma formation under similar conditions.

Quantum Science and Technology
Room 304 - Session QS1-MoA

Scalable Superconducting Qubits, Materials, and Integration

Moderators: Dr. Ekta Bhatia, NY CREATES, **Dr. Aswin Anbalagan**, Brookhaven National Laboratory

1:30pm **QS1-MoA-1 Towards Scalable, Available, and Capable Superconducting Qubits*, Valla Fatemi,*** Cornell University **INVITED**

In this seminar, I will present our team's recent efforts in developing high-performance superconducting qubits. Topics will include improving performance and processing windows of base layer films made from niobium and tantalum on silicon substrates. Particularly, this effort includes a reduction of the substrate temperature well into the back-end-of-the-line process window via use of krypton as a sputtering gas. Transmon qubits with a twenty-micron capacitor gap made from these films exhibit quality factors exceeding fifteen million (coherence times up to 1 millisecond), demonstrating their performance with processing that is compatible with a greater number of tools. Additionally, I will highlight high-performance qubits made with Josephson junctions formed by a resist-free fabrication method and our efforts to make high-performance qubit fabrication more broadly available through developing standard process flows at the Cornell Nanoscale Facility.

This prototype was partially supported by the Microelectronics Commons Program, a DoW initiative, under award number N00164-23-9-G061. Partial funding for shared facilities used in this prototype was provided by the Microelectronics Commons Program, a DoW initiative, under award number N00164-23-9-G061.

2:00pm **QS1-MoA-3 Barrier Height Engineering at V3Si-Si Interfaces for Quantum Device Applications*, Preetha Sarkar,*** Brookhaven National Laboratory*; Zhujun Huang, Ting Cao, Charles Marcus,* University of Washington*; Charles Black, Mingzhao Liu,* Brookhaven National Laboratory

The superconducting A15 phase of vanadium silicide (V_3Si) is a promising candidate for quantum device applications. V_3Si-Si based Josephson junctions can be used to fabricate voltage-controlled transmon qubits, also known as gatemons. Apart from higher temperatures of operation due to the higher T_c (~ 17 K) of V_3Si, these superconductor-insulator-superconductor type gatemons are also expected to have longer coherent times. Because V_3Si is almost perfectly lattice-matched to Si, fabrication of these qubits is compatible with existing CMOS technology.

In order to realize V_3Si-based gatemons, it is crucial to understand how the V_3S-Si Schottky barrier height is tuned by the carrier density in silicon. In this talk, I report a method for reproducibly synthesizing superconducting vanadium silicide on Si substrates at various levels of doping and a systemic temperature-dependent transport study to determine the V_3S-Si Schottky barrier height. It is observed that, as compared to undoped Si, doping increases the barrier transparency by reducing both barrier height and width. Interestingly, n-type doping in Si lowers the barrier height more than p-type doping. We also demonstrate a gate-voltage tunable V_3Si-Si-V_3Si based superconducting field effect transistor.

These results evidence that V_3Si is a suitable platform for realizing voltage-based Josephson field effect transistors (JoFETs) and can have a significant broader impact not only in the field of semiconductor-based quantum computing research but also in the development of novel energy-efficient microelectronics.

2:15pm **QS1-MoA-4 Transition Metal Silicides: A New Class of Material Candidates for Superconducting Quantum Circuit Applications*, Mingzhao Liu,*** Brookhaven National Laboratory **INVITED**

For future superconducting qubits development, implementations that are compatible with silicon-based microelectronics (e.g., CMOS), have the best outlook to enable rapid scale-up and high levels of device uniformity and reliability. This vision takes advantage of the vast knowledge obtained from studying transition metal (TM) silicides as gate and low-resistance interconnect materials in CMOS implementations, and that many TM silicides, such as CoSi2, PtSi, and V3Si, are superconductors. The talk will feature the thin film material synthesis and characterization of several superconducting TM silicides that have transition temperatures ranging from just below 1 K to above 10 K. By using standard nanolithography techniques, these TMSi thin films can be turned into relevant quantum information devices, such as Josephson weak links and microwave resonators. In particular I will discuss the application of PtSi, a B31 noble metal silicide that has superior chemical stability and long superconducting

coherence length (~100 nm), for application in constriction-type, co-planar Josephson junctions.

2:45pm **QS1-MoA-6 Niobium Air Bridge Fabrication and Characterization for Superconducting Quantum Devices**, ***Colin Myers***, *Haozhi Wang, Eli Bader,* University of Maryland, College Park*; Ben Palmer,* Laboratory for Physical Sciences*; Kasra Sardashti,* University of Maryland, College Park

Operation of superconducting qubits at high frequencies and elevated temperatures requires materials with larger superconducting gaps, not only for Josephson junctions but also for surrounding circuit elements such as airbridges and crossovers. This motivates the development of airbridge fabrication using high-gap materials such as niobium (Nb). However, sub-micron Nb airbridges are challenging to realize due to the combined demands of fine lithographic definition, mechanical stability, clean interfaces, and robust Nb deposition. In particular, internal stress, morphology, step coverage, and process compatibility must be carefully controlled to obtain continuous and reliable suspended bridge structures. In this talk, we compare different methods of Nb airbridge fabrication, including two-photon and grayscale lithography. We will also discuss the DC and microwave performance and loss characterizations of various devices, including suspended wires and superconducting resonators.

3:00pm **QS1-MoA-7 Scalable Quantum Computation with Integrated Superconducting Electronics**, ***Igor Vernik***, *Caleb Jordan, Aaron Somoroff, Luigi Di Palma, Alex Kirichenko, Kan-Ting Tsai, Meng-Ju Yu, Jason Walter, Adam Weis, Chris Checkley, Oleg Mukhanov, Daniel Yohannes, Shu-Jen Han,* SEEQC **INVITED**

As quantum computing processors continue to increase in size, there is growing interest in developing cryogenic electronics to address the challenges associated with conventional brute-force approaches to system scaling. Single Flux Quantum (SFQ) technology, implemented using a multilayer niobium (Nb) process and adapted for operation near quantum processors at millikelvin temperatures, offers a promising alternative to remote, bulky, and power-hungry room-temperature electronics. SEEQC's digital quantum management approach places energy-efficient SFQ (ERSFQ) circuits in close proximity to qubits within a multi-chip module (MCM) featuring tightly controlled inter-chip spacing. This architecture enables extremely low power dissipation, compatible with the limited cooling capacity of a typical dilution refrigerator, while maintaining high processing speeds and low error rates. In this presentation, we describe our multilayer fabrication and MCM assembly processes. We demonstrate that, by deploying digital ERSFQ circuitry in close proximity to qubits at millikelvin temperature, all essential functions required to operate a full-stack quantum computer can be realized, including digital qubit charge control, magnetic flux control, and qubit readout.

3:30pm **QS1-MoA-9 Thermal Laser Evaporation of Superconducting Nb Films**, ***Yifei Yan***, *David Catherall, Finley Donachie, Austin Minnich,* California Institute of Technology

Niobium thin films are widely used in superconducting electronics and quantum devices, where film thickness, microstructure, and interfaces strongly influence superconducting properties. Despite mature deposition techniques such as sputtering, evaporative techniques are attractive because their near-equilibrium growth enables improved control over film phase and microstructure. However, conventional evaporation approach is limited for refractory elements such as Nb due to the high temperatures required to reach sufficient vapor pressure. Thermal laser evaporation (TLE) addresses this by using localized laser heating with almost arbitrary power density to reach any desired evaporation temperatures. Here, we report the deposition of Nb thin films using a home-built TLE system, in which a continuous-wave 1kW laser (1070nm) is focused onto a Nb target under ultrahigh vacuum to generate an evaporation flux. We examine the thickness-dependent superconducting transition behavior of the films by physical property measurement system (PPMS). Structural, chemical, and surface morphological properties are characterized using x-ray diffraction (XRD), x-ray photoelectron spectroscopy (XPS), and atomic force microscopy (AFM).

Quantum Science and Technology
Room 304 - Session QS2-MoA

Surfaces, Interfaces, Defects, and Microwave Loss in Superconducting Devices

Moderators: Dr. Suman Bhaumik, TEL Technology Center, America, LLC, **Dr. Drew Rebar**, Pacific Northwest National Laboratory, **Dr. Preetha Sarkar**, Brookhaven National Laboratory

4:00pm **QS2-MoA-11 Control of Defects and Interfaces for High–Coherence Superconducting Qubits**, ***Peter Sushko***, Pacific Northwest National Laboratory **INVITED**

Superconducting qubits have advanced rapidly, yet coherence and device-to-device reproducibility remain limited by material imperfections concentrated at surfaces, buried interfaces, and ultrathin native surface oxides. These regions occupy a small fraction of the device volume, yet can dominate loss via two-level systems associated with defects located there. I will highlight materials science challenges that must be addressed to enable scalable superconducting quantum processors, emphasizing the need for precise synthesis and tightly controlled processing of films and interfaces that form qubits and their circuit elements.

We will cover a few examples of how the combined input from high-resolution microscopic and spectroscopic techniques, together with ab initio simulations, has provided mechanistic, atomic-level insights into the processes leading to the formation of these interfaces and their properties. First, we discuss an atomistic picture of Ta surface oxidation and the formation of a semi-ordered TaO_{1-x} suboxide at the boundary between the amorphous Ta_2O_5 and metallic Ta. Building on this mechanistic understanding, we demonstrate a materials-by-design strategy to suppress Ta oxidation using a reactive Mg and noble-metal capping layers. Beyond free surfaces, we discuss the Ta/sapphire interfacial layer and show that sapphire surface termination prior to Ta deposition controls the heterojunction structure, Ta film orientation, and likely the density of grain boundaries and defect traps in the Ta film. Extending these concepts to Nb, we show how controllable processing can deliberately re-engineer oxides, producing thinner, smoother Nb oxides and improving resistance to oxygen exchange/diffusion. Experiments and simulations together indicate that hydrogen segregates to the oxide/metal interface and can migrate during oxide evolution. Finally, we present a scalable passivation strategy for qubit-grade Nb that uses encapsulation and show how structural characterization and ab initio simulations elucidate the mechanisms of atomic rearrangement and stabilization that suppress oxide formation.

Overall, improving coherence and yield requires atomic-level insight to enable predictive control of oxidation, intermixing, and impurity-induced effects, thereby transforming native interfaces into engineered, reproducible materials systems.

4:30pm **QS2-MoA-13 Microscopic Impact of Sapphire Preparation on Losses in Superconducting Tantalum Thin Films**, ***Aswin Kumar Anbalagan***, *Hyeongjun Koh,* Brookhaven National Laboratory*; Suhas Ganjam,* Yale University*; Ruoshui Li, Daniel Olds,* Brookhaven National Laboratory*; Vesna Stanic,* IBM T. J. Watson Research Center*; Jean-Jordan Sweet,* IBM TJ Watson Research Center*; ChenYu Zhao, Shuoyuan Huang,* Brookhaven National Laboratory*; Jinhyun Cho,* Stony Brook University/Brookhaven National Laboratory*; Ananya Chattaraj, Kim Kisslinger, Sooyeon Hwang, Steven L. Hulbert,* Brookhaven National Laboratory*; Luigi Frunzio, Robert J. Schoelkopf,* Yale University*; Mingzhao Liu, Judith Yang, Andrew L. Walter, Andi M. Barbour,* Brookhaven National Laboratory

Understanding the microscopic origins of dielectric loss in superconducting quantum devices is essential for improving qubit coherence and scalable production. Here, we investigate the relationship between crystalline ordering, interfacial structure, and superconducting loss in tantalum (Ta) thin films deposited on c-plane sapphire substrates prepared using edge-fed film growth (EFG) and heat exchange method (HEM) sapphire. HEM sapphire substrates were chemically cleaned and selectively annealed at 1200 °C in an oxygen-rich environment prior to high-temperature Ta deposition by DC magnetron sputtering. Superconducting measurements reveal that Ta films grown on non-annealed EFG sapphire exhibit lower surface loss factors, higher residual resistivity ratio (RRR), and sharper superconducting transitions compared to annealed HEM sapphire, despite the care taken to fabricate HEM samples with stronger epitaxial ordering that may be conventionally anticipated to improve superconducting performance. Synchrotron X-ray diffraction (XRD) and X-ray reflectivity (XRR) measurements reveal differences in epitaxial ordering, rotational disorder, and interfacial oxide layers. Using four-dimensional scanning

transmission electron microscopy (4D-STEM), Ta grown on both EFG- and HEM-samples were found to exhibit single crystallinity with (111)Ta || (0001) sapphire orientation. However, the HEM-annealed sample contains ~100 nm-wide secondary grains associated with local epitaxial breakdown driven by elastic strain relaxation, whereas the EFG-non-annealed sample shows gradual in-plane lattice rotation without secondary grain formation, suggesting strain accommodation through lattice curvature. Altogether, these results suggest that sapphire surface preparation, substrate homogeneity, and interface chemistry strongly influence microwave loss in superconducting Ta devices and highlight the need for further optimization of sapphire processing and early-stage film growth conditions.

4:45pm **QS2-MoA-14 Engineering the α-Ta/Sapphire Heterostructure: Phase Diagrams, Single-Crystal Growth, and Interface-to-Oxide Characterization for Next-Generation Quantum Devices**, ***Joseph Perry Corbett,*** Miami University Ohio

Superconducting qubits are one of the leading candidates for quantum computers capable of surpassing modern supercomputers on specific problems, with steady progress over the last 20 years increasing both quantum state lifetimes and qubit counts. The recent demonstration of α-Ta thin film qubits with coherence times of 0.5 ms, alongside the well-recognized impetus in the QISE community for fundamental materials science on the insulator/superconductor heterostructure, motivates the work presented here. We perform a comprehensive multi-faceted investigation of sputter-grown Ta thin films on sapphire, integrating studies of phase selectivity, single-crystal epitaxy, and thickness-dependent microstructure alongside first-principles calculations of interfacial energetics and surface oxidation. Phase diagrams constructed for DC magnetron sputtering on c-plane Al_2O_3 (with oxygen partial pressure spanning 5.5×10^{-11} to 2.23×10^{-4} Torr and substrate temperatures from 300 to 900 °C) demonstrate that elevated temperatures exclusively stabilize α-Ta while increased oxygen at low temperatures drives single-phase β-Ta formation, with mixed α/β coexistence at intermediate conditions; complementary measurements resolve phase-dependent surface morphologies and work function values relevant to superconducting performance. Sputter epitaxy at 650 °C followed by UHV annealing at 1000 °C yields single-crystal α-Ta in multiple orientations on c- and a-plane sapphire, as confirmed by XRD pole figures, rocking curves, asymmetric scans, and XRR modeling. Thickness-resolved characterization from 2 to 250 nm identifies three structurally distinct regions (a 0.88 nm pseudomorphic interface, a bulk α-Ta(111) film with terrace widths saturating near 150 nm, and a self-limiting 2.25 nm amorphous oxide), and Van der Pauw transport reveals a superconducting Tc that increases smoothly from 2.9 K at 7.5 nm to 4.2 K at 269 nm, consistent with universal thickness scaling. Complementary DFT calculations rationalize the Ta-rich thermodynamic stability of α-Ta/Al_2O_3 interfaces (with mixed ionic/covalent Ta–O bonding and no oxygen interdiffusion into the film) and the emergence of amorphous TaO once the Ta:O ratio exceeds 1:1. Together, these results provide a quantitative roadmap for phase-selective, orientation-controlled, thickness-tuned α-Ta growth on sapphire for next-generation superconducting qubit platforms.

5:00pm **QS2-MoA-15 Mitigating Vortex Losses in Tantalum Superconducting Resonators Through Defect Landscape Engineering**, ***Rohin Tangirala,*** *Chaman Gupta,* University of Washington*; Benjamin Palmer,* Laboratory for Physical Sciences, University of Maryland*; Yongqiang Wang,* Los Alamos National Laboratory*; Serena Eley,* University of Washington

Tantalum (Ta) has recently emerged as a low-loss material for superconducting circuits, due to its stable native oxide with fewer two-level system (TLS) defects that may cause dissipation and decoherence. Stray and applied magnetic fields can introduce additional energy losses due to the motion of Abrikosov vortices, especially in clean-limit tantalum films. To mitigate this loss channel, we intentionally introduce defects through proton irradiation and lithographically-defined antidots into tantalum superconducting resonators to engineer the vortex pinning landscape and control vortex dynamics. We characterize device performance across a range of applied magnetic fields and conditions relevant to superconducting qubit operation, including single-photon power levels and millikelvin temperatures, in order to quantify losses arising from vortices and explore design considerations for increasing the performance of tantalum resonators under magnetic fields. This may enable the integration of magnetic-field-resilient tantalum resonators into superconducting and hybrid quantum systems.

5:15pm **QS2-MoA-16 A Comparative Study of Niobium Superconducting Resonators on Silicon and 4H-Silicon Carbide Substrates**, ***Marcelo Velasco Forest,*** *Joseph Falvo,* Quantum Collaborative Research Corps & Department of Physics, University of Maryland, College Park*; Kiana Reed,* Department of Physics and Astronomy, University of California, Irvine*; Ivan Lainez, Kasra Sardashti,* Quantum Collaborative Research Corps & Department of Physics, University of Maryland, College Park

Energy loss from two-level systems (TLS) at metal–dielectric and substrate interfaces continues to limit coherence in superconducting quantum circuits. We investigate whether substrate selection and surface preparation can suppress TLS-related loss by comparing niobium (Nb) coplanar-waveguide resonators fabricated on silicon (Si) and 4H-silicon carbide (SiC). Nb films (~150 nm) are deposited by DC magnetron sputtering using a standardized baseline process. Substrate preparation spans a controlled matrix of ex-situ and in-situ treatments, including solvent sonication, O_2 plasma, piranha clean, and HF clean by dip and vapor methods.

TLS-related losses and the effects of different preparation methods were determined from fitting resonator complex transmission, S_{21}, to well-tested theoretical models. We will report a comparison of Si and SiC under identical deposition conditions, as well as the surface preparation procedure that yields the lowest losses for each substrate. The primary outcome is a ranked set of substrate/preparation combinations that maximize single-photon internal quality factor and minimize inferred TLS-related loss.

5:30pm **QS2-MoA-17 Spectroscopy of Two-Level-System Defects via Multilevel Relaxation in a Fixed-Frequency Transmon**, ***Tanay Roy,*** *Xinyuan You, David van Zanten, Francesco Crisa, Sabrina Garattoni, Shaojiang Zhu, Anna Grassellino, Alexander Romanenko,* Fermi Lab

Temporal fluctuations in the coherence of superconducting transmon qubits are widely believed to originate from two-level system (TLS) defects coupled to the qubit. Existing TLS spectroscopy techniques typically rely on qubit frequency tunability or AC-Stark-based approaches, which can introduce additional complexity and offer limited bandwidth. Here, we demonstrate an alternative method for TLS spectroscopy based on monitoring the relaxation dynamics of multiple excited states in a fixed-frequency transmon [1]. By analyzing temporal correlations between multilevel decay processes, we identify signatures of TLS defects that are detuned by more than 100 MHz from the qubit transition yet still significantly impact coherence. Our results establish multilevel relaxation spectroscopy as a simple and broadly applicable technique for probing defect-induced noise in superconducting qubits without requiring flux tunability[1] https://arxiv.org/abs/2602.11127This work was supported by the U.S. Department of Energy, Office of Science, National Quantum Information Science Research Centers, Superconducting Quantum Materials and Systems Center (SQMS), under Contract No. 89243024CSC000002. Fermilab is operated by Fermi Forward Discovery Group, LLC under Contract No. 89243024CSC000002 with the U.S. Department of Energy, Office of Science, Office of High Energy Physics.

Surface Science
Room 305 - Session SS-MoA
Surface Electronic, Magnetic, and Optical Properties

Moderators: Prof. Abner de Siervo, University of Campinas (UNICAMP), **Alexander Sinitskii**, University of Nebraska-Lincoln

1:30pm **SS-MoA-1 Graphene Nanoarchitectonics: Exploring Dimensionality Effects from 0 to 1.X**, ***Aitor Mugarza,*** Catalan Institute of Nanoscience and Nanotecnology - ICN2, Spain **INVITED**

Nanostructuring Graphene Confers Multiple Functionalities to This Material, Making It Attractive to Very Diverse Applications in Electronics, Molecular Sensing and Filtering. For Instance, Semiconducting Gaps Can Be Induced by Reducing Its Dimensions to the Nanometer Scale. At This Scale, Edges Play a Crucial Role in Determining the Physico-Chemical Properties of the Nanomaterial, with the Emergence of Magnetism Localized at Zigzag Edges, or the Capability to Add Functional Groups Being Representative Examples. on the Other Hand, Introducing Pores of Similar Sizes Turns Impermeable Graphene Into the Most Efficient Molecular Sieve Membrane. For Both the Material and Void Components, the Interesting Scale for Applications Is Below 3-5 Nm, a Regime Where Bottom-Up Synthesis Can Be Particularly Efficient.

Here I Report Different Surface-Assisted Methods to Grow *0d* Graphene Quantum Dots with Magnetic Zigzag Edges (1-4), *1d* Nanoribbons Where the Electronic Properties Are Tuned by Controlled Edge Functionalization (5,6), and Nanoporous Graphene Sheets That Combine 1nm Size Ribbons and Pores (7). The Highly Anisotropic Structure of These Weakly Coupled Ribbon Arrays and the Modular Strategy Employed for Their Synthesis Allow Us to Control Their *1.X* Dimensionality by Molecular Bridge Engineering (8), or Even the Realization of 1nm Wide Lateral Heterostructure Superlattices Where Novel Excitonic States Are Predicted (9).

the Novel Electronic States of the Synthesized Nanoarchitectures Are Correlated with the Particular Atomic Structures by Using Scanning Tunnelling Microscopy. Their Potential Application in Devices Is Illustrated by Gate Modulated Transport Measurements in Nanoporous Graphene Sheets.

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2:00pm **SS-MoA-3 Spatially Probing the Topologically Protected Surface State of Bi_2Se_3 to Local Impurities and Defects**, ***Nathan Guisinger***, Argonne National Lab

Low-dimensional materials functioning at the nanoscale are a critical component for a variety of current and future technologies. The exploration of novel quantum materials and architectures to advance quantum information science (QIS) is at the forefront of condensed matter research. There has been tremendous interest in alternative strategies that utilize topologically protected states. Because these states are robust to their local environment, topological QIS offers advantages towards longer coherence time and a more fault tolerant platforms. This talk will discuss our recent atomic-scale study of the well-known topological insulator Bi_2Se_3 that has been doped n-type with magnetic Fe atoms. Specifically, the impact of sub-surface impurities, Se vacancies, and adatoms on the two-dimensional topologically protected surface state. An ultrahigh vacuum low-temperature scanning tunneling microscope was used to perform this study with applied magnetic field up to 9T. Both topographic imaging and spectroscopy were utilized for spatial characterization. This research was performed at the Center for Nanoscale Materials (CNM) at Argonne National Laboratory, which is one of the five Department of Energy Nanoscale Research Centers.

2:15pm **SS-MoA-4 Spectro-Microscopic Characterization of Surface Magnetization in Bulk Fe_3GeTe_2**, *Trevor A. Tyson,* New Jersey Institute of Technology*; Abdullah Al-Mahboob,* ***Jerzy T. Sadowski****,* Brookhaven National Laboratory

The spatial variation of the magnetic structure in Fe_3GeTe_2 has previously been investigated using scanning tunneling microscopy, magnetic force microscopy, X-ray magnetic circular dichroism (XMCD), scanning electron microscopy with polarization analysis, and Lorentz transmission electron microscopy. Here, we employ the XMCD imaging mode of X-ray photoemission electron microscopy (XMCD-XPEEM) to investigate the magnetic domain structure of Fe_3GeTe_2 in zero applied magnetic field. The observed domain configuration follows the expected pattern for thick crystals with strong uniaxial magnetic anisotropy.

To further probe the magnetic texture, we use low-energy electron microscopy (LEEM) with a tilted incident electron beam to image magnetic domain walls. Unlike spin-polarized LEEM, this method does not require specialized sample preparation or a spin-polarized electron source. Instead, magnetic contrast is generated by tilting the incident electron beam relative to the sample surface normal, or equivalently by tilting the sample itself. We demonstrate how the resulting contrast can be analyzed to determine the domain-wall type and to extract critical exponents associated with the surface magnetic behavior.

Acknowledgement: This work is supported by NSF Grant No. DMR-1809931. This research used resources of the Center for Functional Nanomaterials and the National Synchrotron Light Source II, which are U.S. Department of Energy (DOE) Office of Science facilities at Brookhaven National Laboratory, under Contract No. DE-SC0012704.

2:30pm **SS-MoA-5 Surface Electronic Structure of $Sr_3Ir_2O_7$ (001) Thin Films**, ***Peace Adegbite****, M. Zaid Zaz, Yuanyuan Zhang, Arjun Subedi,*** University of Nebraska-Lincoln, USA*; Alpha T N'Diaye,* Lawrence Berkeley National Laboratory*; Kenya Shimada,* Research Institute for Synchrotron Radiation Science, Hiroshima University, Japan*; Takashi Komesu, Xia Hong, Peter Dowben,* University of Nebraska-Lincoln, USA

$Sr_3Ir_2O_7$ is a narrow band-gap Mott insulator and member of the Ruddlesden-Popper strontium iridates. It is a layered material with competing energy scales for strong spin-orbit coupling and Coulombic interactions. The competing energies for band width (W), correlation (U) and spin-orbit coupling affects the surface characteristics in interesting ways. In this study, we investigated the surface electronic behavior and band structure of $Sr_3Ir_2O_7$ (001) thin films, using a variety of surface-sensitive spectroscopy techniques.

Angle-resolved photoemission spectroscopy (ARPES) revealed the presence of a finite density of states at the Fermi level that is localized to the surface, indicating a metallic surface coexisting with an insulating bulk. This surface-localized metallicity is further supported by transport measurements, as the electrical conductivity of $Sr_3Ir_2O_7$ thin films increases with decreasing film thickness. X-ray photoemission spectroscopy shows no measurable band bending with increasing Au overlayer thickness on the $Sr_3Ir_2O_7$ thin film, consistent with the measured linear I-V character and indicating the absence of a Schottky barrier at the $Au/Sr_3Ir_2O_7$ interface. From the valence band dispersion in ARPES, we estimated a light effective hole mass of 0.11 m_0 along the Γ-M direction of the surface Brillouin zone. To obtain a comprehensive view of the electronic structure, the unoccupied band structure was mapped using angle-resolved inverse photoemission spectroscopy and the orbital symmetry of the unoccupied bands at the Sr L-edge was assigned through angle-resolved X-ray absorption spectroscopy.

Furthermore, low energy electron diffraction reveals an anomalous temperature dependence of the surface scattering intensity that contradicts the conventional Debye-Waller behavior. We attribute this behavior to the damping of the normal mode vibrations via thermally activated carriers with increasing temperature.

2:45pm **SS-MoA-6 Revealing the Band Structure of High Entropy Oxides with Angle Resolved Photoemission**, ***Elena Salagre****, Elliot Fuller,*** Sandia National Laboratories

Recent years have seen interest rise for materials that can be tuned beyond traditional means. Compositionally complex oxides (CCOs), also identified as High Entropy Oxides (HEOs), are a unique approach to tailor properties by introducing multiple cations (typically 4+) to a lattice site. Despite such disorder, CCOs often maintain high crystal quality and homogeneity due to entropy stabilization effects. High entropy oxides have been explored as catalyst and as materials for microelectronics, applications in which their surface band structure becomes critical. However, few works have captured the electronic structure of these oxides. Here we reveal how electronic properties emerge due to the competing effects of compositional complexity, disorder and strong correlations. We present a combination of electronic transport and Angle Resolved Photoemission (ARPES) on ABO_3 high entropy oxides both in terms of the A-site and B-site cation substitutions. For the A site substitution by La, Sm, Nd, Gd, Y adds compositional complexity as a fraction substitution (La_{1-x}[Sm, Nd, Gd, Y]$_{x/4}BO_3$) while Sr can be used as a traditional hole dopant to tune the electronic behavior. For B site, a mixture of the transition metals Cr, Mn, Fe, Co, Ni is used to add complexity while tuning *U*, *W*, *Δ* and spin degrees of freedom. Our results present clear evidence that a unified and coherent band structure is maintained in CCOs, even when the valence band is formed by 5 transition metal oxide *d*-levels. Additionally, we explore using compositional complexity in a strongly correlated double exchange metal (LSMO), where it can be used as a tool to systematically explore how new phases emerge, including a crossover regime between correlation and disorder induced behaviors. With these new measurements of the band structure of these CCOs, a better understanding of observed transport and magnetic properties can be achieved.

3:00pm **SS-MoA-7 Unveiling the Surface Electronic and Morphological Properties of the Centrosymmetric Nano-Skyrmion Host $EuAl_4$, *Jarred Grant,*** *David King, Nikiphoros Vlastos, Yuri Dahnovsky, Jinke Tang, TeYu Chien,* University of Wyoming

Centrally symmetric (centrosymmetric) magnets capable of hosting skyrmions have attracted intense interest because they lack the Dzyaloshinskii-Moriya interaction (DMI). In these materials, inversion symmetry is preserved, requiring alternative mechanisms beyond DMI for skyrmion formation and stabilization. Proposals include symmetry-breaking effects such as charge density waves (CDW). The interplay among possible DMI, Ruderman-Kittel-Kasuya-Yosida (RKKY), and four-spin interactions in these systems creates a rich platform for diverse magnetic textures and phases. Centrosymmetric $EuAl_4$ is a particularly promising example, owing to its exceptionally small reported skyrmion size (~3 nm). Direct visualization of these nanoscale skyrmions is highly desirable. Spin-polarized scanning tunneling microscopy (SP-STM) is ideally suited for this length scale; however, key surface properties of cleaved $EuAl_4$, including the cleavage plane, surface morphology, local electronic structure, and termination—remain largely unexplored. In this talk, I will present STM, LEED, and DFT results detailing the cleavage plane, atomic-scale surface morphology, and corresponding dI/dV spectra of cleaved $EuAl_4$(001) single crystals.

*This work was supported by: DMR- 2414748

3:15pm **SS-MoA-8 Engineering Electronic States in High-Entropy Materials: From Disorder-Induced Pseudo Gaps to Gap Tuning in Transition Metal Dichalcogenides*, TeYu Chien,*** University of Wyoming

High-entropy materials provide a unique platform to engineer novel electronic states through extreme chemical disorder. This talk presents scanning tunneling microscopy and spectroscopy (STM/STS) investigations into local electronic structures across two distinct high-entropy systems.

First, we examine the impact of atomic-scale chemical disorder in high-entropy alloys (HEAs). Local d*I*/d*V* spectra reveal the emergence of a disorder-induced pseudo gap at the Fermi level, directly reflecting modifications to the local density of states driven by electron-electron interactions caused by random potentials seen by electron wave function in random elemental distribution environment.

Second, we demonstrate electronic tuning in high-entropy transition metal dichalcogenides (HE-TMDs). By controlling metal compositions, we show a systematic evolution of the tunneling spectrum from low entropy to medium entropy HE-TMDs. Specifically, the characteristic V-shaped d*I*/d*V* spectrum transitions into a distinct U-shaped gap structure. These findings highlight the potential of entropy-stabilized configurations to precisely tailor quantum phases and electronic behaviors at the nanometer scale.

3:30pm **SS-MoA-9 Revealing Cu-Mn Electronic Structure Interaction in Activated $CuMn/Al_2O_3$ Catalyst by Decoupling of Overlapping XPS Spectra*, Yong Yang,*** Shanghaitech University, China*; Rongjia Du,* ShanghaiTech University, China*; Evgeny I. Vovk,* ShanghaiTech University, China, Russian Federation

Mn promoted Cu based catalysts demonstrate high efficiency and stability in various chemical processes including methanol synthesis. Investigation of active centers in bimetallic Cu-Mn catalysts meets certain problems: Mn oxidation state cannot be directly determined because of strong overlapping of Mn and Cu photoelectron and Auger spectra. In this study, a new approach of convoluted background subtraction was proposed to separate the net Mn photoelectron spectra from overlapping Cu signal. The structure of CuAl and CuMnAl catalysts was investigated by XPS, XRD and EXAFS. XPS data were obtained after *in situ* activation and passivation treatments. After dedicated data analysis, the XPS results indicated the interaction and charge transfter between the Cu and Mn species on the CuMnAl catalyst. This study insighted how Mn promoter can effectively tune the electronic states of Cu catalyst; while it also provided a methodology example of separating low intensity Mn photoelectron spectra from overlapped complex background signals that can be aplyed to Mn-Cu or similar multicomponent systems.

4:00pm **SS-MoA-11 Understanding of STS Maps of Strongly Correlated Molecules on Surfaces: Can We Image Molecular Orbitals?*, Pavel Jelinek,*** Institute of Physics of the Czech Academy of Sciences, Czechia **INVITED**

Traditionally, scanning tunneling spectroscopy (STS) of individual molecules is interpreted within the formalism of one-electron molecular orbitals [1]. Although this theoretical approach gives satisfactory agreement with experiment in some cases [2], it is in direct contradiction with the basic principle of quantum mechanics, which excludes direct observation of the wave function [3].

Moreover, recent progress in on-surface synthesis has enabled the preparation of strongly correlated polyradical molecules [1], which are not available by traditional solution-phase synthetic approaches. It is not surprising that interpreting STS maps of such polyradical molecules based on standard one-electron STM theory often fails. In this talk, we will discuss a many-body theoretical framework that enables us to simulate STS maps of strongly correlated molecules accurately [3]. Namely, we will introduce the concept of Dyson orbitals [4] to interpret ionic resonances in STS maps and natural transition orbitals [5] describing spin excitations in STS maps. Finally, we will discuss Kondo orbitals [6] to understand the origin of the spatial Kondo signal in high-spin molecules on metal surfaces.

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4:30pm **SS-MoA-13 Nanoscale Characterization of Metal-Supported Ultrathin Films Using Ultrahigh Vacuum Tip-Enhanced Raman Spectroscopy*, Nan Jiang,*** University of Illinois - Chicago

Metal-supported ultrathin films exhibit unique structural and vibrational properties governed by reduced dimensionality and strong interfacial coupling. Probing these properties at the nanoscale requires techniques that combine high spatial resolution with chemical specificity under well-controlled surface conditions. Here, we utilize ultrahigh vacuum (UHV) tip-enhanced Raman spectroscopy (TERS) to investigate model two-dimensional systems with sub-nanometer resolution.

Our measurements focus on ultrathin films grown on metallic substrates, such as two-dimensional materials and metal oxides. Borophene, a polymorphic two-dimensional boron phase, presents substrate-dependent lattice configurations and anisotropic vibrational responses. UHV-TERS enables identification of distinct vibrational modes associated with different borophene polymorphs and reveals nanoscale structural heterogeneity. In parallel, ultrathin iron oxide films serve as model oxide systems with thickness- and phase-dependent properties. TERS measurements resolve localized phonon modes and provide insight into spatial variations in oxidation state and coordination at the metal–oxide interface.

The UHV environment ensures clean surfaces and reproducible tip–sample junctions, allowing direct correlation between spectroscopic signatures and atomic-scale structure. These results demonstrate the capability of UHV-TERS to probe structure–property relationships in supported ultrathin films with unprecedented spatial resolution. This approach provides a pathway for nanoscale characterization of complex oxide and low-dimensional materials relevant to catalysis and surface science.

4:45pm **SS-MoA-14 Precision Force-Volume HR-AFM Reveals Single-Molecule Reactive Sites and Reactivity Landscapes Quantitatively*, Percy Zahl,*** Brookhaven National Laboratory*; Xinzhe Wang,* Yale University*; Jara Trujillo-Mulero, Emiliano Ventura-Macias,* Universidad Autonoma de Madrid, Spain*; Yunus Dogan, Bugrahan Guner,* Yale University*; Rubén Pérez,,* Universidad Autonoma de Madrid, Spain*; Eric I. Altman, Udo D. Schwarz,* Yale University

Studying molecular interactions at surfaces is crucial for advancing catalytic technologies and addressing numerous challenges in materials science. While three-dimensional atomic force microscopy (3D-AFM), introduced in 2009 [1], enables measurements of tip–sample interactions with sub-angstrom spatial resolution and piconewton force precision, quantitative site-specific information on molecule–molecule interactions has thus far remained inaccessible. This limitation arises because the recovered total tip–sample force contains substantial contributions from the substrate (denoted F_1 and F_2 (see below) as well as from the back part of the tip (F_4), which typically dominate the measured interaction and obscure details in the force (F_3) of interest.

Here, we demonstrate a novel post-processing correction framework that removes these unwanted F_1, F_2, and F_4 contributions. Using the interaction between cobalt phthalocyanine (CoPc)—a prototypical CO_2 reduction catalyst deposited on Ag(111)—and a CO molecule attached to the tip apex, we isolate the CoPc–CO interaction force F_3. This approach reveals site-specific reactivity landscapes and their modulation through $–NH_2$ substitution. Our advance transforms 3D-AFM into a chemically specific and quantitative tool for probing interaction forces between complex molecules, achieving an accuracy previously accessible only through theoretical modeling.

[1] B. J. Alberset al.,Nature Nanotechnology 4, 307 (2009)

[2] Xinzhe Wanget al.,ACS Nano18, 4495 (2024)

Forces assuming a CO terminated metal tip:
F_1: substrate — tip [background]
F_2: background, CO — substrate [background]
F_3: molecule — CO [the one of interest]
F_4: metal apex of tip — molecule [the main enemy]

5:00pm **SS-MoA-15 Statistical Adsorption Mapping and 3D-AFM Characterization of Cobalt Phthalocyanine (CoPc) on Au(111)**, ***Bugrahan Guner***, *Yunus E. Dogan,* Yale University*; Percy Zahl,* Brookhaven National Laboratory*; Xinzhe Wang,* Oak Ridge National Laboratory, USA*; Eric I. Altman, Udo D. Schwarz,* Yale University

Molecule-substrate interactions play a critical role in molecular adsorption because local atomic registry, reconstructions, and related surface strain can influence where molecules adsorb, how they orient, and how strongly they interact with the surface. Au(111) is one of the most widely used model substrates for such studies, as it is chemically stable, atomically well-defined, and exhibits the characteristic herringbone reconstruction, which creates distinct fcc, hcp, domain-wall, and elbow/kink regions. Cobalt phthalocyanine (CoPc) is also a widely studied model molecule due to its relevance in substrate-supported molecular catalysis [1].

To examine how the reconstructed Au(111) surface guides CoPc adsorption, we employ low-temperature scanning tunneling microscopy to first identify the positions and orientations of individual adsorbed CoPc molecules, followed by a statistical analysis where molecules are assigned to specific reconstruction regions while considering their distance to the nearest elbow. This allows adsorption near elbows/kinks, along herringbone/domain-wall regions, and within fcc/hcp domains to be compared systematically.

This analysis is then connected to three-dimensional atomic force microscopy (3D-AFM) measurements, where frequency-shift data collected at different tip-sample distances are used to reconstruct local interaction forces between the sample and a tip functionalized by attaching a CO molecular to its apex [2-3], which yields complementary force-sensitive information on molecule-substrate coupling and chemically relevant interactions. Together, these approaches connect surface reconstruction, molecular organization, and local interaction forces, providing a framework for understanding how structured metal substrates influence molecular catalyst behavior.

References

[1] Y. Wu et al., Nature 2019, 575, 639.

[2] X. Wang et al., ACS Nano 2024, 18, 4495.

[3] M. Z. Baykara et al., Beilstein J. Nanotechnol. 2012, 3, 637.

5:15pm **SS-MoA-16 Energy-Resolved Low-Energy Electron Microscopy as a Quantitative Metrology for EUV Photoresist Films**, ***Peter Sun,*** *Chang-Yong Nam, Jerzy Sadowski,* Brookhaven National Laboratory

Extreme ultraviolet (EUV) lithography drives photoresists toward thinner films, smaller features, and tighter line-edge roughness (LER), placing new demands on the characterization of resist behavior. Resist chemistry is governed by low-energy secondary electrons (<20 eV) generated from 13.5 nm photons, but transient surface charging shifts the effective landing energy throughout exposure, leaving film response at these energies unresolved by existing metrology.

We address this gap with charging-compensated low-energy electron microscopy and diffraction (LEEM/LEED) as a quantitative metrology platform for next-generation EUV resist films. Using 25 nm PMMA as a model system irradiated at 5–20 eV, we monitor the diffuse diffraction response and resolve the landing energy and surface potential. A conductance-based charging model extracts the total electron yield and dissipation parameters, enabling a dynamic electron-energy ramping scheme that locks the landing energy and turns LEEM/LEED into a controllable, energy-resolved metrology for resist films.

The energy-resolved method enables studies of resist-degradation performance and efficiency, including stochastic energy diffusion correlated with LER, and supports next-generation EUV and beyond-EUV resist development.

This research is supported by the U.S. Department of Energy Office of Science Accelerate Initiative Award 2023-BNL-NC033-Fund. This research used resources (XPEEM/LEEM end station of the ESM beamline) of the Center for Functional Nanomaterials and the National Synchrotron Light Source II, which are the U.S. Department of Energy (DOE) Office of Science facilities at Brookhaven National Laboratory, under Contract No. DE-SC0012704.

5:30pm **SS-MoA-17 DFT Insights into Electronic Modulation of Cobalt Sites for N_2O Decomposition on Ni-Doped Spinel Oxides**, *Hyung Chul Ham,* ***Chi Hun Lee,*** Inha university, Republic of Korea*; Su Keun Kuk, Jong-Min Lee, Hyuk Jae Kwon,* Samsung Advanced Institute of Technology, Republic of Korea

Nitrous oxide decomposition on transition-metal oxide surfaces is controlled by the adsorption and conversion of N_2O-derived intermediates, as well as by the ability of the surface to release oxygen. In this study, we use density functional theory calculations to investigate the surface reaction mechanism of N_2O decomposition on Co_3O_4(110) and $NiCo_2O_4$(110) spinel surfaces, which serve as representative models for oxidized shells formed on Co–Ni co-exsolved nanoparticles. Particular attention is given to how Ni incorporation modifies the surface reaction energetics and the electronic structure of Co-centered active sites.

Our calculations show that N_2O activation occurs near surface octahedral Co sites on both Co_3O_4(110) and $NiCo_2O_4$(110). The reaction proceeds through a bent trans-$N_2O_2^{2-}$ intermediate, consistent with experimentally observed hyponitrite-like surface species. Compared with Co_3O_4(110), $NiCo_2O_4$(110) stabilizes adsorbed N_2O more strongly and lowers the energetic penalty for forming the trans-$N_2O_2^{2-}$ intermediate. Transition-state calculations further show that Ni incorporation reduces the activation barrier for hyponitrite decomposition into N_2 and surface oxygen species. In addition, the subsequent O_2 formation step becomes more favorable on $NiCo_2O_4$(110), which can be attributed to weaker binding of surface oxygen species.

Electronic-structure analyses reveal that the improved reaction energetics originate from Ni-induced restructuring of Co-centered active sites. Ni incorporation modifies metal–oxygen covalency and stabilizes hybridized metal 3d–N 2p states involved in N_2O adsorption, as supported by projected density of states and crystal orbital Hamilton population analyses. In addition, surface octahedral Co sites exhibit a surface-induced spin-state change, suggesting that the spin-polarized electronic structure of these sites contributes to N_2O activation and intermediate conversion.

These results indicate that Ni-modified Co_3O_4 spinel surfaces enhance N_2O decomposition by simultaneously promoting N_2O adsorption, hyponitrite intermediate decomposition, and oxygen release. More broadly, this work highlights how surface composition and electronic structure, including spin-state effects, can be tuned to design non-noble-metal oxide catalysts for greenhouse-gas decomposition.

Thin Films
Room 317 - Session TF1-MoA
Thin Films for Energy

Moderators: Prof. Dr. Adriana Creatore, Eindhoven University of Technology, **Prof. Mark Losego**, Georgia Institute of Technology

2:00pm **TF1-MoA-3 TFD Messier Mid-Career Award Lecture: Growth Mechanisms and Properties of Thin-Film Ceramics for Energy Applications**, ***Per Eklund,*** Uppsala University, Sweden **INVITED**

This invited presentation for the AVS Thin Film Division's Russel F. Messier Mid-Career Award Lecture gives an overview of my research in the energy area and fundamental growth mechanisms. For thermoelectric devices, I present an overview of our work on multicomponent CrN-, ScN-, and $Ca_3Co_4O_9$-based thin films. The semiconducting early transition metal nitrides have emerged as an unexpected class of materials for thermoelectric energy harvesting. CrN exhibits n-type conduction with a

high power-factor enabled by a high electron concentration thermally activated from N vacancies, and alloys can be made of rocksalt-$Cr_{1-x}Sc_xN$. Multicomponent alloying of ScN and CrN in alloys such as CrMoVWN or combinations thereof offer further possibilities for tailoring the thermoelectric properties and growth conditions. We have developed textured and nanoporous hase-pure $Ca_3Co_4O_9$ thin films. These can further be deposited on flexible mica substrates, enabling flexible inorganic thermoelectric thin films that withstand repeated bending, and as free-standing films.

For growth on mica, an outstanding question is the growth of stress-free epitaxial films by van der Waals epitaxy (vdWE). Unlike conventional epitaxy, vdWE allows stress-free growth of thick films with oriented crystals without dislocations even for large film-substrate lattice mismatches. However, vdWE of non-layered materials is often presumed or claimed on layered substrates such as mica without experimental evidence. We have shown that the growth of rocksalt ScN and NiO films on mica(001) occurs by conventional epitaxy, which should be the default assumption for non-layered materials unless vdWE isexplicitly proven. In contrast, for layered materials on mica, the situation is far more complex, and an atomistic understanding of film/substrate interface structure that explains and predicts vdWE has remained elusive. We have unveiled atomistic interface mechanisms for vdWE of MoO_3 and VO_2 on mica showing negligible strain buildup in continuous epilayers, confirming vdWE. Ab initio computations showing interface energy minima for these orientations correlate with high cross-interface proximity between Mo atoms in alpha-MoO3 and K in mica conducive for maximal vdW attraction. These insights on interface structure and energetics provide a framework for predicting vdWE for different film/substrate combinations and designing of stress-free and/or standalone epitaxial films of layered materials on layered substrates such as mica.

2:45pm **TF1-MoA-6 Enhancing Energy Storage Performance via Minimal Doping in $SrTiO_3$ Thin Films**, ***Saeed Almishal***, *Joseph Petruska, Jon-Paul Maria,* Penn State University

We investigate a controlled minimal doping strategy for enhancingenergy storage performance in Mn-substituted SrTiO3 thin films by introducing nanoscale polarization disorder through Ti/O defect dipoles.We develop robust X-ray fluorescence calibration methods, enabling reliable quantification of Mn concentrations down to ~0.25% in bulk ceramics. We subsequently grow thin films by pulsed laser deposition on Pt/sapphire substrates,monitoring crystalline qualitywithX-ray diffractionandsurface roughness using atomic force microscopy.We additionally utilizeX-ray photoelectron spectroscopyfor chemical analysis and scanning electron microscopy to measurefilm thickness.We systematically characterize our thin film capacitors with tungsten-top electrodes through polarization-electric field measurements, breakdown testing, and energy storage analysis as functions of dopant concentration, film thickness, and measurement frequency. We identify an optimal Mn concentration of 1.75% at 350 nm thickness, providing the best compromise between polarization, breakdown field, efficiency, and reproducibility, delivering room temperature recoverable energy density ~87 J/cm3 at remarkably high 86% efficiency, compared to pure SrTiO3 ~5 J/cm3 and ~ 30% respectively, when measured at 10KHz frequency. Overall, our results demonstrate that minimal chemical perturbations can produce substantial enhancements in energy storage behavior.

3:00pm **TF1-MoA-7 Interfacial Engineering of the HTL-Perovskite Interface in Perovskite Solar Cells Using Atomic Layer Deposition**, ***Alexandra Hurd***, *Md Aslam Uddin, Oluka Okia, Neil Dasgupta,* University of Michigan, Ann Arbor

Perovskite solar cells (PSCs) are the leading low-cost, easily manufacturable photovoltaic alternative to commercial silicon, with efficiencies rivaling that of silicon. However, the interface between the perovskite absorber and hole transport layer (HTL) remains a critical barrier for the long-term operational stability of p-i-n PSCs. Nickel oxide is a highly effective inorganic HTL due to its high hole mobility, wide bandgap, and intrinsic stability. However, the trivalent nickel states required for hole conductivity are thought to contribute to perovskite degradation at the NiO-perovskite interface via redox and acid-base reactions[1]. Some strategies have been implemented in the literature to passivate this interface, including self-assembled monolayers, other organic and inorganic interlayers, and doping of the NiO[2,3]. However, there are limited studies that employ chemical control of the HTL-perovskite interface via vacuum processing methods to improve interfacial stability.

This work explores atomic layer deposition as a method for precise tuning of the nickel oxide film and NiO-perovskite interface. By performing post-deposition anneals in different gaseous environments, we control surface oxidation states of NiO. We examine trends between HTL electrochemical properties and interfacial stability for NiO-only and NiO with an ultrathin inorganic buffer layer. Surface energy and chemistry of the films are characterized by water contact angle goniometry and XPS, respectively. We conduct heat and light stability tests of encapsulated HTL-perovskite junctions and characterize degradation using X-ray diffraction and photoluminescence spectroscopy. Interfacial toughness of the interface is also characterized with mechanical testing. By identifying trends in interfacial stability and toughness with various NiO surface properties, we inform interfacial engineering of the interface to improve operational stability of PSCs and take steps toward their commercialization.

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[2]Zhou W., Fang Y., et al., Solar Energy Materials and Solar Cells, (2026), 296, 114079

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3:15pm **TF1-MoA-8 Regulating early-stage chemistry enables certified open-circuit voltage of 847 mV in wide-bandgap kesterite Cu2ZnSnS4 thin-film solar cells**, ***Ao Wang***, *Kaiwen Sun, Xiaojing Hao, Martin Green,* University of New South Wales, Australia

On the path to carbon neutrality, increasing photovoltaic (PV) penetration requires continuous cost reduction and efficiency advancement. It drives the need for developing earth-abundant, stable, and low-cost wide-bandgap materials that are compatible with Si-based tandem cells. Wide-bandgap kesterite Cu_2ZnSnS_4 (CZTS) is widely regarded as a promising candidate, yet its certified efficiency remains capped below 11.5% with an open-circuit voltage (V_{OC}) under 750 mV. Although researchers have long identified reducing the V_{OC} deficit as critical, achieving substantial improvement in this emerging technology has proven challenging.

In this work, we overcome this long-standing bottleneck by simultaneously achieving a certified V_{OC} of 847 mV and a record efficiency of 12.4% (previous results summarized in Table 1). This work sets a new benchmark for wide-bandgap CZTS, delivering a certified V_{OC} near 850 mV, which is the first beyond 800 mV and nearly 100 mV higher than the prior record.

Table 1. Certified results of wide-bandgap Cu_2ZnSnS_4 solar cells

V_{OC} (mV)	Efficiency (%)	Bandgap (eV)	Reference
731	11.0	1.50	Nat Energy 3, 764–772 (2018)
748	11.4	1.53	Nat Energy 10, 255–265 (2025)
709	11.5 (active-area)	1.50	Nat Energy 10, 630–640 (2025)
847	12.4	1.57	This work

More importantly, we reveal why the widely adopted strategy of designing a Cu-poor/Zn-rich composition, though guided by numerous theoretical calculations, has failed to deliver substantial performance advancement. Despite the well-controlled initial global composition, the spatial local chemistry before crystallization is more critical and can deviate significantly. In practice, the strong reactivity of Cu with S during annealing often leads to a Cu-rich surface, making it difficult to preserve the designed composition.

Here, we employ a ‘structured two-stage Cu’ strategy that enriches Cu-S bonding at the film surface, thereby lowering the driving force for Cu out-diffusion. The stabilized environment simultaneously suppresses diffusion-induced secondary phases and segregation, bridging the gap between global design and local chemistry to ensure the desired crystallization chemistry and pathway. Consequently, benign defects are promoted while detrimental species are suppressed, leading to a significant enhancement of the effective carrier lifetime.

Beyond CZTS or even Cu-based chalcogenides, this strategy is expected to apply broadly to multinary thin-film materials containing elements with contrasting chemical reactivities. Furthermore, the concept is not limited to vacuum deposition, but can also guide solution processing and other scalable fabrication methods.

3:30pm **TF1-MoA-9 Perovskite Photovoltaics on Flexible Foils: Reliability, Scaling, and Pathways to Market**, ***Vivek Babu***, Verde Technologies **INVITED**

Metal-halide perovskite photovoltaics have attracted strong interest because they combine high efficiency with the potential for lightweight, flexible, and low-cost manufacturing. These features create a unique value proposition for applications where conventional silicon photovoltaics are limited by weight, rigidity, or installation constraints. Examples include space power, high-altitude platforms, unmanned aerial vehicles, and building- or vehicle-integrated photovoltaics.

However, moving perovskite photovoltaics from promising laboratory devices to reliable products requires solving challenges beyond initial power conversion efficiency. Flexible thin-film foils introduce practical constraints related to substrate handling, film uniformity, mechanical robustness, encapsulation, interconnection, and long-term environmental stability. As device area increases from small cells to mini-modules and panels, local defects and non-uniformities can strongly affect yield, reproducibility, and reliability.

In this invited talk, I will discuss the opportunities and barriers for commercializing flexible perovskite solar modules on polymer and metal foils. The presentation will focus on the connection between application requirements, manufacturing choices, and reliability expectations. Particular attention will be given to the challenges of scaling laboratory processes to larger-area flexible formats, maintaining device performance across the full panel area, and developing test protocols that reflect real operating conditions such as thermal cycling, humidity, illumination, mechanical stress, and radiation exposure.

Finally, I will discuss possible pathways toward market adoption, including the role of pilot-line manufacturing, inline quality control, accelerated reliability testing, encapsulation strategies, and early application targets where lightweight and flexible solar modules can provide clear system-level value. The goal is to highlight what is needed for flexible perovskite photovoltaics to move from high-performance prototypes toward manufacturable and bankable energy products.

Thin Films
Room 317 - Session TF2-MoA

Fundamentals of TF I

Moderators: Joe Becker, Kurt J. Lesker Company, **Prof. Subhadra Gupta**, University of Alabama

4:00pm **TF2-MoA-11 The Origins of Mxene Optical Properties**, ***Zahra Fakhraai,*** University of Pennsylvania **INVITED**

The functional properties of most 2D materials are well defined by their chemical composition. In contrast, for metal-organic complexes, the organic ligand can play a key role in controlling the electronic band structure of the complex. In this presentation, I will discuss the optical properties of MXenes, a relatively new class of highly conductive two-dimensional materials. MXenes are 2D transition metal carbides that are typically made by etching of a 3D crystal. In the prototypical $Ti_3C_2T_x$ MXenes, the termination state depends on the synthesis, etching, and delamination processes, which together result in mixed terminations consisting of =O, -OH, -F, and/or -Cl groups. In addition to being metallic, $Ti_3C_2T_x$ MXenes also show a broad near-infrared (IR) optical extinction (~1.5 eV), which has been widely attributed to a localized surface plasmon resonance (LSPR). However, using experimental measurements and density functional theory (DFT) calculations, we demonstrate that in mixed-terminated $Ti_3C_2T_x$ MXenes, this low-energy band is an interband transition specifically arising from oxygen-terminated ($Ti_3C_2O_2$) MXene. As such, we establish that in addition to the chemical structure, post-synthetic variations in MXene terminating groups can dramatically alter their band structure and optical properties. For example, we show that in $Ti_3C_2Cl_2$, where -Cl is the predominant termination, the low-energy transition vanishes, resulting in strongly metallic properties. In thin films, this property change can lead to the design of novel optical properties, such as hyperbolicity, while engineering the band structure can produce transparent optical regions in the IR spectral range. These variations in band structure due to termination states could play a significant role in the light-matter interactions in MXenes, result in electron-phonon coupling effects, and affect their thermal stability at high temperatures.

4:30pm **TF2-MoA-13 Optical and Structural Properties of Ga_2O_3 Thin Films Deposited by Reactive and Non-Reactive Sputtering**, ***Marcell Gajdics,*** *Ildikó Cora, Dániel Zámbó, Zsolt Horváth Endre, Béla Pécz,* HUN-REN Centre for Energy Research, Hungary

The ultrawide bandgap semiconductor, Ga_2O_3 has numerous potential applications in the fields of optoelectronics and high-power electronics. Gallium oxide thin films can be grown by a variety of methods, among which radio frequency sputtering is a commonly used technique, as it allows highly uniform layers to be deposited at low temperatures. In most cases, a ceramic Ga_2O_3 target is used for the sputter deposition of Ga_2O_3. In our work, we present an alternative method, i.e. reactive sputtering of a liquid Ga target. We have shown that by using this technique, layers close to the ideal stoichiometry can be deposited with higher deposition rate than by using a Ga_2O_3 target. The optical properties (e.g. refractive index) were studied as a function of the oxygen concentration in the films. Post-deposition heat treatments were also performed on the amorphous as-deposited layers to study the annealing-induced structural and optical changes. The crystallization and phase evolution were investigated by X-ray diffraction and transmission electron microscopy; in the latter case, both ex situ and in situ measurements were performed. It was found that the crystallization of Ga_2O_3 occurs in two steps: in the first step, the formation of the metastable γ-Ga_2O_3 phase was observed, and then, as a result of further annealing, the thermodynamically stable β-Ga_2O_3 appears. The photoluminescence emission and the optical bandgap were also measured at different annealing temperatures, and the results were correlated with the structural properties. The two crystalline phases have distinct emission spectra, and the photoluminescence of the β-Ga_2O_3 is also shown to depend on the annealing atmosphere.

4:45pm **TF2-MoA-14 Tailoring the Optical Response of Ultrathin GZO Films Through Process and Microstructural Control**, ***Kyu Ri Choi,*** *Miroslava Marinova, Geetika Chitturi, Jae Ik Choi, Vladimir Shalaev, Alexander Kildishev, Alexandra Boltasseva,* Purdue University

Gallium-doped zinc oxide (GZO) is an attractive transparent conducting oxide for epsilon-near-zero (ENZ) photonics due to its tunable optical response, reduced loss, and suitability for ultrafast photonic applications. Here, we investigated the influence of thickness, deposition temperature, and laser repetition rate on the structural and optical properties of pulsed laser-deposited GZO thin and ultrathin films on Si substrates. Films with thicknesses from 5 - 260 nm were characterized using spectroscopic ellipsometry, X-ray diffraction, and STEM/EDS measurements. A central component to our analysis was the identification of an amorphous SiOx-GZO interfacial layer that strongly affected the optical response in the ultrathin regime. Films grown at 200 °C exhibited increasing crystallinity and grain size with thickness, resulting in reduced optical loss and a blueshift of the ENZ wavelength, indicative of enhanced metallicity and reduced grain-boundary scattering. In contrast, room-temperature films showed limited crystallinity evolution and suppressed ENZ tunability. Transfer-matrix simulations revealed that the ENZ modal response depends strongly on both film thickness and minimum refractive index, with robust ENZ-mode excitation sustained for sub-50 nm films with refractive index minima below 0.6. These results establish key process-structure-property relationships for tailoring ENZ behavior in GZO ultrathin films for ultrafast and nonlinear nanophotonic platforms.

5:00pm **TF2-MoA-15 Plasma-Driven Microstructural Evolution in TaC Thin Films Deposited by DC, RF, and HiPIMS Sputtering**, ***Tainara Coutinho de Carvalho,*** *Jon-Paul Maria,* Penn State University

Controlling the microstructure of TaC thin films is essential for applications requiring high hardness, thermal stability, and chemical inertness, where functional performance is strongly governed by growth kinetics during deposition. Although DC, RF, and HiPIMS sputtering generate plasmas with distinct and well-known energetics, their comparative influence on TaC microstructural evolution under equivalent deposition rates remains insufficiently understood.

In this work, TaC films were deposited by DC, RF, and HiPIMS magnetron sputtering while systematically varying methane flow, working pressure, substrate temperature, target-to-substrate distance, deposition power, and film thickness. Structural and microstructural characterization was performed by XRD and SEM for all films, with TEM investigations on representative samples to understand microstructure at finer length scales.

Phase formation showed strong sensitivity to methane availability, with cubic TaC predominating under most conditions and Ta_2C forming only at low methane flow during RF deposition, suggesting that limited reactive carbon supply under RF plasma conditions favors the formation of metal-rich carbide phases. Despite comparable deposition rates, each sputtering mode produced distinct grain morphologies, highlighting the strong influence of plasma energetics and species transport on growth pathways. DC deposition promoted faceted grains within a narrow methane range, RF induced a transition from elongated Ta_2C grains to triangular TaC grains, and HiPIMS stabilized triangular morphologies across a broader methane window, adding a kick pulse to HiPIMS growth progressively suppressed this anisotropic growth behavior. Total pressure and target-to-substrate distance produced distinct morphological responses in DC and HiPIMS films, reflecting differences in collisional transport and arrival energy of the depositing species, whereas substrate temperature produced comparatively limited effects.

Changes in deposition power and film thickness revealed that these morphological transitions are associated with shifts in the balance between nucleation density and competitive grain growth. Ultimately, this work highlights how plasma-driven growth kinetics can be leveraged to design carbide thin films with tunable and application-specific microstructures.

5:15pm **TF2-MoA-16 Optimization and Stabilization of Stress in SiO_x for Piezoelectric Thin Films Stress Compensation**, ***J Goodman***, *Burcu Dursun,* The Pennsylvania State University*; Gavin Frueh, Kenneth Buffo, Casey DeRoo,* The University of Iowa*; Paul Reid,* Harvard & Smithsonian Center for Astrophysics*; Hanyuan Liang, Thomas Jackson, Susan Trolier-McKinstry,* The Pennsylvania State University

Lead zirconate titanate (PZT) thin films on Si substrates experience tensile stress due to the difference in thermal expansion coefficients between Si (2.3–4.5 × 10^{-6}/K) and PZT (5.5–8.0 × 10^{-6}/K)[1,2]. Stress in the PZT films and their electrode stacks leads both to deformation of the substrate, and to lower piezoelectric coefficients due to suppressed domain wall motion[2]. One method being investigated to counteract this tensile stress is the use of a compressive compensation layer. SiO_x thin films are being investigated for this application as the compressive stress generated by SiOx films can be tailored as a function of sputtering pressure[3]. Thus, depositions can be adjusted to compensate for substrate distortion generated by the PZT films and their electrode stacks during fabrication. The goal of this work is to characterize the magnitude and stability of the stress generated during SiO_x deposition.

For this work, SiO_x films were deposited onto Si wafers using radio frequency magnetron sputtering at chamber pressures between 2.5 and 3.0 mTorr. The thicknesses of the SiO_x films ranged from 180 to 1220 nm, with the indexes falling between 1.60 and 1.90. The high refractive index relative to SiO_2 (1.46)[4] indicates that the deposited films are oxygen deficient.

The compressive stress generated was between 330 and 490 MPa immediately following deposition, which is sufficient to compensate for the expected stress in the actuator stack (180±20 MPa/µm).

However, the compressive stress in the deposited SiO_x layers decreased over a seven-month period, dropping by >90 MPa in some cases. This decrease in compressive stress over time can be stabilized through growth of an Al2O3 barrier layer immediately following SiO_x deposition. Films covered in Al_2O_3 had a smaller change in stress, <±5 MPa, over the same period. The Al_2O_3 layers for this work were grown using atomic layer deposition at 200˚C with Trimethylaluminum (TMA) and H_2O precursors. Work on characterizing the generation and degradation of stress created by SiO_x will be reported, as well as work on stabilizing the stress state with an Al_2O_3 passivation layer.

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2D Materials
Room 304 - Session 2D+QS-TuM

Novel Quantum 2D Materials

Moderators: Fei Yao, University at Buffalo, **Roland Kawakami**, The Ohio State University

11:00am **2D+QS-TuM-13 Watching 2D Materials Form: Real-Time Atomic-Scale Visualization of TMD Growth and Crystallization Pathways**, ***Raymond Unocic***, *Prajakta Prabhune, Aidan Cotton,* North Carolina State University*; Caitlin Obrero,* Stanford University*; Suman Jaiswal, Masoud Mahjouri-Samani,* Auburn University*; Kyungnam Kang, Kai Xiao,* Oak Ridge National Laboratory **INVITED**

Achieving control over 2D material functional properties requires direct insight into the dynamic pathways that drive nucleation, crystallization, and growth. Aberration-corrected scanning transmission electron microscopy (STEM), coupled with in situ capabilities, has emerged as a powerful platform that can be used to directly observe these processes with atomic-scale spatial resolution and under a range of synthesis conditions. In this work, we investigate thermolysis-driven growth and pulsed laser deposition (PLD)-derived amorphous-to-crystalline transformations for 2D transition metal dichalcogenides (TMDs). Using MEMS based heating microchips, controlled heating experiments were performed to directly visualize the evolution of amorphous precursor phases into crystalline layered structures, revealing the atomic-scale pathways governing growth and phase evolution. By systematically varying thermal conditions and electron dose, we aimed to establish correlations between processing parameters and the resulting kinetic and energetic landscapes that dictate crystallization behavior. To further uncover hidden relationships within the transformation dynamics, we employ data analytics and machine learning approaches to quantify atomic trajectories and to identify transient states. The direct observation of these transformations provides unprecedented insight into the role of local structural rearrangements and transient intermediate states in governing the evolution of final material architectures. These findings establish a foundation for predictive synthesis strategies and enable atomic-scale control over TMD growth pathways.

11:30am **2D+QS-TuM-15 Airgap-Mediated Remote Epitaxial Control of Bandgap Opening in Bilayer Silicene on Semiconductor Substrates**, ***Kumar Vishal,*** Wright University

Bilayer silicene (BLSi) is a promising silicon-compatible 2D material for future nanoelectronic channels, but practical bandgap engineering requires simultaneous strain retention, substrate interaction control, and release from growth templates. We use first-principles density functional theory to model epitaxial and remote-epitaxial BLSi on lattice-mismatched semiconductor substrates, with emphasis on Ga- and Sb-terminated GaSb surfaces. Substrate-induced biaxial tensile strain is used to flatten and electronically activate BLSi, while the BLSi/substrate separation is varied to emulate an airgap interlayer that suppresses direct chemical bonding.The calculations reveal three interaction regimes governed by optimized interface spacing, surface termination, electron transfer, and residual buckling. For Ga-terminated GaSb, direct epitaxy relaxes to a strongly bonded interface at Δd0 = 0.817 Å, producing a 112 meV bandgap but limiting transferability. Increasing the spacing creates a metastable remote-epitaxial regime at Δd0 ≈ 2.6–2.9 Å, where electron density at the interface drops below 0.075 Å^-3 and the bandgap becomes tunable in the 20–30 meV range. At larger spacing, interfacial charge transfer becomes negligible and BLSi approaches the strained free-standing limit near 57–59 meV. For Sb-terminated GaSb, the weaker Si-Sb interaction enables a wider practical tuning window: an airgap of approximately 3.0–4.3 Å gradually opens the BLSi bandgap from near zero to 57 meV while maintaining a weakly coupled, releasable interface.These results show that an atomically controlled airgap can function as a passive remote-epitaxial layer, preserving lattice-mismatch strain while preventing irreversible covalent bonding. The approach offers a low-complexity route for tuning bilayer silicene electronic structure and for integrating strain-engineered 2D silicon materials with scalable semiconductor device processing.The technical details above are grounded in your uploaded paper, including the DFT modeling, GaSb_Ga/GaSb_Sb comparison, three interface-spacing regimes, electron-density reduction, and tunable bandgap results.

11:45am **2D+QS-TuM-16 Synthesis and Characterization of Two-Dimensional Indium Gallium Nitride (2d $In_xGa_{1-x}N$) via Graphene Encapsulation**, ***Krishnan Mekkanamkulam Ananthanarayanan***, *Soukyoon Kim, Md Farhan, Nutifafa Y. Doumon, Adri van Duin, Joshua Robinson,* The Pennsylvania State University

Group-III nitrides are widely explored semiconducting material for optoelectronics including light-emitting diodes (LEDs), photodetectors, solar cells and lasers; however, quantum applications such as single photon emitters, tunnel junctions and quantum sensors remain unrealized. Atomically thin two-dimensional (2D) nitrides are predicted to have large tunable bandgap than the bulk counterpart via quantum confinement with electronic and optical properties for wide spectrum of applications such as deep UV light emitters, single photon sources and other optoelectronic devices. First-principles calculations predict 2D $In_xGa_{1-x}N$ to possess a tunable bandgap ranging from 1.7 to 4.1 eV depending on the composition. However, experimental realization of large area 2D nitrides growth other than hBN remains elusive due to 3D growth induced by surface energy constraints. Graphene encapsulation has paved the way for realization of MOCVD growth of 2D GaN_x (E_g≈5eV), InN_x (E_g≈2eV) and AlN_x (E_g≈9eV). The significant limitation in the MOCVD growth of 2D nitrides via graphene encapsulation is the 3D island formation on top of graphene and small domain growth. In this study, we have synthesized large-area 2D $In_xGa_{1-x}N$ by intercalation of 2D In_xGa_{1-x} alloy at the interface of EG/SiC using confinement heteroepitaxy (CHet) and followed by ammonolysis to intercalate nitrogen to counter the 3D island formation. The high energy interface between epitaxial graphene (EG) and silicon carbide (SiC) efficiently stabilizes the metal and other compounds into confined 2D crystalline form. The intercalation of tunable 2D In_xGa_{1-x} metal alloy composition by changing the relative elemental composition of the precursor using CHet technique have been previously demonstrated. XPS, cross sectional transmission electron microscopy (TEM), energy dispersive X-ray spectroscopy (EDS) and AES mapping provides evidence of ~100 μm^2 2D $In_xGa_{1-x}N$ at the EG/SiC interface and determine the III-alloy nitride composition. The electron energy loss spectroscopy (EELS) and UV-vis spectroscopy extract the energy bandgap of 2D $In_xGa_{1-x}N$ with varying alloy compositions. The vertical transport measurements of the heterostructure are carried out using conductive atomic force microscopy (C-AFM) using a conductive SiC substrate. Scanning electron microscopy (SEM) and AFM validate the reduced 3D island formation. The surface morphology of 2D III-nitride consists of graphene wrinkles, tears and nitrogen trapped bubbles formed underneath the EG. We combine the study with ReaxFF reactive molecular dynamics simulations to elucidate the mechanism of graphene bubbles formation and the role of EG, In and Ga.

Atomic Scale Processing Mini-Symposium
Room 316 - Session AP+EL+EM+PS+TF-TuM

Area Selective Processing and Patterning

Moderators: Prof. Dr. Greg Parsons, North Carolina State University, **Dr. Silvia Armini**, IMEC, Belgium

8:00am **AP+EL+EM+PS+TF-TuM-1 ASCEND: A Novel Solution-Based Method To Control Deposit Composition and Placement**, *Jevalyne Vienes,* ***Amy Walker,*** University of Texas at Dallas

We introduce a novel selective deposition process called ASCEND, or "Additive and Surface Control of Electroless Nanostructure Deposition." ASCEND integrates mechanistically-informed and well-controlled extensions of electroless deposition (ELD) and chemical bath deposition (CBD). It uses hybrid ELD-CBD conditions and patterned surfaces to deposit strongly adherent metallic and metal chalcogenide films and nanowires. It is inexpensive, easily scaled, and compatible with technologically relevant substrates. We illustrate ASCEND using Cu and CuS deposition. First, we employ ethanolamine additives in Cu ELD using dimethylamine borane (DMAB) on –OH and $–CH_3$ terminated alkanethiolate self-assembled monolayers (SAMs) either to deposit nanowires or perform area-selective deposition. Using monoethanolamine or triethanolamine copper nanowires are formed at the junction of patterned –OH/$–CH_3$ terminated SAMs. In contrast using diethanolamine, area selective deposition is observed in the $–CH_3$ terminated SAM area. Using TOF SIMS data we show that monoethanolamine and triethanolamine adsorb vertically (or at an angle) with the amine group interacting with the $–CH_3$ terminated SAM and leaving the hydroxyl groups free to interact with the bath components. This causes repulsion of the DMAB reducing agent, hindering deposition on the $–CH_3$ terminated SAM areas leading to nanowire formation. In contrast,

diethanolamine adsorbs flat on $–CH_3$ terminated SAMs and no nanowire formation is observed; rather area-selective deposition occurs.

In the second experiment we control the deposit composition in Cu ELD using thiourea, which is a common bath additive, on -OH, -COOH and $–CH_3$terminated SAMs. At < 10^{-2} M thiourea, Cu films are deposited on all substrates. At ≥ 10^{-2} M the deposited layers are copper sulfides. At pH 5 and pH 9, the film is composed of CuS for all functionalized SAMs studied, while at pH 12 the deposit is Cu_2S. We attribute this to the role of thiourea in the bath. At low concentrations, thiourea acts as a complexing and reducing agent, while at high concentrations (> 10^{-2} M) the dominant reaction is thiourea hydrolysis leading to the formation of copper sulfides. Finally, exploiting this understanding we demonstrate a simple method to deposit layered Cu/Cu_xS and CuS nanowires on patterned SAM substrates by changing the TU concentration in the bath.

8:15am **AP+EL+EM+PS+TF-TuM-2 Using Acetylacetates to Control Chemical Reactivity and Physical Properties of Surfaces***, **Andrew Teplyakov**,* University of Delaware

Over the last few years, the applications of various acetyl acetates in tuning both chemical reactivity of surfaces in deposition and etching processes and physical properties of the interfaces and thin films have received a substantial attention both from fundamental perspective and from applications point of view. This presentation will analyze the chemistry of several acetylacetates, including the ligands formed on surfaces by acetylacetone (acacH), hexafluoroacetylacetone (hfacH) and 1,1,1-trifluoroacetylacetone (tfacH) and the implications of this chemistry in area-selective atomic layer deposition (AS-ALD), atomic layer etching (ALE), and tuning optoelectronic properties of oxide surfaces and thin films. The effects of the gas-phase keto-enol equilibrium and the acid/base properties of oxide surfaces on the adsorption mechanisms will be discussed. The applications of this knowledge to design non-growth and growth surfaces for ALD and to propose new chemistries for ALE of 2D materials will be demonstrated.

8:30am **AP+EL+EM+PS+TF-TuM-3 Atomic Layer Etching for Advanced Logic Devices***, **Masanaga Fukasawa**,* National Institute of Advanced Industrial Science and Technology (AIST), Japan **INVITED**

The dimensions of advanced logic devices require atomic-level control of variability, and atomic-layer etching (ALE) is a promising technique to meet this requirement. By separating adsorption and desorption, ALE improves controllability compared with conventional RIE. Currently, however, the long process time—leading to increased manufacturing cost—remains a major challenge, and thus industrial adoption has been limited. Nevertheless, in next-generation highly scaled 3D transistors such as CFETs, further improvements in etch selectivity, mitigation of pattern loading, and reduction of etch-induced damage are required. As a result, the importance of ALE is expected to increase [1].

To further improve etch selectivity, we have developed a technique that integrates area-selective deposition (ASD) and ALE within a single etching chamber to achieve ultra-high etch selectivity [2]. In atomic-scale processes such as ALD and ALE, understanding surface reactions and process performance at the atomic level enables more precise process design through the combination of individual reaction steps. Moreover, this approach is beginning to be adopted not only for ASD + ALE but also for ASD + RIE [3] in various process modules. In particular, with High-NA EUV lithography reducing resist thicknesses to below 30 nm, extremely high etch selectivity becomes even more critical. Thus, integration schemes that combine ASD with RIE/ALE will play an increasingly important role.

Regarding low-damage processing, although several studies have reported blanket-level evaluations, examples that demonstrate practical-level performance have been limited. In this work, we applied ALE or RIE to the bottom-break step of contact hole etching and compared the resulting electrical characteristics of contact chains. The results clearly show that ALE provides superior performance [4].

ALE delivers the controllability, reproducibility, and integrability required for next-generation semiconductor technologies, and elevates semiconductor fabrication to a new level of precision. I believe ALE will become increasingly essential in advanced logic device manufacturing.

Acknowledgement: This paper is based on results obtained from the project, “Research and Development Project of the Enhanced Infrastructures for Post-5G Information and Communication Systems” (JPNP20017), subsidized by New Energy and Industrial Technology Development Organization (NEDO).

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9:00am **AP+EL+EM+PS+TF-TuM-5 Band Practice: Tuning Gold's Workfunction Through NHC d-Band Interactions***, **Sean Barry**,* Carleton University, Canada*; Wai Tung Shiu, Paul Ragogna,* Western University, Canada

N-heterocyclic carbenes (NHCs) have emerged as robust small-molecule inhibitors (SMIs) for modifying metal surfaces, yet a quantitative understanding of their influence on surface electronic structure remains limited. Here, we investigate the modulation of the d-band center of a gold surface by NHC adsorption using a combination of solution- and vapour-phase deposition. Four structurally distinct NHCs were deposited on Au substrates, and the resulting interfaces were characterized using X-ray photoelectron spectroscopy (XPS), ultraviolet photoelectron spectroscopy (UPS), and time-of-flight secondary ion mass spectrometry (ToF-SIMS).

All NHCs formed stable monolayers on Au, with surface coverages that depended on both molecular structure and deposition method, ranging from 1.88 to 3.56 NHC/nm^2. UPS measurements revealed significant reductions in the Au work function (up to ~1.2 eV), with vapour-deposited films exhibiting larger shifts, consistent with differences in interfacial structure and electron redistribution. Analysis of the valence band spectra shows a systematic lowering of the Au d-band center upon NHC adsorption, indicating increased filling of antibonding states and weakened adsorbate–metal interactions.

Three primary factors governing d-band modulation were molecular orientation and the formation of $Au(NHC)_2$ adatom complexes, which lead to enhanced electron donation. Surface coverage plays a critical role, with higher coverages producing stronger modulation due to increased adsorbate–metal interactions. Finally, ligand electronics, particularly backbone substitution, influence the NHC's σ-donating ability and thus the extent of electronic perturbation at the interface.

This presentation will discuss the structure-function relationships of NHC substitution and coverage as well as absorption interactions.

9:15am **AP+EL+EM+PS+TF-TuM-6 Inhibition of SiO_2 by plasma treatments for bottom-up gap-fill applications***, **Aurelia Trevisan**, Adrie Mackus, Erwin Kessels,* Eindhoven University of Technology, The Netherlands

As the features in electronic devices become smaller, top-down processes based on lithography need eventually to be complemented by bottom-up processes such area selective atomic layer deposition (AS-ALD). Although ALD allows for conformal deposition on 3D features, it is challenging to fill high aspect ratio (AR) trenches without the formation of defects such as voids and seams in the middle. To obtain a defectless bottom-up gap-fill of a trench by ALD, the growth per cycle (GPC) of the employed ALD process should be lower at the top of the trenches than at the bottom. Different approaches that result in a decreased GPC on the top of AR trenches for seamless gap-fill have been studied employing molecular inhibition species[1] and NH_3 plasma pre-treatments.[2]

In this work, we investigated the mechanisms of inhibition of SiO_2 by NH_3, N_2/H_2 and SF_6/H_2 plasma exposures aiming at the application of such plasma pre-treatment for achieving gap-fill with SiO_2. We exposed the SiO_2 surface to NH_3, N_2/H_2 and SF_6/H_2 plasma at different conditions and we studied the surface chemistry by reflection-absorption infrared spectroscopy (RAIRS). For a NH_3 plasma exposure, we found that the substitution of the OH groups with NH_2 groups is almost complete[3] at low NH_3 pressure from the comparison of the areas of the OH peak (~3740 cm^{-1}) in the RAIRS spectra acquired after the plasma exposures at different NH_3 pressures. Next, to investigate the inhibition of the SiO_2 surface by plasma, RAIRS spectra were also obtained after dosing the Si precursor, bis(diethylamino)silane (BDEAS), with and without the plasma treatment step. From the IR spectra, we found that the amount of adsorbed BDEAS molecules on SiO_2 pre-treated with NH_3 plasma (60s, 0.01 mbar) is reduced by ~82%.

A NH_3 plasma pre-treatment was added before the dose of the precursor to every cycle of the SiO_2 PE-ALD process. The effect of the NH_3 plasma pre-treatment on the growth was investigated by conducting spectroscopic ellipsometry (SE) after every cycle. When the NH_3 plasma pre-treatment was added, a 53% reduction of the GPC was obtained. We expect this reduction to be enough to achieve gap-fill of high AR trenches, which will be studied by cross-sectional transmission electron microscopy.

References

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9:30am **AP+EL+EM+PS+TF-TuM-7 Precursor Isomerization-Enabled Etching Amplification: A Novel Route to Area Selective Deposition of SiOC Films**, ***Xiaocheng Huang***, *Junjie Zhao,* Zhejiang University, China

Self-aligned patterning via area selective deposition (ASD) is a promising approach to mitigate overlay variations challenges in photolithography for advanced nanomanufacturing. However, it remains difficult to achieve area selective deposition when the adsorption and/or film growth on the target non-growth surface (NGS) exceeds that on the target growth surface (GS). We developed an etching amplification strategy based on precursor isomerization for selective deposition of SiOC when adsorption and/or film growth was higher on the target NGS than on the target GS. *In-situ* DRIFTS demonstrated that V_3D_3 cyclosiloxane undergoes ring-opening on CoO_x surfaces. This ring-opening reaction significantly enhances the etching rate under O_2/Ar plasma by 243% compared to the pristine pV_3D_3, as confirmed by *in-situ* QCM measurements. *In-situ* QCM during ASD cycles showed higher mass gain on CoO_x than on SiO_2 during V_3D_3 deposition steps; however, the subsequent etching step completely removed the adsorbed species from the NGS due to etching amplification. By integrating deposition and etching processes, we achieved selective deposition of a ca. 18.36 nm thick SiOC film on pre-patterned Co/SiO_2 substrates with nearly 100% selectivity. This work sheds light upon etching amplification by precursor isomerization for developing highly selective ASD processes.

9:45am **AP+EL+EM+PS+TF-TuM-8 A Novel Hybrid Approach to Area-Selective Deposition: Combining Two Strategies for Blocking Growth**, *Jay Swarup, James Jensen, Gokul Rajagopal,* ***James Engstrom,*** Cornell University

Area-selective atomic layer deposition (AS-ALD) has emerged as a promising bottom-up nanofabrication strategy for next-generation semiconductor manufacturing, where continued device scaling makes conventional lithographic patterning increasingly difficult and costly. Selectivity can be achieved by passivating non-growth surfaces (NGS) with blocking molecules while permitting growth on designated growth surfaces (GS), and it depends critically on precursor chemistry, blocking molecule identity and application method, and reactor temperature. Here we systematically investigate two blocking strategies for AS-ALD of Al_2O_3 targeting selective growth on Cu (GS) with suppression on SiO_2 (NGS) using BDMADA-Al, a bulky, non-pyrophoric precursor [1]. We employ *in situ* real time quartz crystal microbalance (QCM) techniques, coupled with selected *ex situ* techniques including X-ray photoelectron spectroscopy (XPS).The first strategy employs sequential dosing of a small molecule, while the second strategy introduces a co-adsorbate dosed simultaneously with the precursor to enable competitive adsorption at NGS reactive sites. In the first strategy, dimethylamido trimethylsilane (DMATMS) was applied repetitively in an ABC-type cycle (T = 285 °C), which produced modest blocking efficacy, where detectable growth from QCM could be delayed for the first ~ 20 cycles, while Al is clearly observed with XPS after 40 cycles.In the second strategy we also employ an ABC-type cycle, but also introduce a co-adsorbate dosed simultaneously with BDMADA-Al at T = 120 °C.We examined six different co-adsorbates, all possessing reactive functional groups, which revealed stark differences in blocking efficacy depending on the co-adsorbate used.Three co-adsorbates did not enhance blocking but, rather, produced linear (with exposure time) CVD-like growth during the combined precursor/co-adsorbate pulse.In contrast, three co-adsorbates yielded *complete blocking* of growth on SiO_2 for at least 40 cycles of ALD, confirmed by both QCM and XPS.In order to verify the operative mechanism of competitive adsorption we varied both the partial pressure of the co-adsorbate and the reactor temperature.We found that by either decreasing the partial pressure of the co-adsorbate, or increasing the temperature led to less effective blocking of growth, confirming the mechanism based on competitive adsorption.These results demonstrate that an approach that combines two strategies can produce synergy and a more effective method to enable area selective deposition.

[1]J. V. Swarup, H.-R. Chuang, J. T. Jensen, J. Gao, A. L. You and J. R. Engstrom, J. Vac. Sci. Technol. A **43**, 022404 (2025).

11:00am **AP+EL+EM+PS+TF-TuM-13 Probing Reactivity at Heterointerfacial Sites Using Area Selective Atomic Layer Deposition**, *Shani Monadeev,* ***Oz M. Gazit***, *Alexander Stook,* Technion Israel Institute of Technology, Israel

Background

Heterointerfaces are a sub-class of defects arising from atomic mismatches across material boundaries. These coordinatively unsaturated sites modulate the electronic and geometric structure of catalysts to facilitate specific reactive adsorption, activation, and transformation of reactant molecules.[1] In electronic devices the critical heterointerfaces are “buried” between the layers,[2] whereas for catalysts, the reaction performance can depend on both the buried interfaces (i.e. metal support interactions) and on the exposed heterointerfacial (defect) sites, interacting with substrate and product molecules, see **Scheme 1**.

Results and discussion

In the current work, we use a bottom-up area selective atomic layer deposition (AS-ALD) to form supported thin layer raft-like oxides. To facilitate the AS geometry, we developed a new approach, which uses NaCl nanocrystals as masking domains during the ALD process. This unique approach allows us to apply this methodology onto silicon wafers and on different surface area particulate silica support materials. The HRSEM-EDS (Energy Dispersive Spectroscopy) mapping in **Figure 1** shows an example of a well-defined multilayer structure, formed following the sequential deposition of TiO_2 (≈20 nm) and subsequently Al_2O_3 (≈20 nm) layers onto an NaCl-mask before and after mask removal. Leveraging on the strength of AS-ALD we study the structure, binding energy, strain and more of the exposed heterointerface, aiming to decuple those from the exposed basal plan and bulk effects. We compare our AS-ALD materials to materials obtained using a top-down deposition of thin nanosheets of layer double hydroxides. All materials are extensively characterized using XPS, DRIFT-IR, HRSEM and HRTEM, grazing angle-WAXS and probe molecules TPD-MS. The functionality of the heterointerfacial sites is tested using Aldol type condensation reactions for the conversion of biomass derived platform molecules as a target and probe reaction.

References

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11:15am **AP+EL+EM+PS+TF-TuM-14 Area-selective Atomic Layer Deposition of Al2O3 on SiNx with Aminosilane-Functionalized SiO2 as the Nongrowth Surface**, ***Andrew Kaye,*** Colorado School of Mines*; Bhushan Zopé,* Intermolecular, Inc.*; Xinjian Lei, Ronald Pearlstein, Haripin Chandra, Agnes Derecskei,* EMD Electronics*; Sumit Agarwal,* Colorado School of Mines

SiO_2 and SiN_x are two of the most extensively used dielectric materials in semiconductor manufacturing. Previously, we showed that area-selective ALD of Al_2O_3 can be achieved on SiN_x by passivating the SiO_2 surface with aminosilanes. Using *in situ* attenuated total reflection Fourier-transform infrared (ATR-FTIR) spectroscopy (see Figure 1), we will show that the aminosilanes react with both the SiO_2 and SiN_x surfaces, but the coverage of aminosilanes on the SiN_x surface is incomplete, which does not prevent ALD of Al_2O_3 from dimethylaluminum isopropoxide (DMAI) and H_2O, but simply introduces a nucleation delay of 5-10 cycles. However, selective growth of Al_2O_3 on SiN_x was limited to ~1 nm at which point DMAI started to react with the SiO_2 surface to nucleate film growth.

Based on these initial studies, our hypothesis was that there are residual Si–OH groups that remain on the SiO_2 surface react with DMAI to initiate growth of Al_2O_3. We have also shown that DMAI likely coordinates with Si–O–Si groups on aminosilane-functionalized SiO_2 films, which also leads to nucleation; therefore, simply reducing the surface Si–OH group density is inadequate. To extend the nucleation delay on SiO_2, we created a set of plasma-deposited SiO_2 surfaces with a controlled density of surface Si–OH groups by first preheating from the deposition temperature of 150 °C up to 500 °C, and then by cooling the substrate to a lower temperature prior to ALD of Al_2O_3. We used aminosilanes with different size head groups to study the uptake of aminosilanes and the steric blocking effects of both Si–OH and Si–O–Si sites to block Al_2O_3 ALD. The headgroup size did not significantly impact the initial uptake of aminosilanes with the same size leaving groups (see Figure 2). Using *in situ* ellipsometry, we show that aminosilanes with larger head groups resulted in more selective growth on SiN_x over SiO_2. Next, we showed that increasing the aminosilane dose increased the nucleation delay of Al_2O_3 ALD on both SiO_2 and SiN_x surfaces due to increased coverage, but selectivity did not improve significantly. Finally, we show that using a two-step aminosilane passivation scheme with sub-saturation doses of a large aminosilane and then a small aminosilane resulted in >3 nm of selective Al_2O_3 ALD on SiN_x over SiO_2 surfaces (see Figure 3).

11:30am **AP+EL+EM+PS+TF-TuM-15 Beyond Two-Color Selectivity: Area Selective Deposition on Multi-Oxide Surfaces Using Small Molecules Inhibitors**, ***Benjamin Sanhueza**, Marc J. M. Merkx, Wilhelmus M. M. Kessels,* Eindhoven University of Technology, Netherlands*; Tania E. Sandoval,* Universidad Tecnica Federico Santa Maria, Chile*; Adriaan J.M. Mackus,* Eindhoven University of Technology, Netherlands

Area-selective deposition (ASD) using small molecule inhibitors (SMIs) emerges as a promising bottom-up alternative, enabling selective deposition on growth areas (GAs) while inhibiting the non-growth areas (NGAs). Although ASD has shown strong potential, most studies are limited to two-surface-selectivity, which does not capture the multi-material complexity of modern semiconductor devices.[1]. In this context, we investigate the selectivity of SiO_2 ASD in a multi-oxide system by evaluating the role of different SMIs and their impact on inhibition selectivity, with relevance on 3D memory [2] and 3D logic devices.[3]

Here, we employ a previously developed SiO_2 ASD process on Al_2O_3 and SiO_2 surfaces,[4] using the bis(diethylamino)silane (BDEAS) precursor, H_2 and O_2 plasma as co-reactants, and different SMIs. Building on this process, we investigate multi-surface selectivity by introducing ZrO_2 as an additional third oxide surface.

Among the SMIs investigated, acetylacetone (Hacac) is presented as a representative case. *In situ* reflection–absorption infrared spectroscopy (RAIRS) shows that Hacac reacts with ZrO_2, achieving surface saturation and up to 96% blocking of a single BDEAS dose, which is comparable to that observed on Al_2O_3 as an NGA. Preliminary results further indicate that the H_2 plasma pre-treatment increases the density of isolated and vicinal –OH groups, enhancing Hacac coverage and improving blocking up to 99.5%, demonstrating the strong influence of this plasma pre-treatment on the ZrO_2 surface.

In situ ellipsometry measurements show that ZrO_2 acts as an effective NGA, exhibiting a nucleation delay of up to 28 cycles (~2.6 nm of selective SiO_2 deposition). Remarkably, similar selectivity is achieved on both Al_2O_3 and ZrO_2 surfaces, indicating consistent inhibition behavior across different oxides.[1], [5]

In addition to the results of this case study, it will be discussed that the choice of SMIs can tune inhibition behavior enabling different growth across surfaces. In this way, the loss of selectivity can be preferentially initiated on one NGA prior to another through SMI selection, enabling controlled thickness variations across different materials.

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11:45am **AP+EL+EM+PS+TF-TuM-16 Surface Hydroxyl Topology and Relative Orientation Effects on Surface-Inhibitor Reactivity: Revisiting Chemical Passivation in Alumina and Zirconia.**, *Lucas Lodeiro, Nicolás Rozas-Castro,* Universidad Tecnica Federico Santa Maria, Chile*; Dennis Hausmann, Rachel Nye de Castro,* Lam Research Corporation*; Adriaan Mackus,* Eindhoven University of Technology, Netherlands*; **Tania Sandoval**,* Universidad Tecnica Federico Santa Maria, Chile

Hydroxylated metal oxide surfaces are paramount for catalysis and thin–film processing. In this context the reduction of surface reactivity via molecular inhibitors or chemical passivation is a common and necessary practice. Small–molecule inhibitors (SMIs) such as acetylacetone (Hacac) and acetic acid (HAc) are widely employed to inhibit growth by reactive site consumption on hydroxylated oxides.[1] Despite their ubiquitousness, the influence of **surface site configuration** on inhibitor reactivity remains unexplored.

Experimental evidence that chemically distinct hydroxyl motifs exhibit different reactivities toward SMIs is available.[2] In this work, we revisit the chemical passivation of hydroxylated alumina and zirconia by SMIs, with emphasis on the role of surface site configuration, defined as a combination of Local Topology and Relative Orientation of hydroxyl groups on metal oxide surfaces. Rather than treating hydroxylated sites as a whole entity, we examine how geometrically and electronically distinct surface motifs modulate inhibitor binding modes and reactivity.

Considering that systematic exploration of all possible site configurations rapidly becomes challenging due to the large chemical space, we further investigate whether simple surface descriptors, derived from local electronic structure and geometry, can provide predictive insight into surface reactivity toward SMIs. Our goal is to identify descriptor trends (e.g., charge distribution, coordination, or accessibility metrics) that correlate with inhibitor adsorption behavior, enabling informed prioritization of surface motifs prior to exhaustive site screening.

By linking surface site configuration, inhibitor-surface reactivity and descriptor–based analysis, this work aims to understand the nuances in the chemical passivation of metal oxide surfaces, and provides guidance to design descriptor–informed screening strategies.

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[2] J. Phys. Chem. C, 2022, 126, 4845–4853

12:00pm **AP+EL+EM+PS+TF-TuM-17 Can pFA Invert Selectivity? The Chemistry of TiO_2 Nucleation on Chlorinated and Aminated Si(111) Surfaces During Thermal Atomic Layer Deposition**, ***Tyler Parke**, Andrew Teplyakov,* University of Delaware

Recently, the near-atomic level precision offered by atomic layer deposition (ALD) has been exploited by developing area-selective schemes which can be used to fabricate complex three-dimensional nanostructures, such as modification of a substrate's surface functionality to induce a "selectivity inversion" between growth surfaces (GS) and non-growth surfaces (NGS). This is a newly developing technique, which has only been demonstrated thus far with few vapor-phase treatments, and which requires a molecular level understanding of the chemistry between surface and modifying reactant, as well as between modified surface and precursor. Here, single-crystal Si(111) surfaces terminated with hydrogen [H-Si(111)] or chlorine [Cl-Si(111)] monolayers, which are typically NGS's in thermal TiO_2 processes, are proposed as potential substrates to modify with a basic amine, para-fluoroaniline (pFA), and invert their selectivity. Amination with pFA is demonstrated to selectively modify the H-Si(111). Thermal TiO_2 ALD is subsequently attempted to test the aminated surface's capability as a GS or NGS. The fundamental chemistry of the interaction between the pFA and either surface, as well as between the aminated surface and ALD precursors $TiCl_4$ and tetrakis(dimethylamido)titanium (TDMAT), are probed with a combination of X-ray photoelectron spectroscopy (XPS), Fourier transform infrared spectroscopy (FT-IR), density functional theory (DFT), and time of flight secondary ion mass spectrometry (ToF-SIMS) in order to determine the structure of the aminated surface and understand its effect on reactivity under ALD conditions.

Applied Surface Science
Room 319 - Session AS-TuM

Applied Surface Science in Action I

Moderators: Dr. Michael Eller, University of Mississippi, **Dr. Samantha Rosenberg**, Kairos Power

11:00am **AS-TuM-13 Considerations when Developing Standards and Tools for Surface Chemical Analysis**, ***Justin Gorham**, Donald Windover,* National Institute of Standards and Technology (NIST) **INVITED**

Surface chemical analysis, like other disciplines, rely on harmonized methods and benchmarking materials in order for results from the same technique to be reproducible from institute to institute. These harmonized methods are often incorporated into documentary standards which contain the details analysts require to conduct a process (e.g. prepare sample(s); calibrate the tool(s); conduct the measurement(s); analyze data; reporting requirements; etc.). Benchmarking materials are often co-developed during standards work as either a classification of reference materials or simply materials of known purity. As the name implies, these benchmarking materials are often employed as a tool for checking/calibrating a given property of a tool (e.g. linearity of energy scale). This presentation will focus on considerations and tools employed in the development of standards from a surface analysis perspective. Discussion will be held on both the development and maintenance of standards. Additionally, discussion will focus on the use case of NIST benchmarking materials known as research grade test materials (e.g. Hafnium oxide, Titanium Nitride, etc), currently under development, to advance measurements in the semiconductor community specifically as it pertains X-ray based measurements (e.g. XRR, XPS, XRF).

11:30am **AS-TuM-15 Might a Tiered Approach to Reviewing and Reporting Help Improve the Quality of XPS Results Appearing in Publications?***, **Don Baer,*** Pacific Northwest National Laboratory

Anecdotal evidence, confirmed by detailed analysis, highlights widespread inadequacies in XPS data and analysis reported in scientific literature. As XPS is increasingly utilized across various fields, researchers without specialized XPS knowledge often collect, analyze, and report data. These papers are often reviewed by experts in the subject matter, not in XPS, leading to missing or incomplete instrumental, data, and analysis information appearing in journals. Consequently, the quality and reliability of XPS results are difficult to assess, and flawed data is frequently published. Although this issue is not unique to XPS, this talk focuses on the reviewing and reporting of XPS information.

Surface analysis experts have worked to provide guidelines for less experienced XPS users. However, there remains a gap between the information reported in journals, what would comply with ISO and ASTM standards, the expectations of reviewers, and what is really needed. Research by Karel Gaskel revealed that most standard-required information is not reported, reflecting a disconnect between ideal reporting practices and practical journal requirements. Standards often focus on full repeatability, which can be burdensome and not always relevant, yet more information is needed than is typically provided to ensure data quality and relevance.

To address these challenges, a tiered approach to reviewing and reporting XPS data is suggested for discussion. A model might include three levels: i) **Credibility Level:** Data follows generally accepted practices and is adequate for its stated purpose in journals or reports, especially when XPS is not a primary analysis method used in the paper; ii) **Archive Level:** Data and analysis are of high quality, with sufficient detail about the instrument, sample, and analysis to allow for inclusion in databases and to provide context and purpose; **Reference/Fully Repeatable Level:** Full information is provided, enabling experts to replicate experiments and qualify the data as "reference data" of standard quality.

The need for thorough and appropriate reporting grows as artificial intelligence and data archiving become more prevalent. Adequate information is necessary for AI systems to identify high-quality data, and for archives to maintain meaningful records. A tiered approach might offer a practical guide for improving both the reporting and review of XPS data, aligning reporting requirements with the intended use and ensuring data quality across various applications. The challenge is identifying what each of these, or other, levels would mean in practice and how they might be described with clarity.

11:45am **AS-TuM-16 Strategies for Reducing Charging of Insulating Samples in Auger Electron Spectroscopy***, **Juergen Scherer,*** Physical Electronics

Auger Electron Spectroscopy (AES) is a powerful surface-sensitive analytical technique widely used to probe the elemental and chemical composition of materials at the nanoscale. Its high spatial resolution makes AES uniquely valuable for applications ranging from microelectronics and thin films to failure analysis and advanced materials. However, a persistent challenge in AES is the analysis of materials that are insulating or contain insulating regions, which represent a large and growing fraction of technologically relevant materials. Charge accumulation under electron beam irradiation can lead to spectral distortion, peak shifting, signal loss, and, in severe cases, the inability to obtain meaningful data.

This presentation discusses practical strategies for reducing and managing charging effects during AES analysis of insulating and heterogeneous samples. Emphasis is placed on understanding the physical origins of charging phenomena and how instrument configuration, experimental conditions, and sample preparation choices can be leveraged to mitigate their impact. Through illustrative examples, the talk highlights how thoughtful control of measurement parameters can substantially improve data quality, reproducibility, and reliability when working with challenging samples. By focusing on realistic scenarios encountered in routine AES measurements, this work aims to provide users with actionable insights for extending the applicability of AES to a broader class of insulating and heterogeneous materials.

12:00pm **AS-TuM-17 The Binary Residual Map and the Automated Determination of the Transfer Function Cutoff for the Fourier Filtering of X-ray Photoelectron Spectroscopy Data***, **Matthew Linford,*** *Alvaro Lizarbe, Maksym Gerashchenko, Tyler Andersen, Jonathan Nelson,* Brigham Young University*; David Aspnes,* NC State

We recently proposed that the Fourier denoising of X-ray photoelectron spectroscopy (XPS) data may have a legitimate place in XPS data processing (*J. Vac. Sci. Technol. A,* **2025**, *43*, 033401). For example, the denoising of spectra becomes critical when they are to be used for training artificial intelligence (AI) systems. In this talk, we discuss two new data analytical tools we have developed that greatly facilitate the Fourier denoising of XPS and other types of data. The first is the Binary Residual Map™. The binary residual map color codes the residuals from large numbers of fits or smooths and combines them into a single figure. The transition in a binary residual map where longer runs of a single color disappear is generally where good fitting or denoising is taking place. In addition, we have developed an algorithm, which we will discuss, that finds a reasonable position for the transfer/filter function in reciprocal space for denoising. This feature will be important both for newer users that may be unsure about Fourier analysis and also for fully automating the denoising of XPS data.

Biomaterial Interfaces

Room 321 - Session BI1-TuM

Biomaterials and Nanomaterials Fabrication I

Moderators: Prof. Joe Baio, Oregon State University, **Prof. Sapun Parekh**, University of Texas at Austin

8:00am **BI1-TuM-1 Engineering the Human Sense of Touch as the Finger-Object Interface***, **Charles Dhong,*** University of Delaware **INVITED**

The human sense of touch is a basic sensory experience, and for those who are visually impaired, a critical source of information. Technologies that interface with the sense of touch or "haptics" have seen progress over the years, but remain limited in the variety of sensations that these devices can reproduce and are nowhere near the the ability to recreate everyday sensations, especially when we compare these haptic technologies to vision or sound.

In this talk, we will show how the mechanical forces generated at the finger-object interface through adhesion and friction phenomena can be leveraged to control, or study, the human sense of touch. Mechanical forces generated at this interface give rise to tactile sensations and ultimately fine touch perception. Manipulating this mechanical interface through surface chemistry, polymer chemistry, and thin-film mechanics can give rise to new kinds of haptic devices while also enabling fundamental investigations into the perception of touch. We will end this talk by giving examples of how advances in the finger-object interface can enable widespread applications, from new insights into sensory neuroscience, to new accessibility technologies, and to medical diagnostics.

8:30am **BI1-TuM-3 Curvature-Programmed Polymer Interfaces via Condensed Droplet Polymerization***, **Rong Yang,*** Cornell University

Polymer interfaces with micro- and nanoscale convex topographies offer powerful routes to control optical response, imaging, sensing, and biointerfacial interactions. However, conventional lithography and self-assembly approaches often face tradeoffs among scalability, geometric tunability, and fabrication complexity. Here, we introduce condensed droplet polymerization (CDP), a one-step, template-free strategy in which condensed monomer droplets serve as nanoscale reactors to generate polymeric micro- and nanodome arrays with programmable size, curvature, and surface coverage. To make CDP predictive rather than empirical, we develop a theoretical framework that integrates monomer condensation, polymerization kinetics, droplet evaporation, and geometric arguments. This model rationalizes dome height and radius through the measurable droplet base radius, enabling accurate prediction of final dome geometry from synthesis conditions and monomer reactivity despite the stochastic nature of condensation. The resulting curvature-programmed interfaces exhibit distinct optical functions, including light focusing and magnification, with potential utility for high-resolution visualization of subwavelength features and biological specimens. As a biointerface demonstration, biphilic microdome arrays fabricated from poly(2-hydroxyethyl methacrylate) reduce *Pseudomonas aeruginosa* colonization without changing macroscopic wettability, suggesting a curvature-driven antifouling mechanism. Early evidence further supports its capability to program

immune cell functions. Together, CDP and the accompanying predictive model establish a scalable platform for designing polymer thin-film architectures with controlled curvature. This approach provides new opportunities for morphology-by-design in optical, sensing, and biointerfacial applications

8:45am **BI1-TuM-4 RF Pulsed Plasma Modified Composite Scaffold for Enhanced Anti-Microbial Activity and Accelerated Wound Healing***, **Ajinkya Mahadev Trimukhe**,* University of Milan Bicocca, Italy*; Jose Savio Melo,* Bhabha Atomic Research Centre, India*; Deepa Chaturvedi, Ratnesh Jain, Prajakta Dandekar, Rajendrasing Deshmukh,* Institute of Chemical Technology, India

This study entails the successful synthesis of a biodegradable microporous agarose-chitosan composite scaffold and modifying its surface with diphenyldiselenide (DPDSe), by using low-pressure RF pulsed plasma for enhanced wound-healing applications. The scaffolds' synthesis composition was optimized at a 3:1 agarose-to-chitosan ratio and 4% polymer concentration. The optimized RF plasma treatment parameters for depositing DPDSe on the scaffold surface were at a pulse rate of $5_{ON}/15_{OFF}$ (ms) for 80 minutes. The plasma-modified scaffold surfaces demonstrated superior antibacterial activity against Gram-positive bacteria *S. aureus* and *S. epidermidis*, achieving inhibition zones up to 24 mm and 26 mm, respectively, while maintaining excellent biocompatibility, with 91.9% and 88.6% cell viability for HaCaT and HadF cells, respectively. Surface characterization revealed enhanced hydrophilicity, with contact angles decreasing from 89° to 33°, and from XPS analysis, it was observed that there was increased oxygen content from 19.82% to 21.87%, and successful selenium deposition at an atomic concentration of 1.01%. *In vivo* studies using albino Wistar rats demonstrated accelerated wound healing, with plasma-modified scaffolds achieving 100% wound closure by day 14, compared with 16 days for untreated scaffolds, accompanied by enhanced collagen synthesis, evidenced by a hydroxyproline content of 5.96 µg/mL. The selenium-modified scaffolds showed comparable efficacy to standard Betadine treatment while offering practical advantages as solid dressing materials, making them promising alternatives for treating challenging wounds.

9:00am **BI1-TuM-5 Engineering Curvature-Controlled Polymer Dome Biointerfaces via Condensed Droplet Polymerization***, **Haobo Xu**, Rong Yang,* Cornell University

Surface-attached dome morphologies are ubiquitous in nature but remain difficult to reproduce synthetically due to limited control over geometric parameters such as curvature. Here we introduce condensed droplet polymerization (CDP), a synthesis strategy that leverages condensed monomer microdroplets as discrete microreactors to produce surface-attached polymer dome arrays with precisely tunable geometry. The potential of CDP for functional interface design is demonstrated in two contexts. Inspired by dome-shaped morphologies on crustacean shells, we investigate antifouling behavior and identify an optimal intermediate dome size (~10 µm) with targeted curvature that significantly suppresses *Pseudomonas aeruginosa* attachment despite a globally hydrophobic surface. In addition, sub-micron dome arrays significantly increase extracellular vesicle yield from M1-polarized murine macrophages (J774A.1), suggesting that curvature-defined biointerfaces can regulate plasma membrane dynamics, particularly the inward budding process associated with the endocytic pathway, thereby promoting the subsequent production and release of extracellular vesicles. These results establish CDP as a versatile platform for engineering curvature-controlled interfaces for antifouling materials and cell-regulating biomaterials.

Biomaterial Interfaces

Room 321 - Session BI2-TuM

Biomaterials and Nanomaterials Fabrication II

Moderators: Ali Rafati, Medtronic, Inc., **Dr. Christopher So**, Naval Research Laboratory

9:15am **BI2-TuM-6 Tuning Biopolymer Surface Wettability through Plasma Copolymerization***, **Morgan Hawker**, Alexzandria Kubik, Mackenzie Jackson, Kristina Closser,* California State University, Fresno

Plasma, the fourth state of matter, is a partially ionized gaseous mixture and versatile tool for controlling interactions at biointerfaces. Polymers are ubiquitous biomaterials and tailoring how the polymer device interfaces with the biological environment is paramount to controlling its function. For example, promoting favorable cell-surface interactions is needed for tissue engineering devices, whereas preventing bacterial attachment is favorable to prevent infection at the device surface. Plasma-enhanced chemical vapor deposition is a versatile technology to control interactions at the biomaterial/biological environment interface through adding a conformal protective film that encases the polymeric device below. The film is obtained through interfacing a polymer substrate with the plasma (partially ionized gas mixture). Plasma species such as radicals and cations undergo gas-phase reactions, and products from those reactions form the conformal film. Plasma copolymerization is a related strategy that utilizes a mixed feedgas of two or more plasma precursors, whereby conformal coating surface properties can be controlled by simply varying the feedgas composition.

This study reports a previously unexplored combination of plasma precursors – pentane and acrylic acid – to deposit coatings with tunable chemistry and wettability on silk fibroin constructs. Five pentane/acrylic acid feedgas compositions were utilized, ranging from 100%, 75%, 50%, 25%, and 0% pentane by pressure. Plasma deposited coating properties were evaluated through water contact angle goniometry and x-ray photoelectron spectroscopy. Coating static water contact angle values were tunable between >90 degrees to <55 degrees depending on the feedgas composition, which correlated to surface chemical composition. Plasma diagnostics and density functional theory were used to evaluate plasma precursor fragmentation, providing further insights into plasma/surface interactions. This library of plasma-modified silk-based materials can be used to design biomaterial surfaces that are optimally situated for the intended biomedical setting.

9:30am **BI2-TuM-7 Capture of Rare Earth Metals Using Bio-Inspired Polymeric Materials***, **Gillian Kropp**, Kailey Richard, Kenan Fears, Okhil Nag,* U.S. Naval Research Laboratory

Rare earth metals, largely comprised of lanthanides, are essential materials for a wide range of applications, including electronics, imaging and diagnostic technology, and energy systems. However, in nature these metals are found dispersed at low concentrations and mixed with other metals, making them challenging to locate, extract, and chemically isolate. Therefore, developing materials with high selectivity and tuneability is crucial to the separation and extraction of these lanthanides. Peptoids are a class of biomimetic molecules that are expanding the landscape of materials used for therapeutics, diagnostics, and metal chelation. In fact, with the development of new synthetic and automated strategies, peptoid-based materials are highly versatile and tunable. Our goal is to leverage this tuneability to design, synthesize, and characterize materials for selective rare earth metal extraction.

9:45am **BI2-TuM-8 Materials Science / Properties of Transformational Uncoated and Multifunctional/Best Biocompatible Ultrananocrystalline Diamond (Uncd) Coated-Bioactive Bovine Nanohydroxyapatite Scaffolds for Transformational Bone Tissue Engineering***, **Orlando Auciello**,* Texas State University and Original Biomedical Implants*; Angelica Castillo-Paza,* Centro de Investigación y Estudios Avanzados, Mexico*; Leon Bernal-Alvarez,* Universidad Nacional Autónoma de México*; Dorian Cañon-Davila,* Centro de Investigación y Estudios Avanzados, Mexico*; Lerma Chan-Chanc,* Universidad Nacional Autónoma de México, Campus Juriquillalerma@, Mexico*; Rafael Ramírez-Bona,* Centro de Investigación y Estudios Avanzados, Mexico*; Mario Rodriguez-Garciad,* Universidad Nacional Autónoma de México, Campus Juriquilla, Mexico

Abstract

This Talk will be focused on describing materials science and characterization ofphysicochemical properties of hydroxyapatite (HAp) scaffolds and HAp scaffolds coated with a unique transformational best biocompatible (because made of Carbon atoms /element of life in human DNA, cells, molecules) Utrananocrystalline Diamond (UNCD) coating (HAp-UNCD) produced by a patented microwave plasma chemical vapor deposition (MPCVD) and Hot filament Chemical Vapor Deposition (HFCVD) process. The studies involved complementary analytical techniques and biological assays, namely:

1. Scanning Electron Microscopy (SEM) revealed scaffolds' pore structure, critical for bone regeneration / formation and associated EDS chemical analysis showing Ca, P and C atoms.
2. High Resolution Transmission Electron Microscopy (HRTEM) revealed nanoscale structures of HAp and HAp-UNCD scaffolds; and Energy Dispersive Spectroscopy (EDS) analysis confirmed the presence of P on HAp and C atoms in the UNCD coating on HAp scaffolds.

3. X-ray Diffraction (XRD) analysis revealed HAp-UNCD crystalline structure before/after immersion in HBSS, revealing excellent inertness of the UNCD-coated HAp.
4. Raman spectroscopy provided chemical analysis of original HAp and UNCD-coated HAp, before and after immersion in Hanks' Balanced Salt Solution (HBSS).
5. Infrared (IR) analysis revealed carbonate ions on scaffolds' surfaces.
6. X-ray Photoelectron Spectroscopy (XPS) analysis revealed transformational chemical interactions between atoms in HAp scaffolds and in UNCD coated HAp scaffolds.
7. *In vitro* cytotoxicity assays showed NO-cytotoxicity in HAp and HAp-UNCD scaffolds.
8. N_2 adsorption-desorption analysis showed mesoporosity in both scaffolds.
9. Mineral content analysis showed Na / Mg atoms, important elements for bone cells' growth.
10. .
11. Application of Integrated UNCD-coated commercial Ti-alloy dental implants in HAp in maxillary bones demonstrated a new transformational UNCD-coated DIs-maxillary bone integration

Biomaterial Interfaces
Room 321 - Session BI3-TuM
Characterization of Biological and Biomaterials Surfaces

Moderators: Dr. Sebastian Diaz, Naval Research Laboratory, **Prof. Roberto Eguiluz**, University of California Merced

11:15am **BI3-TuM-14 ToF-SIMS Analysis of Tissue Microenvironments and Tumor Growth Progression***, **Lara Gamble**, Daniel Graham,* University of Washington

Tissue microenvironments are a complex ecosystem of cell and non-cellular (e.g. chemical signaling molecules). The regulation of cell growth, metastatic potential, and drug resistances are associated with the microenvironments around solid tumors. Time-of-flight secondary ion mass spectrometry (TOF-SIMS) is a sub-micron spatial resolution imaging mass spectrometry technique used for chemical imaging. Here a combination of ToF-SIMS and H&E staining are used to analyze mouse pancreatic tissue slices by imaging tumors in a *pIns-MycER^{TAM}/p53$^{-/-}$* mouse model. TOF-SIMS was performed with an ION-TOF TOF.SIMS 5-100 instrument (ION-TOF GmbH, Münster, Germany) equipped with a liquid metal ion gun (LMIG) for analysis and an electron flood gun for charge neutralization. Analyses of the *pIns-MycER^{TAM};p53$^{-/-}$* tumor microenvironment has identified and mapped molecules that play key roles in tumor metabolism and growth including nucleic acids, organic acids and lipids, as well as inorganic ions. Evidence is provided of significant metabolic change occurring within *Myc*-driven *β* cell tumors and surrounding stromal region over a 12-day period and demonstrate that TOF-SIMS imaging is a useful tool for spatial characterization of metabolite changes in the *Myc* model. Analyses provide evidence that significant metabolic changes occur in the tumor microenvironment in response to *Myc* activation and that the metabolic profiles of the tumor and the stroma differ dramatically.

11:30am **BI3-TuM-15 Molecular Analysis of Small Extracellular Vesicles by Nanoprojectile Secondary Ion Mass Spectrometry***, **Pierre Hirchenhahn**, Stanislav Verkhoturov, Victoria Cura, Ravi Jada,* Texas A&M University*; Thanh Qui Nguyen, Daheui Choi,* Mayo Clinic*; Michael J. Eller,* University of Mississippi*; Alexander Revzin,* Mayo Clinic*; Emile A. Schweikert,* Texas A&M University

Small extracellular vesicles (SEVs) are biological objects of 30 to 150 nm. They serve as communication line between cells and their environment through the transport of lipids, proteins and genetic material. Because they carry tissue- and health-status-specific biomarkers, SEVs are highly promising candidates for disease diagnosis and monitoring. However, their strong chemical heterogeneity makes their characterization particularly challenging. Current analytical techniques generally provide only partial or averaged information, preventing a comprehensive understanding of SEVs molecular diversity. In this context, Nanoprojectile Secondary Ion Mass Spectrometry (NP-SIMS) appears as a powerful solution. Unlike conventional SIMS approaches, NP-SIMS operates in an event-by-event mode, where the analyte is impacted by a single nanoprojectile at a time. The nanoprojectiles used are Au_{400}^{4+} clusters accelerated to 100 kV, generating craters of only 10–20 nm in diameter. The secondary ions emitted from each individual impact are mass analyzed and recorded separately, providing unprecedented molecular lateral resolution and sensitivity. A critical challenge for NP-SIMS investigations is the preparation of suitable capture surfaces ensuring both high EV density and minimal aggregation, so that each nanoprojectile impacts only a single vesicle. To address this issue, plasma-cleaned silicon wafers were functionalized with successive layers of (3-Aminopropyl)triethoxysilane (APTES) and glutaraldehyde prior to EV incubation. The different preparation steps and resulting surface chemistry were assessed through a combination of NP-SIMS, X-ray photoelectron spectroscopy (XPS), and scanning electron microscopy (SEM). Finally, the validity of the developed preparation protocol was demonstrated using hepatic extracellular vesicles.

This work was supported by NIH grant number 5R01DK134661.

11:45am **BI3-TuM-16 Nanoscale Characterization of Bio-Nanomaterials Using Nano-Projectile Secondary Ion Mass Spectrometry***, **Christelle Guillermier**,* Bienne Technology*; Michael Eller,* University of Mississippi*; Stanislav Verkhoturov,* Texas A&M University*; Richard Rickman,* Bienne Technology*; Emile Schweikert,* Texas A&M University

Advances in nanoparticle biomaterial engineering have made accurate characterization of these systems increasingly important. Many modern nanoparticle designs are multifunctional, resulting in complex and often heterogeneous composition, including hybrid and core/shell architectures, particles functionalized with multiple ligands, asymmetric particles, sensing platforms, and targeted therapeutic carriers each presenting distinct analytical challenges.

To address these challenges, we present Nano Projectile Secondary Ion Mass Spectrometry (NP-SIMS), a variant of conventional SIMS that enables nanoscale molecular analysis of individual nanoassemblies. In contrast to conventional SIMS, which relies on continuous ion beams with spatial resolutions typically limited to ~30 nm, NP-SIMS employs ~2 nm gold nanoprojectiles delivered as isolated impacts separated in both time and space. A time-of-flight (ToF) mass spectrum is acquired from each individual impact event. Each nanoprojectile probes a nanovolume approximately 10 nm in diameter, allowing nanoassemblies to be analyzed one-by-one rather than as ensemble averages. This event-by-event acquisition approach enables the direct identification of colocalized molecular species within complex nanoassemblies.

Here, we present several examples illustrating the application of NP-SIMS to the characterization of complex biomaterial nanoassemblies. First, NP-SIMS was used to analyze extracellular vesicle (EV) population heterogeneity at single-EV resolution and to distinguish hepatocyte-derived EVs from liver cancer EVs based on differences in surface marker expression. Second, we demonstrate the determination of DNA ligand loading and ligand density on DNA functionalized metal nanoparticles, specifically anisotropic gold nanostars and isotropic gold nanospheres with comparable surface areas. Third, NP-SIMS was applied to the analysis of a mixture of nanoparticles containing identical metal cores (3–5 nm in diameter) but functionalized with ligands of different chain lengths (decanethiol, tetradecanethiol, and hexadecanethiol). Using NP-SIMS, we determined the relative abundance of the three nanoparticle populations on the surface.

These examples demonstrate the capability of NP-SIMS to characterize molecular composition, heterogeneity, and surface functionalization within complex nanoscale biomaterial systems at the level of individual nanoassemblies, providing analytical information inaccessible through ensemble-averaged measurements.

12:00pm **BI3-TuM-17 Interactions of Divalent Metal Cations with Phosphate Headgroups in Monolayers at the Air/Water Interface***, **Sadia Afroz**, Paul S. Cremer,* Pennsylvania State University

The binding of divalent metal cations to negatively charged monolayers in aqueous solutions is a complex process that depends on the supramolecular arrangement and spacing of the headgroups at the air/water interface. Previous literature showed that binding of Mg^{2+} and Ca^{2+} to the $PIP(4,5)P_2$ head groups has significant impact on interactions between $PIP(4,5)P_2$ and protein by changing the orientation of the head group and ordering of the acyl chain. Moreover, Ca^{2+}forms contact ion pairs with $PIP(4,5)P_2$ head groups, whereas Mg^{2+}preferentially forms solvent-shared ion pairs. Herein, Sum Frequency Generation (SFG) vibrational spectroscopy was employed to probe the water structure and mode of ion binding with two different PA species, 1,2-dilauroyl-sn-glycero-3-phosphate (DLPA) and 1-stearoyl-2-hydroxy-sn-glycero-3-phosphate (LPA). It was found that increasing the PA charge density and fraction deprotonation increased the binding affinity in both cases, but LPA showed stronger sensitivity than DLPA. These data also suggested that differences in the binding behaviour between $Ca^{2+}$and Mg^{2+}arose from the molecular-level details of the binding mechanism. The spacing of the headgroup was important and the

phosphate moieties could be closer together with LPA (1 tail) compared to DLPA (2 tail). This study provides important insights into the mechanisms underlying the binding of divalent cations to PA, which may have implications for understanding cellular signaling.

Electronic Materials and Photonics
Room 318 - Session EM-TuM

Advanced Devices and Materials for Photonic, Sensing, and Quantum Applications

Moderators: Dr. Erica Douglas, Sandia National Laboratories, **Dr. Seth King**, University of Wisconsin - La Crosse, **Prof. Leland Nordin**, University of Central Florida, **Somil Rathi**, Arizona State University

11:00am **EM-TuM-13 Low-Loss Single Mode AlN-Based CMOS-Compatible Platform for Quantum Photonic Integrated Circuits**, ***Bogdan Dryzhakov***, *John Serafini, Bernadeta Srijanto, Steven Randolph, Kyle Kelley,* Oak Ridge Natinal Laboratory

Quantum photonic technologies require scalable integrated platforms that combine low-loss routing from the UV to IR, controlled modal confinement, nonlinear optical functionality, and fabrication compatibility. Single-mode photonic circuit operation is critical for quantum applications, requiring waveguide geometries that suppress parasitic higher-order modes; however, the reduced dimensions and tighter tolerances needed for modal confinement amplify sensitivity to sidewall roughness, etch damage, dimensional nonuniformity, and scattering loss. Aluminum nitride (AlN) offers a promising CMOS-compatible material platform, combining wide-bandgap transparency, environmental robustness, ferroelectric functionality, and intrinsic χ(2) nonlinearity. We present an end-to-end AlN quantum photonic integrated circuit platform, targeting $\chi^{(2)}$ nonlinear processes for on-chip quantum light generation. Building a suitable fabrication stack required studies spanning lithography across organic, metal, and dielectric masking strategies, reactive ion etching optimization, and modeled design principles. The demonstrated nonlinear photonic platform achieves single-mode operation at 1550 nm with propagation losses as low as ~1 dB cm^{-1} and Q-factors exceeding 10^5. These results establish ferroelectric AlN as a viable platform for scalable quantum interconnects and integrated quantum technologies.

11:15am **EM-TuM-14 Elvamide Nylon as a Versatile and Tunable Alignment Layer in Liquid Crystal Devices**, ***Joshua Levy***, National Academies of Sciences, Engineering, and Medicine*; Zoey Davidson, Jakub Kolacz, Christopher Green, Christopher Spillmann,* US Naval Research Laboratory

Liquid crystal (LC) alignment layers are essential for uniform molecular orientation in LC devices, governing anchoring strength, pretilt angle, and optical performance. Polyimide (PI), the most widely used alignment layer material, requires aggressive solvents (NMP) and curing temperatures >200°C, precluding integration with thermochemically sensitive photonic substrates. Furthermore, PI exhibits significant absorption in the blue-UV spectral ranges, limiting its utility in broadband LC-tunable photonic devices like phase shifters, tunable filters, ring resonators, and variable optical attenuators. Nylon Elvamide 8023R is a methanol soluble, room-temperature-processable alternative that has been used in LC devices for decades, yet no systematic characterization relating processing parameters to alignment layer performance has been reported. This work presents the first thickness-correlated characterization of spin-coated Elvamide 8023R on ITO glass using liquid crystal E7. Elvamide films were spin coated across a range of concentrations (Figure 1(a)), and atomic force microscopy confirmed uniform, continuous film formation at both the microscale (Figure 1(b)) and nanoscale, where individual nylon fibrils are resolved prior to rubbing (Figure 1(c)). Following unidirectional rubbing (Figure 2(a)), orientation mapping and histograms reveal a dramatic shift from randomly oriented fibrils (Figure 2(b)) to strongly aligned fibrils (Figure 2(c)), with the nematic order parameter increasing 12-fold from S=0.066 to S=0.828. Film thickness scales approximately linearly with spin concentration (Figure 3(a)), with continuous films formed down to ~1.7 nm with high film uniformity, below that achievable using polyimide. Polar anchoring energy, measured using the Yokoyama-van Sprang high-field method, remains approximately constant across all concentrations (Figure 3(b)), with a mean value of E_a=1.58×10^{-4} J/m^2, exceeding the strong anchoring threshold by 10-fold. Pretilt angle, measured via the Scheffer-Nehring crystal rotation method, exhibits concentration-dependent behavior below 0.0625%, then saturates at α=1.19°±0.10° (Figure 3(c)), revealing a mechanism for tuning LC pretilt through coating thickness without compromising anchoring strength. FTIR and UV-Vis spectroscopy further confirmed high optical transmissivity from UVB through IR, addressing PI's UV absorption limitations. These findings make Elvamide 8023R a compelling alignment layer material for LC-tunable photonic devices operating over a wide range of the electromagnetic spectrum, particularly where low processing temperatures, minimal optical loss, and ultra-thin films are required.

11:30am **EM-TuM-15 Rolled-up metamaterials (RUMMS) for infrared imaging**, ***Gokul Nanda Gopakumar***, *Stephanie Law,* Pennsylvania State University

Subwavelength information about an object is carried by waves with large wavevectors. The diffraction limit is caused by the rapid evanescent decay of these large wavevector modes at the surface of a material. Hyperbolic materials allow light with large wave vectors to propagate within the material without decaying exponentially close to the surface. These materials have a negative real part of the permittivity tensor along at least one direction and a positive permittivity along at least one other direction, leading to an open isofrequency surface, in contrast to the closed isofrequency surface of normal materials. In a flat hyperbolic material, the sub-diffractional information will still exponentially decay once it leaves the hyperbolic medium. However, in a rolled-up hyperbolic material, the wavevector of the light decreases as it propagates radially, and the image is magnified, enabling propagation beyond the surface.

In this work, we present rolled up semiconductor-based infrared hyperbolic metamaterials. We fabricate these structures by using a strained bilayer that can be released from the substrate. The strained bilayer is grown using III-V semiconductors in a molecular beam epitaxy system. It comprises of a compressively strained bottom layer and tensile strained top layer grown on top of a sacrificial layer. A heavily doped III-V semiconductor is grown on top and this layer acts as an optical metal in the IR. Fabrication of rectangular mesas is done using standard lithographic and wet etching techniques. Finally, a wet etch that selectively removes the sacrificial layer is used to gradually release the strained bilayer, causing it to roll up. By changing the alloy composition, we tune the stress in the bilayers to change the diameter of the rolled-up tube. The number of turns in the rolled-up tube can also be increased by increasing the etching time. The result is a RUMM that has alternating layers of dielectric and metal in the radial direction.

The growth of the strained bilayer and determination of the strain are evaluated using high resolution X-ray diffraction. Scanning electron microscopy is used to image the rolled-up tubes and correlate their diameter to the bilayer strain. Finally, infrared spectroscopy will be used to measure the optical properties of the RUMMs. This is the first step in creating a fully semiconductor-based curved hyperbolic metamaterial that can be used in subdiffractional imaging in the IR wavelength range.

11:45am **EM-TuM-16 Optical Data Storage Materials**, *Yuanbing Mao,* ***Venkata Daggupati***, Illinois Institute of Technology

To satisfy the demand for further data growth and low energy consumption storage, the exploration of new optical data storage (ODS) recording materials has drawn intensive attention. However, the lack of suitable persistent and optically stimulated luminescence materials with deep-level traps is still the bottleneck of such applications. We have recently explored solid-state optical materials and tuned their optical properties, and ultimately engineering their desirable trap characteristics, for such applications. Particularly, by tailoring their trap depth, density and distribution, we have improved their optical information storage performance. Moreover, synergistic stimulation of these phosphors has been demonstrated as multimode storage media for ODS applications. Hence, other than demonstrating trap engineering as an effective way to tune luminescence properties of solid-state optical materials for ODS application, this talk will offer deep insights into their fundamental trapping and recombination processes and lay a strong foundation for multi-functional optical materials in future innovations.

12:00pm **EM-TuM-17 High-Mobility Electron Transport and Mid-Infrared Optical Properties of Sputter-Deposited InN**, ***Ryan Spangler***, Pennsylvania State University*; Jacob Shusterman,* Oak Ridge National Laboratory*; Josh Nordlander,* Pennsylvania State University*; Anton Ievlev,* Oak Ridge National Laboratory*; Jon-Paul Maria,* Pennsylvania State University

InN is a wurtzite group-III nitride that strongly favors high unintentional *n*-type conductivity, especially when grown by sputter deposition. This capacity for high carrier concentrations (>10^{19} cm^{-3}), when combined with

the high mobilities allowed by the low electron effective mass of InN, makes this material a promising candidate for semiconductor plasmonics in the mid- to near-infrared. In this work, we demonstrate a sputter-deposition process that uses high working gas pressures (>100 mTorr) to achieve favorable transport properties of heteroepitaxial InN on AlN-buffered C-plane sapphire. Within this processing space, we find the Hall mobility increases significantly with film thickness, achieving a value of 840 $cm^2/V \cdot s$ at a thickness of 240 nm, significantly higher than other reports of sputtered InN.[1-3] We perform X-ray diffraction and atomic force microscopy to characterize the high film quality. We also use time-of-flight secondary ion mass spectrometry (ToF-SIMS) depth profiles to assess whether impurities such as O, H, and C can account for the high background carrier concentrations ($>10^{19}$ cm^{-3}) of the unintentionally doped material. We further dope the InN films with Ge to control the infrared optical properties, increasing the carrier concentration to nearly 10^{22} cm^{-3} to induce plasma frequencies ranging from 5.5 µm to 1.6 µm as measured by infrared variable angle spectroscopic ellipsometry (IR-VASE). As expected, however, the Hall mobility begins to fall at high Ge doping levels, which could increase optical losses at near-infrared frequencies. This work showcases the potential for tunable, high-mobility sputter-deposited InN and Ge:InN in IR plasmonic and optoelectronic applications.

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Light Source Enabled Science
Room 319 - Session LS-TuM

Light Source Enabled Energy Science

Moderators: Dr. Andi Barbour, Brookhaven National Laboratory, **Dr. Philip Ryan**, Argonne National Laboratory, USA

8:00am **LS-TuM-1 Surface Sensitive and In-Situ Characterization of Perovskite Materials for Energy Conversion**, ***Juanita Hidalgo,*** New York University **INVITED**

Developing new energy conversion technologies is a critical scientific challenge to address global energy demand and global warming. Perovskite-type materials are particularly important because they exhibit electronic and or ionic conductivity, enabling a wide range of energy-related applications, including photovoltaics, fuel cells, and electrolysis cells. Lead halide perovskites (APbX3) have emerged as promising absorber layers for low-cost solar cells, while perovskite oxides (ABO3) are widely used as electrodes and catalysts in solid-state electrochemical systems. However, the perovskite crystal structure can be unstable and undergo phase transformations under external stressors. To investigate the surface structural and chemical properties of these materials, my work employs advanced synchrotron-based in-situ characterization techniques, including grazing-incidence wide-angle and small-angle x-ray scattering (GIWAXS/GISAXS) and near-ambient-pressure X-ray photoelectron spectroscopy (NAP-XPS). First, my talk will address the instability of lead halide perovskites under exposure to humidity and air, and the complex relationship between structure, properties, and performance in solar cell applications. Using in-situ GIWAXS, we investigated the undesired phase transformations that occur under humid air and humid nitrogen environments, revealing a synergistic effect between water and oxygen that accelerates degradation. Second, I will discuss the high-temperature reduction of perovskite oxides, which leads to the formation of embedded metal nickel nanoparticles through a process known as exsolution. These nickel nanoparticles can act as catalysts for electrochemical reactions relevant to energy conversion and storage. Using simultaneous in-situ XPS and GISAXS, we tracked nanoparticle formation through the reduction of nickel oxide to the metallic state and the corresponding structural evolution observed by GISAXS. Therefore, understanding the mechanisms governing perovskite phase transformations and establishing correlations between structure, chemistry, and properties is essential for tuning and optimizing these materials to achieve more robust, stable, and efficient energy technologies for real-world applications.

8:30am **LS-TuM-3 Energy Science Research Using In Situ and Operando Soft X-ray Spectroscopy at the National Synchrotron Light Source II: Science Highlights and Future Plans**, ***Iradwikanari Waluyo,*** Brookhaven National Laboratory

From catalysts and fuel cells to batteries and corrosion-resistant superalloys, the In situ and Operando Soft X-ray spectroscopy (IOS, 23-ID-2) beamline at the National Synchrotron Light Source II (NSLS-II) at Brookhaven National Laboratory (BNL) provides versatile experimental techniques to enable impactful science. The IOS beamline provides capabilities for ambient pressure X-ray photoelectron spectroscopy and X-ray absorption spectroscopy for revealing the dynamic evolution of the chemical and electronic states of energy materials under realistic working conditions. I will present recent research highlights, including (1) characterizing the surface chemical state of single-atom alloy model catalysts under oxidizing and reducing conditions, (2) understanding the reaction mechanism of industrially relevant heterogeneous catalytic reactions such as CO_2 hydrogenation, CH_4 conversion, and ethylene epoxidation, and (3) optimizing novel materials synthesis through tunable metal exsolution from perovskites. I will also give an overview of ongoing short term and long term upgrades with the aim to enable multi-modal ambient pressure soft X-ray spectroscopy at IOS, which will allow researchers to obtain comprehensive electronic and chemical information for energy materials in operating conditions at relevant time scales.

8:45am **LS-TuM-4 Operando Soft X-Ray Spectroscopy of Electrochemical Interfaces: From Reaction Cell and Sample Design to Mechanistic Insight**, *Santosh Kumar,* Diamond Light Source Ltd., UK*; James J. C. Counter,* University of Manchester, UK*; David C. Grinter, Matthijs A. van Spronsen, Pilar Ferrer,* Diamond Light Source, UK*; Christopher M. Zalitis, Tugce Eralp Erden,* Johnson Matthey Technology Centre, UK*; Roger A. Bennett,* University of Reading, UK*;* ***Georg Held,*** Diamond Light Source, UK

Synchrotron-based *operando* soft X-ray photoelectron spectroscopy (XPS) and near-edge X-ray absorption fine structure (NEXAFS) enable element-specific probing of electrochemical interfaces under realistic conditions but require advanced reaction cell and sample designs to bridge aqueous electrochemistry and vacuum-based detection. We present a modular spectro-electrochemical flow cell and window-free working electrode assembly (WEA) compatible with near-ambient-pressure XPS and NEXAFS. The platform combines interchangeable SiN_x or polymer membranes (such as Nafion™) with controlled hydration, enabling stable in-situ measurements under electrochemical operation. Using CuO_x- and IrO_x-based electrodes, we demonstrate tracking of redox processes, surface hydration, and oxygen evolution chemistry. *Operando* XPS and NEXAFS reveal potential-dependent metal oxidation and the formation of reactive oxygen species, providing direct insight into reaction mechanisms at electrochemical interfaces. This approach establishes a versatile methodology for soft X-ray studies of electrocatalysts.

References

1. *Catalyst-Coated Mesoporous Carbon–Membrane Electrode Assembly for In-situ Soft X-ray XPS and NEXAFS Studies of Electrocatalytic Interfaces*, **ACS Electrochemistry** (2026) DOI: 10.1021/acselectrochem.5c00554.
2. *An Electrochemical Flow Cell for Operando XPS and NEXAFS Investigation of Solid–Liquid Interfaces*, **J. Phys. Energy** 6,036001 (2024). DOI: 10.1002/cctc.202400937

9:00am **LS-TuM-5 Substrate-Mediated Doping Reshaping Interfacial Energetics in Organic Electronics**, ***Xiane Li***, *Slavomir Nemsak,* Advanced Light Source, Lawrence Berkeley National Laboratory

Energy level alignment (ELA) at electrode/organic-semiconductor interfaces governs charge generation, transport, and injection in organic electronic and energy-conversion devices. However, ELA is typically characterized under ultra-high vacuum, whereas practical devices operate in ambient environments where water is ubiquitous. The influence of water on interfacial energetics therefore remains largely unresolved. Here we probe the evolution of ELA in the presence of water using operando ambient-pressure X-ray photoelectron spectroscopy combined with Kelvin probe measurements. We find that water molecules strongly reshape the interfacial electronic structure by screening the spontaneous charge transfer that forms interface dipoles under vacuum. This screening suppresses dipole formation at interfaces, lowers or increases the work function of the system, and promotes electron or hole accumulation in the

organic semiconductor, resulting in pronounced substrate-mediated n-doping/p-doping. Our findings reveal a previously unrecognized environmental influence on ELA, establishing water as a key regulator of substrate-mediated interfacial energetics in organic electronic systems.

9:15am **LS-TuM-6 Investigation on Topotactic Phase Transition of $LaCoO_3$ Thin Films with in Situ XRD and Ambient Pressure Hard X-Ray Photoelectron Spectroscopy**, *Hyunsuk Shin, Youngmin Yun,* Gwangju Institute of Science and Technology, Republic of Korea*; Okkyun Seo,* National Institute for Materials Science, Japan*; Seongeun Kim,* Chosun University, Republic of Korea*; Minsik Seo, Dongwoo Kim,* Gwangju Institute of Science and Technology, Republic of Korea*; Hojoon Lim,* Myongji University, Republic of Korea*; Hojun Oh, Subin Jang, Kyungmin Kim, Sae Hyun Kang,* Gwangju Institute of Science and Technology, Republic of Korea*; Adrian Hunt, Iradwikanari Waluyo,* Brookhaven National Laboratory*; Do Young Noh,* Gwangju Institute of Science and Technology, Republic of Korea*; Hyon Chol Kang,* Chosun University, Republic of Korea*;* ***Bongjin Simon Mun****,* Gwangju Institute of Science and Technology, Republic of Korea

To understand the correlation between the structure phase transition (SPT) and electronic/chemical properties of LaCoO3 (LCO), multimodal techniques, including in situ XRD, I-V measurement, and ambient pressure hard X-ray photoelectron spectroscopy (AP-HAXPES) are employed. Especially, AP-HAXPES not only allows operando analysis under wide pressure and temperature ranges, but also provides the direct bulk sensitive information of the electronic/chemical states. The AP-HAXPES measurement overcomes the difference of the probing depths between conventional XPS and XRD, thereby providing bulk-sensitive chemical/electronic structure information under reaction condition. The observed oxidation states in core level spectra, Co 2p, clearly showed that the oxygen vacancies play an important role in the SPT of LCO thin films. Importantly, the analysis of the valence band (VB) spectra of AP-HAXPES showed the presence of enlarged band gap formation, demonstrating the presence of the complex interplay between the oxygen vacancies and electronic structure. The modified VB structures across the SPT are also compared to the in situXRD and transport measurements.

9:30am **LS-TuM-7 Advances in Hydrogen Technology Enabled by Synchrotron X-ray Methods***, **Nicholas Strange**,* SLAC National Accelerator Laboratory, United States Minor Outlying Islands (the) **INVITED**

Hydrogen energy represents a critical frontier in securing the United States' long-term energy resilience and global technological dominance. Achieving cheap, sustainable, and equitable hydrogen production at scale requires rapid advancement of the underlying materials science and process technologies, a challenge that has mobilized significant federal investment and a growing network of national laboratory partnerships. This talk will highlight previous and ongoing research within the materials science division at the Stanford Synchrotron Radiation Lightsource (SSRL), contextualized within the broader scopes of the HyMARC, H2NEW, H2NUC, HydroGEN, and HyBlend energy materials networks (i.e., DOE-led consortia uniting national laboratories around hydrogen production, storage, and transport).

The hydrogen R&D landscape is undergoing a decisive shift from foundational discovery toward application-focused development of materials optimized for specific performance and durability requirements. American leadership in this transition is essential, both to drive down the cost of clean hydrogen production and to establish the domestic industrial base necessary for long-term energy independence. *In situ* and *operando* X-ray scattering measurement designs developed at SSRL will be discussed, with results presented from a selection of collaborative projects aimed at accelerating this national effort.

Multifunctional and Hybrid Microsystems
Room 318 - Session MC-TuM

Multifunctional and Hybrid Microsystems: MEMS and Bio Applications

Moderators: Prof. Dr. Jesse Berezovsky, Case Western Reserve University, **Prof. Dr. Jaesung Lee**, University of Central Florida

8:00am **MC-TuM-1 Ultralow-Dissipation Diamagnetically Levitated Graphite Rotors for Gyroscopic Inertial Sensing***, **Samira Yasmin**, Pooja Roy,* University of Central Florida*; Yunong Wang, Philip Feng,* University of Florida*; Jaesung Lee,* University of Central Florida

Rotational degrees of freedom are nearly unconstrained, making levitated rotors compelling candidates for next-generation inertial sensors. By eliminating mechanical anchors entirely, this approach suppresses the dominant loss pathways—support loss and friction—that limit the performance of conventional gyroscopes. Here we report on a diamagnetically levitated pyrolytic graphite rotor platform operating under high vacuum, characterized through ringdown measurements, and analyzed toward practical gyroscopic readout.

The rotor is laser-machined from highly oriented pyrolytic graphite, which exhibits strong negative magnetic susceptibilities ($\chi_x = \chi_y = -85\times10^{-6}$, $\chi_z = -450\times10^{-6}$) enabling passive, stable levitation above a concentric permanent-magnet assembly integrated beneath a custom PCB. The annular rotor geometry (inner radius 2.175 mm, outer radius 4.175 mm, mass ~95 mg) concentrates rotational inertia at large radius.

Rotational actuation and sensing are implemented via a closed-loop system combining a 633 nm laser interferometer, FPGA-based digital timing, and a high-voltage (200 V) electrostatic pulse drive. The optical contrast between the graphite rotor arms and the PCB surface generates a periodic photodetector signal, from which the FPGA extracts instantaneous rotation speed and generates phase-synchronized drive pulses. Under vacuum conditions of 80−100 μTorr, where gas damping is substantially reduced, the rotor is driven to 410 RPM, after which free ringdown is recorded. The rotational speed decay follows $\Omega(t) = \Omega_0 e^{-\gamma t}$, yielding an extracted damping constant of $\gamma = 1.9\times10^{-4}$/s.

The measured γ and I_z directly set the thermomechanical noise floor, expressed as an angular random walk (ARW). At 410 RPM and room temperature, the thermal-noise-limited ARW is estimated at 2.28×10^{-4} °/√h, with a projected improvement to 9.1×10^{-5} °/√h at 1100 RPM. To connect this platform to practical gyroscopic operation, we derive an analytical scale factor linking optically measured out-of-plane rim displacement to input angular rate through the coupled tilt dynamics of the spinning rotor. Under the nearly symmetric rotor approximation in the weak-damping limit, the estimated scale factor is $S = 3.02\times10^{-5}$ m/(rad/s), implying that a 1 nm displacement resolution at the rotor rim translates to an angular-rate resolution of ~40 μrad/s upon full gyroscope readout implementation.

These results establish a quantitative performance framework for diamagnetically levitated graphite rotors, highlighting vacuum environment, spin-axis inertia, and tilt stiffness as the primary design levers for advancing sensitivity in compact, anchor-free rotational inertial sensors.

8:15am **MC-TuM-2 Influence of Fluid Dynamics on a Halide-Suppressor Electrolyte for Copper Electrodeposition in High Aspect Ratio Through Silicon Vias***, **Jessica McDow**, Matthew Jordan,* Sandia National Laboratories

Through silicon vias (TSVs) are essential for three-dimensional microelectronic integration, enabling enhanced electrical and thermal connectivity. Copper electrochemical deposition (ECD) with halide-suppressor chemistries has achieved void-free, bottom-up filling of high aspect ratio TSVs[1]. However, the interplay between hydrodynamics, ion transport, and suppressor adsorption kinetics within these recessed features remains incompletely understood.

This work combines experimental electrochemical depositions and computational fluid dynamics (CFD) modeling to understand the critical role of fluid flow in governing copper deposition profiles within TSVs of a 70 μm diameter and 625 μm depth. Cyclic voltammetry (CV) on rotating disk electrodes reveals that increased rotation rates enhance suppressor replenishment, shifting the re-inhibition potential and diminishing hysteresis associated with the s-shaped negative differential resistance (S-NDR) behavior. Electrochemical deposition experiments demonstrate that rotation rate modulates deposition uniformity: low rotation rates lead to void formation due to insufficient suppressor transport, while excessively high rotation rates cause premature plating termination near the via opening due to enhanced suppressor adsorption.

CFD simulations confirm that convective flow penetrates only the upper ~100 μm of the via, establishing a hydrodynamic boundary layer where suppressor concentration approaches bulk levels, sustaining suppression and limiting deposition at the via mouth. Below this region, transport is diffusion-dominated, enabling concentration gradients that promote bottom-up filling. By strategically modulating rotation rates—starting at 400 rpm, increasing to 1000 rpm, then returning to 400 rpm—void-free filling is achieved with a 33% reduction in plating time from 18 to 12 hours.

These findings highlight the complex balance between convective and diffusive transport in controlling suppressor dynamics and copper deposition within TSVs. Understanding and harnessing fluid dynamic effects are crucial for optimizing scalable, high-throughput TSV filling processes in advanced 3D integration technologies.

[1] Schmitt, R. P.; Menk, L. A.; Baca, E.; Bower, J. E.; Romero, J. A.; Jordan, M. B.; Jackson, N.; Hollowell, A. E. Void-Free Copper Electrodeposition in High Aspect Ratio, Full Wafer Thickness Through-Silicon Vias with Endpoint

Detection. *J. Electrochem. Soc.* **2021**, *167* (16), 162517. https://doi.org/10.1149/1945-7111/abd56e.

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8:30am **MC-TuM-3 Redefining Dynamic Limits of MEMS Resonators via Nonlinear Dynamics*, Hanna Cho,*** The Ohio State University **INVITED**

As resonant MEMS approach fundamental material and performance limits, new design paradigms are required to enable the next generation of sensing and timing technologies. Nonlinear dynamics are increasingly recognized as a pathway to overcome the constraints of conventional linear operation. Among these, internal resonance (InRes), in which two or more vibrational modes are nonlinearly coupled through integer frequency ratios, provides opportunities for dynamic range extension, frequency stabilization, and controlled intermodal energy transfer. Unlike traditional MEMS devices operating within narrow linear regimes, InRes enables energy exchange between coupled modes, allowing stable resonance to be maintained under large excitation levels and environmental perturbations. In this talk, I will present recent advances in understanding and engineering InRes in MEMS resonators through combined theoretical modeling and experimental validation. In particular, I will demonstrate how InRes can passively suppress frequency drift by anchoring the primary mode response to an InRes condition, effectively mitigating amplitude-to-frequency conversion induced by nonlinear effects. These insights have direct implications for the development of timing references with long-term frequency stability, as well as for the design of high-performance inertial sensors with larger scale factors. The results illustrate the emerging potential of nonlinear resonance as a transformative design paradigm for next-generation MEMS technologies.

9:00am **MC-TuM-5 Multifunctional AlN-Based MEMS Resonator Platforms for Advanced RF Filtering and Sensing Applications*, Mingyo Park,*** Pennsylvania State University **INVITED**

Next-generation wireless systems (5G and emerging 6G) are driving demand for RF nano/micro-electromechanical (N/MEMS) acoustic resonators that operate across the 3–30 GHz band. Future RF front-ends require compact, high-performance devices that deliver low insertion loss, wide bandwidth, multi-band compatibility, and robust high-power operation — requirements captured by the resonator figure of merit, FoM = $Q \times kt^2$. Pushing acoustic resonators toward higher frequencies, however, demands aggressive reduction of piezoelectric film and electrode thicknesses, introducing compounding mechanical and electrical losses that ultimately limit performance.

This talk will discuss recent progress in thin-film piezoelectric MEMS resonators built on ultra-thin epitaxial AlN and AlScN. AlScN has emerged as a particularly attractive piezoelectric due to its enhanced electromechanical coupling relative to conventional AlN. By pairing high-quality epitaxial films with optimized resonator geometries, film bulk acoustic resonators (FBARs) operating near 19 GHz [1] have demonstrated strong potential for compact filtering solutions in next-generation RF front-ends, while surfacing the central challenges of mm-wave acoustic design: electrode loss and material quality at extreme thinness.

Beyond passive filtering, piezoelectric MEMS resonators can also be engineered to support nonlinear electromechanical functionality through mechanical frequency comb generation [2]. When driven beyond a critical threshold, single or coupled resonators exhibit strong nonlinear modal interactions that produce equally spaced spectral lines in the mechanical domain. These phononic frequency combs can evolve from a few discrete sidebands into broad, tunable spectral clusters as device geometry, modal coupling, and drive conditions are varied. The resulting nonlinear dynamics offer a route to on-chip multi-frequency signal generation without the complexity of external circuitry.

Taken together, high-frequency acoustic filtering and nonlinear comb generation point toward a broader class of reconfigurable RF microsystems built on the AlN/AlScN piezoelectric material family. Such devices could enable compact filters, low-power frequency sources, spectral processors, and multi-frequency sensing architectures for future wireless and sensing networks. The talk will close by reflecting on how materials engineering, resonator design, and nonlinear dynamics can be combined to expand the functionality of piezoelectric MEMS well beyond conventional RF filtering.

[1] M. Park, et al., EDL.,2024 [2] M. Park, et al., JMEMS.,2019.

9:30am **MC-TuM-7 Electrochemical Sensing of Hormonal Serotonin Levels in Crayfish*, Sydney Overton,*** *Kanishka Balamurugan, Jens Herberholz, Reza Ghodssi,* University of Maryland College Park

The neurotransmitter serotonin (5-hydroxytryptamine, 5-HT) has been implicated as a key biomarker that regulates a range of neurobehavioral functions, including playing a prominent role in modulating social behavior across species. Here, we refined a surface-modification method to enable detection of endogenous (i.e., naturally occurring), nanomolar concentrations of 5-HTfrom crayfish hemolymph (i.e., blood) collected from communally housed (COMs) animals and those isolated for one (1-day ISOs) or seven days (7-day ISOs). The three-electrode sensor for measuring 5-HT is comprised of a carbon-fiber microelectrode (CFME) working electrode, Pt counter electrode, and Ag/AgCl reference electrode. Previous *in vivo* measurements utilized a CFME electrochemically etched (EC) then dip-coated into a carbon nanotube (CNT)-Nafion dispersion (EC/CNT-Nafion). However, to match the electrochemical sensor's detection sensitivity, crayfish were injected with 5-HT. Here, we optimized the surface modification to improve signal-to-noise and sensitivity for *in vitro* 5-HT detection by dip-coating then electrochemically etching (CNT-Nafion/EC). Doing so improved the signal-to-noise ratio 2.8x and maintained the limit of detection from previous fabrication (60nM), enabling successful measurements of endogenous 5-HT *in vitro.*

To investigate how social isolation affects serotonergic mechanisms, we measured hormonal 5-HT in hemolymph from isolated and communally housed crayfish utilizing our CNT-Nafion/EC CFME.Voltammetry results show a clear oxidation peak at 0.29 V, demonstrating detection of un-spiked, hormonal 5-HT. Our findings indicate that 5-HT levels change in response to social isolation, and these changes are species-dependent. 7-day ISOs *Procambarus* (*P. clarkii)* crayfish exhibited a major increase in 5-HT compared to COMs, whereas *Faxonius* (*F. Spp*) crayfish hormonal concentrations of 5-HT peaked in 1-day ISOs. 7-day ISOs *P. clarkii* crayfish contained an average of 581.2nM 5-HT in their hemolymph, a 307.6% increase from COMs, and1-day ISOs did not have significantly higher concentrations compared to COMs. By comparison, *F. spp* 5-HT concentrations in 1-day ISOs were 867.5nM, a 540.1% increase in hormonal 5-HT concentrations compared to COMs, and 7-day ISOs 5-HT concentrations matched COMs.

The *in vitro* results demonstrate the sensor's utility for studying 5-HT dynamics and exhibit results strongly suggesting an underlying effect of social isolation on hormonal 5-HT. Moreover, our findings provide an exciting avenue for future studies, including those providing higher temporal fidelity on 5-HT changes that modulate neural activities and corresponding behaviors.

9:45am **MC-TuM-8 Development of Dissolvable Cantilevers for Localized Oral Drug Delivery*, Yung Priscilla Lai,*** *Joshua Levy, Reza Ghodssi,* University of Maryland

Therapeutics to treat inflammatory bowel disease can cause severe systemic side effects. Localized drug delivery in the gastrointestinal (GI) tract can lower these side effects and increase drug efficacy. Our team has developed an ingestible device that can deliver drugs on-demand in the intestines with multiple cantilever actuators (Fig. S1a). The strained cantilever beams act as springs that can drive the penetration of drug-loaded microneedles into inflamed areas. The current polymer cantilevers made of polyether ether ketone (PEEK) films remain rigid but are not dissolvable, leading to risks of retention and unforeseen consequences as they remain in the body after drug delivery. Dissolvable and biocompatible cantilevers provide a safer alternative for targeted drug delivery in the GI tract.

The difficulty in using dissolvable polymer films as cantilevers arises from their low mechanical strength and stress relaxation under strain, undermining their ability to deploy drugs into the GI mucosa. We can improve these properties by changing the film's degree of crosslinking while maintaining film dissolution. Several crosslinked films were investigated: 1) polyvinyl alcohol (PVA), 2) PVA with citric acid (PVA-Citric) baked at 120°C for 4 hours, 3) freeze-thaw crosslinked PVA with 1M NaCl (PVA-NaCl), and 4) PEEK as a control. Polymer films were cut to size with a CO_2 laser cutter as the cantilever's length dictates its delivery range, ensuring the drug can reach inflamed areas further above the device surface (Fig. S2a). The films were then characterized for their blocking force (Fig. S1b and Fig. S2a), dissolution (Fig. S1c), and stress relaxation (Fig. S1d).

We measured the blocking force at the cantilever tip to evaluate whether polymer films could deliver drug-loaded microneedles without tissue damage. Crosslinking parameters that can provide higher blocking force at

large cantilever displacements were identified. (Fig. S2a, PVA-NaCl and PVA-Citric vs. PEEK). Moreover, higher citric acid content appeared to increase film swelling for cantilever dissolution (Fig. S2b, PVA-Citric 80:20). Further materials optimization will enable lower PVA stress relaxation (Fig. S1d and Fig. S2c) while maintaining high blocking force and film dissolution.

Nanoscale Science and Technology
Room 320 - Session NS-TuM

Multimodal Techniques in Surface and Interface Engineering at the Nanoscale

Moderators: Dr. Aubrey Hanbicki, Laboratory for Physical Sciences, **Prof. Deep Jariwala**, University of Pennsylvania

8:00am **NS-TuM-1 Foundation Models for 2D Materials Research**, ***Haozhe "Harry" Wang,*** Duke University **INVITED**

Foundation models are transforming the discovery, fabrication, and characterization of two-dimensional materials — moving the field toward autonomous laboratories in which AI plans, executes, and interprets experiments with minimal human guidance. In this talk, I will present three complementary advances from our group that together demonstrate a foundation model-native pipeline spanning synthesis, microscopy, and spectroscopic analysis of 2D materials.

First, I will introduce ATOMIC (Autonomous Technology for Optical Microscopy and Intelligent Classification), a foundation model-powered system for zero-shot autonomous microscopy of 2D semiconductors. Without any task-specific training, ATOMIC achieves 99.7% classification accuracy, showing that large vision models can autonomously navigate, image, and interpret nanoscale features at scale. Second, I will present SpectraNET, a curated benchmark of experimental spectroscopic data designed to bridge the gap between frontier AI capabilities and real-world materials characterization. SpectraNET provides standardized evaluation tasks for large language models applied to spectral analysis; through chain-of-thought prompting, we systematically improve inference performance while exposing the current boundaries of AI-driven spectral interpretation. Third, I will describe an LLM-guided chemical vapor deposition platform in which a reasoning-capable language model acts as an autonomous process controller for 2D material synthesis. Leveraging a structured recipe library and one-shot growth recommendations, the system achieves high-yield synthesis toward user-specified targets — dramatically reducing the experimental iteration traditionally required in nanomaterial fabrication.

Taken together, these efforts outline a concrete roadmap for AI-driven laboratories that close the loop from growth to characterization to discovery, accelerating the pace of 2D materials innovation.

8:30am **NS-TuM-3 Controlled Non-Volatile Modulation of Optical Dispersion in Monolayer Tungsten Disulfide via Ferroelectric Polarization Patterning**, ***Yuhong Cao,*** *Deep Jariwala,* University of Pennsylvania

The manipulation of optical properties, including reflection, refraction, polarization, phase, and frequency, has long been central to advancing photonic and optoelectronic technologies. However, existing electro-optical approaches rely on volatile mechanisms that require continuous power consumption. Here, we demonstrate strong, nonvolatile modulation of optical dispersion in monolayer tungsten disulfide (ML WS_2) using patterned ferroelectric domains in aluminum scandium nitride (AlScN). By locally poling ferroelectric domains into opposite states, we achieve substantial manipulation of the complex refractive index ($\Delta n > 0.7$, $\Delta k > 0.4$) and excitonic energy shifts (~50 meV) in ML WS_2, comparable to previous gate-tuning approaches while eliminating continuous power consumption. We introduce an asymmetric screening model that reveals how ferroelectric polarization induces carrier-density-dependent Coulomb screening, leading to distinct excitonic behaviors between electron- and hole-doped regions. Furthermore, we demonstrate a gate-free lateral p-n homojunction with a rectification ratio of 6×10^3, formed through spatial carrier redistribution. These findings establish ferroelectric/2D heterostructures as a powerful platform for nonvolatile optical dispersion engineering, enabling energy-efficient, reconfigurable photonic and optoelectronic devices.

8:45am **NS-TuM-4 Enhanced Ferroelectricity in Ultrathin Compositionally Graded AlScN**, ***Zekun Hu,*** *Haiwei Zhang, Rajeev Kumar, Yuhong Cao, Xiaolei Tong, Pedram Yousefian, Hyunmin Cho, Bongjun Choi, Chao-Chuan Chen, Yunfei He, Kefei Bao, Chloe Leblanc, Eric Stach, Roy Olsson, Deep Jariwala,* University of Pennsylvania

Ferroelectric $Al_{1-x}Sc_xN$ is a promising BEOL-compatible material platform for nonvolatile microelectronics because of its large polarization, wide bandgap, and compatibility with scalable nitride processing. However, aggressive thickness scaling remains limited by the coupled tradeoff among switchability, leakage, dielectric breakdown, ferroelectric stability, and control of the as-grown polarization state. Here, we report the first experimental demonstration of enhanced ferroelectricity in a 20 nm gradient AlN/AlScN/AlN heterostructure. By incorporating AlN interfaces together with compositional grading across the film thickness, the heterostructure modifies the polarization and dielectric response while preserving robust ferroelectric switching in the ultrathin regime. The gradient composition is directly verified by transmission electron microscopy, and, importantly, the heterostructure enables deterministic control of the as-grown polarization state on the same substrate, providing a distinct advantage for scalable integration and comparative device fabrication. Compared with uniform AlScN controls of similar thickness, the gradient heterostructure exhibits a 21.2% higher breakdown field, a 52.2% increase in coercive field, ~10% higher remanent polarization, a 17% lower permittivity, and approximately 40× higher resistivity, while maintaining comparable endurance. The combination of reduced permittivity, enhanced dielectric strength, strengthened polarization response, controlled polarization state, and strongly suppressed leakage suggests that gradient engineering with AlN interfaces improves field control and ferroelectric stability in ultrathin wurtzite nitrides. Importantly, this heterostructure design also enables scaling to a 5 nm AlN/AlScN/AlN sandwich structure containing only a 2 nm $Al_{0.64}Sc_{0.36}N$ ferroelectric layer, whereas a directly deposited 5 nm $Al_{0.64}Sc_{0.36}N$ film does not exhibit functional ferroelectric switching. These results establish a direct correlation between heterostructure design and ferroelectric performance, demonstrating that compositional grading and interfacial engineering together provide an effective route to stabilize and enhance ferroelectricity at reduced thickness. This strategy provides a pathway for further scaling of AlScN-based ferroelectric films, which may enable lower-voltage operation and higher-density integration in future nitride-based memory.

9:00am **NS-TuM-5 Functionalization-Driven Surface Assembly of Hexavanadate Molecular Memristors**, ***Dejia Kong,*** *Daniel Mejia Rodriguez, Amity Anderson, Wenjin Cao, Shuai Zhang,* Pacific Northwest National Laboratory*; Eric Z. Liu,* University of California at Santa Barbara*; Jonas Lorenz, Kirill Monakhov,* Leibniz Institute of Surface Engineering (IOM), Germany*; Venkateshkumar Prabhakaran, Oliva M. Primera-Pedrozo, Xue-Bin Wang, Niranjan Govind, Zbynek Novotny, Grant E. Johnson,* Pacific Northwest National Laboratory

Polyoxometalates (POMs) represent a class of molecular materials with significant potential for next-generation electronics, but their application requires precise control of their electronic properties on surfaces and in addressable arrays. This study investigates the electronic structures and self-assemblies of Lindqvist hexavanadate polyoxometalates (V_6POMs) on highly oriented pyrolytic graphite (HOPG). Using ion soft landing (ISL), we deposited intact, mass-selected V_6POMs functionalized with azide, succinate, and hydroxyl groups. X-ray photoelectron spectroscopy (XPS) confirms the retention of the V^{5+} oxidation state upon deposition. High-resolution scanning tunneling microscopy/spectroscopy (STM/S), supported by density functional theory (DFT) calculations, reveals a key finding: while isolated V_6POMs are semiconducting, their lateral aggregation, driven by hydrogen bonding between organic linkers, substantially reduces the molecular transport gaps. This demonstrates that the electronic properties of surface-supported V_6POMs may be tuned by controlling both the choice of organic functional group and the degree of aggregation. These results establish a clear pathway toward developing chemically programmable, multi-state resistive switching elements for future memristive devices and energy-efficient microelectronics.

9:15am **NS-TuM-6 Scalable HfN Based AlScN Ferroelectric Diode Memories for High-Temperature Operation up to 500 °C**, ***Chao-Chuan Chen,*** University of Pennsylvania*; Tzu-Yu Peng,* National Taiwan University, Taiwan*; Yunfei He, Zekun Hu, Kefei Bao, Roy Olsson,* University of Pennsylvania*; Yu-Jung Lu,* Academia Sinica, Taiwan*; Deep Jariwala,* University of Pennsylvania

Ferroelectric AlScN has attracted significant attention for next-generation non-volatile memory applications owing to its large remanent polarization,

high thermal stability, and CMOS compatibility. However, the intrinsically high coercive field of AlScN results in large operating voltage, while aggressive thickness scaling is often limited by increased leakage current, premature breakdown, and unstable ferroelectric switching behavior. To address these issues, HfN has emerged as a promising bottom electrode material because its small lattice mismatch with AlScN enables coherent interface formation and reduced leakage current, potentially facilitating ultrathin and thermally robust ferroelectric devices.

In this work, HfN-based AlScN ferroelectric diode memories with different AlScN thicknesses (20 and 45 nm) and different oxide interlayers (Al_2O_3 and HfO_2) were investigated to evaluate the effects of thickness scaling and interface engineering on high-temperature ferroelectric operation. The influence of oxide interlayers on switching characteristics, leakage current, and self-rectifying behavior was also compared. Electrical characterizations, including DC, AC switching, and PUND measurements, were performed over a wide temperature range from room temperature to 500 °C to evaluate thermal stability and ferroelectric switching behavior under elevated-temperature operation.

Stable ferroelectric switching behavior was successfully maintained up to 500 °C under both AC and DC measurements. Both 20 nm and 45 nm AlScN devices demonstrated stable ferroelectric operation over a wide temperature range. A gradual reduction in coercive field with increasing temperature was observed, indicating thermally assisted polarization switching and reduced switching voltage. In the 45 nm devices, the remanent polarization reached |2Pr| values of ~150 μC/cm^2 and further increased at higher temperatures, suggesting enhanced polarization switching behavior. Although leakage current increased at elevated temperature, the devices retained clear ferroelectric switching characteristics and finite self-rectifying behavior with on/off ratio of ~10. In addition, the effects of AlScN thickness and oxide interlayers on switching stability and leakage behavior were systematically compared. These results highlight the thermal robustness and scalability of HfN-based AlScN ferroelectric diodes for high-temperature non-volatile memory applications.

9:30am **NS-TuM-7 Imaging Atomic Dynamics in Real-Time: Current Capabilities and Future Horizons at SLAC MeV-UED**, ***Alexander Reid***, SLAC National Accelerator Laboratory **INVITED**

High-brightness radio-frequency photocathode technology enables the generation of ultrashort electron bunches for a variety of frontier application. In the megaelectronvolt (MeV) energy range, these bunches serve as a powerful probe of atomic dynamics at the timescale of lattice vibrations, chemical reactions and phase rearrangement. MeV electrons combine ultrashort durations (<100 fs), with high momentum resolution, tens-of-nanometer scattering depths, and low energy deposition. The MeV ultrafast electron diffraction facility at SLAC National Accelerator Laboratory leverages these properties to allow sensitive measurement of atomic motions in solid, liquid and gas phase systems. This presentation details the current MeV-UED instrument at SLAC, its scientific achievements and the ongoing developments. A special focus will be emerging opportunities in in-situ, in-operando and multi-modal measurements capabilities.

11:00am **NS-TuM-13 Cavity Electrodynamics of Van der Waals Heterostructures**, ***James McIver***, Columbia University **INVITED**

Van der Waals (vdW) heterostructures host many-body quantum phenomena that can be tuned *in situ* using electrostatic gates. These gates are often microstructured graphite flakes that naturally form plasmonic cavities, confining light in discrete standing waves of current density due to their finite size. Their resonances typically lie in the GHz - THz range, corresponding to the same μeV - meV energy scale characteristic of many quantum effects in the materials they electrically control. This raises the possibility that built-in cavity modes could be relevant for shaping the low-energy physics of vdW heterostructures. However, capturing this light-matter interaction remains elusive as devices are significantly smaller than the diffraction limit at these wavelengths, hindering far-field spectroscopic tools. Here, we report on the sub-wavelength cavity electrodynamics of graphene embedded in a vdW heterostructure plasmonic microcavity. Using on-chip THz spectroscopy, we observed spectral weight transfer and an avoided crossing between the graphite cavity and graphene plasmon modes as the graphene carrier density was tuned, revealing their ultrastrong coupling. Our findings show that intrinsic cavity modes of metallic gates can sense and manipulate the low-energy electrodynamics of vdW heterostructures. This opens a pathway for deeper understanding of emergent phases in these materials and new functionality through cavity control.

11:30am **NS-TuM-15 Dynamical Control of Tip-Induced Light-Matter Interactions at the Surface of Quantum Materials**, ***Kyoung-Duck Park***, Pohang University of Science and Technology (POSTECH), Republic of Korea **INVITED**

Structure, function, dynamics, and interactions are fundamental concepts for understanding physical systems in nature. Among them, light-matter interactions have been a central subject of modern optics and condensed matter physics. However, conventional optical approaches have largely been limited to the classical regime at the microscale because of the diffraction limit. Recent advances in plasmonic nanocavities and tip-enhanced nano-spectroscopy have opened new opportunities to induce and probe light-matter interactions at the nanoscale. Nevertheless, these two approaches have mostly developed independently: plasmonic nanocavities can strongly enhance optical fields but lack spatially resolved spectroscopic access, while tip-enhanced nano-spectroscopy provides nanoscale optical information but has rarely been used as an active platform to dynamically control light-matter interactions. In this talk, I will introduce the concept of tip-enhanced cavity-spectroscopy (TECS) as a unique approach to induce, probe, and dynamically control tip-induced light-matter interactions at the surface of quantum materials. By using a plasmonic tip as a movable and tunable nanocavity, TECS enables nanoscale access to strong and ultrastrong light-matter interactions, including regimes where quantum tunneling and cavity-induced modification become important. This platform allows the optical, mechanical, polarization, and electrical degrees of freedom of the tip-sample junction to be actively controlled in real time. I will further discuss several emerging directions enabled by this concept. First, we exploit the extremely high local pressure generated by a nanoscale tip, reaching the GPa scale, to directly modify lattice structures and electronic properties at material surfaces. Second, we demonstrate dynamic control of near-field polarization by incorporating adaptive optics into near-field spectroscopy. Third, we develop conductive TECS, in which electrical current is directly introduced through the cavity junction to control local electronic and optical responses. These advances establish tip-induced light-matter interactions as an active and dynamically controllable platform for nanoscale spectroscopy, imaging, and quantum-material manipulation.

12:00pm **NS-TuM-17 Magneto – THz Correlated Electronic Behavior at the Nanoscale Through Scanning Near-Field Optical Microscopy**, ***Samuel Haeuser***, Iowa State University*; Richard H.J. Kim,* Ames National Laboratory*; Randall K. Chan,* Iowa State University*; Joong-Mok Park, Thomas Koschny,* Ames National Laboratory*; Jigang Wang,* Iowa State University

Probing real space magnetic responses at terahertz (THz) scales is challenging but highly desired, as the local responses are less affected by the topologically trivial inhomogeneity that is ubiquitous in spatially averaged measurements. We explore a variety of material sets that contain strong electronic correlation behaviors at the nanoscale. Inherent properties of materials directly provide us with a playground of electrons but generally require special circumstances to manifest coherently. For example, $ZrTe_5$ hosts topologically protected helical edge states localized to atomically sharp boundaries, where magnetic fields can tune preferred electrical channels. $Pr_{(1-x)}Ca_xMnO_3$ hosts the colossal magnetoresistance transition from an insulator to a metal that has long been described to originate as nanoscopic phase transition on the order of the crystal lattice itself, also tuned by the combination temperature and magnetic field. Both systems are not guaranteed to remain under high energy excitations that may break such states. Thus, to probe the nanoscale electron correlated phenomena we apply a custom-built cryogenic magneto-THz/infrared scattering-type scanning near-field optical microscopy (cm-sSNOM) platform. We resolve the nanoscale, THz spectroscopic evolution of the magnetic field-driven colossal magnetoresistance transition [1] and magnetic brightening of helical edge states in quantum spin Hall transport [2].

[1] S. Haeuser, et al., "Terahertz-nanoscale visualization of the microscopic spin-charge architecture of colossal magnetoresistive switching" arXiv:2603.07941

[2]S. Haeuser, et al., "Magnetic Brightening and Nanoscale Imaging of Spin-Polarized Helical Edge Modes," **Nature Nanotechnology**, in press (2026) arXiv:2605.04883

Plasma Science and Technology
Room 315 - Session PS1-TuM

High Aspect Ratio and Cryogenic Etching I

Moderators: Prof. Kenji Ishikawa, Nagoya University, Japan, **Dr. Eric Miller**, IBM

8:00am **PS1-TuM-1 Challenges in Etching High Aspect Ratio Patterns for Memory Devices**, *Seokhyun Lim, Wonbong Jung, In-Joong Kim, JungHwan Um,* ***Sung-Il Cho,*** Samsung Electronics Co., Republic of Korea **INVITED**

Since the first V-NAND was introduced in 2013, high aspect ratio contact(HARC) etching has become the most critical technology for developing 3D devices. As aspect ratio of vertical patterns increases, both profile fidelity and throughput become more demanding. Consequently, the etch-rate reduction known as aspect ratio dependent etching(ARDE) must be overcome first, and traditional development has focused on raising ion energy to meet this requirement. Recently, however, the requirement to minimize local variations, such as distorted patterns and abnormal critical dimensions, has grown substantially. For example, non-circular patterns in vertical-channel structures induce abnormal operation because of undesirable electric field distributions. This deformation is mainly caused by non-uniform polymer deposition and bent ion trajectories, which has led the semiconductor industry to adopt precise waveform control and polymer management technologies. Increasing ion energy, meanwhile, narrows the arcing margin of the equipment and raises charge-up damage concerns. The recently intorduced cryogenic etching can mitigate these problems associated with high bias power, but it brings its own set of requirements. At present, industrial cryogenic etching is limited to etch SiO2 and SiN selective to organic hardmasks. Therefore, a broader range of chemistries and plasma conditions should be exploited for various applications. In this presentation we will outline the various technical obstacles that arise in HARC etching and propose development directions to address them.

8:30am **PS1-TuM-3 High-Aspect-Ratio Carbon Hard-Mask Etch Using High-Density Plasma and a Novel Additive Gas Chemistry**, ***Koki Mukaiyama,*** *Shuji Funada, Ryusuke Seino, Maju Tomura, Yoshihide Kihara,* Tokyo Electron Miyagi Limited, Japan

In 3D NAND flash memory manufacturing, carbon is commonly used as a hard mask for channel-hole etching. As the number of stacked memory cells increases, the carbon mask must be made thicker, necessitating high-aspect-ratio (HAR) etching. Current carbon-mask etch processes employ oxygen with a sulfur-containing additive using high-density inductively coupled plasma (ICP) with high applied bias. Because sulfur-based sidewall protection becomes insufficient at high aspect ratios, process conditions that narrow the mask openings are often adopted to prevent enlargement of the critical dimensions (CDs). However, this narrowing restricts radical transport to the feature bottom, substantially reducing the etch rate in HAR regions. To address this issue, we focused on additive gas chemistry. Since the discovery of sulfur-containing additive gases [1,2], no additive gas that outperforms them has been reported. In this study, we introduced a novel additive gas (hereinafter referred to as “Gas A”) into oxygen plasma and evaluated its effects on etching characteristics. We found that Gas A reacts with carbon to form a passivation layer on the sidewalls even at high aspect ratios, yielding smaller hole CDs than those obtained with sulfur-based protection. In addition, Gas A removes deposits from the mask openings and suppresses CD narrowing at the openings during etch progression, while leaving the mask itself intact. Because fewer reactive species are consumed at the sidewalls and the mask openings remain larger, more radicals and ions can reach the HAR regions. As a result, the etch rate is enhanced while hole CDs are reduced. Furthermore, combining Gas A with sulfur-containing gases results in additional etch-rate enhancement and CD reduction. Using Gas A enables HAR etching of carbon masks thicker than 4 μm with feature diameters of approximately 100 nm.

[1] M. Pons *et al*., Jpn. J. Appl. Phys. 33 (1994).

[2] J. K. Kim *et al*., J. Vac. Sci. Technol. A 31 (2013).

8:45am **PS1-TuM-4 Passivation-less Etching in Cryogenic Regime**, ***Hiroto Ohtake,*** *Radhe Agarwal, Alvaro Garcia, Tina Dhekial-Phukan,* Applied Materials Inc.*; Han Luo,* Applied Materials Inc., Canada*; Jeong Hwan Kim, Teris Liu,* Applied Materials Inc.

As semiconductor devices continue scaling, feature dimensions have become increasingly narrow. These trends impose requirements on highly anisotropic etching in confined spaces. Conventionally, vertical etch profiles are achieved with passivation gases, such as oxidizing species, fluorocarbons, or oxygen halogenides, to suppress lateral etching of silicon. However, excessive passivation gas addition is causing etch stop or top clogging. Therefore, reducing or eliminating passivation gases is highly desirable.

Cryogenic etching technology might offer a promising path for passivation-less anisotropic etching. At cryogenic substrate temperatures, physisorption of reactive species is enhanced, while spontaneous chemical reactions are suppressed. As a result, a higher concentration of radicals can be delivered effectively to the etch front without excessive lateral attack. But high pressure and high source power impact the sidewall etch even at cryogenic temperature.

In this study, plasma operation at low pressure (0.5 mTorr) and low RF power (50 W) with cryogenic substrate temperature was stabilized in a 300 mm diameter etching chamber through optimization of the coil and top structure. To validate the concept, carbon etching was employed as a model. Under low-pressure and low-power conditions, the ion-to-radical flux ratio increases, enabling directional etching even in a pure oxygen plasma without passivation additives. By lowering the substrate temperature from −40 °C to −90 °C, the ratio of vertical to lateral carbon etch rates improved substantially from 2.8 to 7.2. This indicates that spontaneous reactions are significantly reduced at cryogenic temperatures, allowing the formation of anisotropic profiles with reducing the use of passivation gases. The anisotropy was also found to be sensitive to process pressure. At −90 °C, the vertical-to-lateral etch rate ratio decreased to 3.7 when the pressure was increased to 10 mTorr. Plasma simulations indicate that lower pressures yield a higher ion-to-radical ratio, which directly contributes to enhanced anisotropy.

In conclusion, cryogenic etching under low-pressure and low-power conditions might be a promising approach for next-generation semiconductor etching, enabling highly anisotropic profiles with less passivation chemistries.

9:00am **PS1-TuM-5 The Evolution of CVD-C Mask Profile During High-Aspect-Ratio Hole Etching**, ***Mitsuhiro Omura,*** *Li Wu, Junichi Hashimoto, Chihiro Sakamoto, Chihiro Abe, Yuta Manabe, Hirotaka Tsuda, Toshiyuki Sasaki,* KIOXIA, Japan

The advent of AI has increased the importance of semiconductor devices in modern technology. New generations of 3D flash memory have joined logic devices and DRAM as key components enabling this new era. To meet the increasing bit density demand, flash devices incorporate an ever-increasing number of word lines. These, in turn, complicate the dry etching of memory holes, which form the space for channels and functional thin films. This high-aspect-ratio memory hole etching process requires precise profile control, with challenges such as low mask selectivity, necking, clogging, bowing, striation, hole bottom distortion, etc[1].

Here, we focus on the issue of mask sidewall encroachment known as ‘necking’. The mechanism behind this effect has been simulated by considering polymer deposition from neutrals and ion sputtering using a vertical cross section perspective [2]. In this analysis, we turn our attention to the neck shape revealed in the less understood horizontal cross section. We began by etching a typical SiO/SiN film stack in a fluorocarbon-mixed gas plasma. The test structure also contained a CVD-deposited carbon (CVD-C) hard-mask with a dense hole pattern. We then observed the neck shape on the CVD-C mask in a horizontal cross section for two types of hole patterns in equilateral and isosceles triangle arrangements. Distortion in the isosceles triangles far exceeded that shown in the equilateral triangles despite identical processing conditions. By observing the evolution of mask surface morphology, we find that early local mask erosion at the narrower hole-to-hole spaces in the isosceles triangle arrangement eventually leads to significant variation in the mask height remaining. This variation might lead to neck profile variation such as height, width, and taper angle in a vertical cross section. We speculate that variation in the remaining height of the CVD-C mask could lead to inconsistent neck profiles which manifest in the horizontal cross sections as hole distortion.

References

[1] G. S. Oehrlein et al., J. Vac. Sci. Technol. B 42(4), 041501 (2024).

[2] D. Kim et al., Thin Solid Films 515, 4874 (2007).

9:15am **PS1-TuM-6 ASSD Student Award Finalist Talk: Plasma Chemistry and Cryogenic Control of Etching, Passivation, and Surface Modification in Hydrogenated Amorphous Carbon Thin Films**, ***Jhonatan Gil Romero,*** *Kenneth Lathrum, Seonhee Jang,* University of Louisiana

Hydrogenated amorphous carbon (a-C:H) is used as a hard-mask material for semiconductor patterning, which requires a precise balance between

etch rate, passivation, surface roughness, wettability, optical response and oxide/a-C:H selectivity. This work maps how plasma chemistry, cryogenic temperatures, inductively coupled plasma (ICP) and radio frequency (RF) power in the etching process tune these coupled responses.

a-C:H films were deposited on Si (100) by plasma-enhanced chemical vapor deposition (PECVD) using a cyclohexane precursor at room temperature. They were processed in an inductively coupled plasma deep reactive ion etching (ICP-DRIE) system under RF-only or ICP+RF power modes. Four primary fluorine gases (SF_6, CF_4, CHF_3, and C_4F_8) and three secondary gases (O_2, Ar, and N_2) were evaluated across temperatures between -120 and 20 °C and pressures between 3.333 and 9.999 Pa. Film thickness and optical constants were measured by ellipsometry, surface morphology and roughness by atomic force microscopy (AFM), and wettability by a contact-angle goniometer. Tetraethyl orthosilicate (TEOS) oxide was used to determine TEOS/a-C etch selectivity, calculated when both films had positive net etch rates.

Under fixed ICP+RF power, gas chemistry controlled the transition between film removal and passivation. Oxygen (O_2) containing mixtures yielded the highest etch rates, led by CF_4+O_2 at median 2.43 nm/s versus 1.03 nm/s for CF_4. Fluorocarbon-rich chemistries suppressed etching or promoted net film growth: CF_4+CHF_3 yielded the lowest median etch rate at 0.10 nm/s, while C_4F_8 and CF_4+C_4F_8 showed median growth rates of 1.12 and 0.562 nm/s. Cryogenic conditions (-30 to -120 °C) increased median passivation growth relative to 20 °C by 84% for CF_4+C_4F_8. Under ICP+RF, C_4F_8 passivation also increased root mean square (RMS) roughness by 140%, relative to CF_4 at 0.1834 nm. Passivation further increased hydrophobicity, with median change in contact angle (ΔCA) up to +6.94°. In contrast, O_2-assisted etching produced hydrophilic surfaces, with median ΔCA reaching -33.1° for RF-only CF_4+O_2. The highest selectivity value was 2.740 for CF_4+CHF_3 under ICP+RF. ICP+RF power enhanced a-C:H removal in 13/16 paired (RF-only) comparisons; lowering pressure increased ICP+RF etch rate but reduced selectivity by 28%. Optically, passivation increased the final extinction coefficient by 33.5%, and CF_4+O_2 etching by 67.6% relative to CF_4.

These results define the process windows for O_2-assisted a-C:H removal, fluorocarbon passivation, and pressure/power tradeoffs, providing a framework for balancing TEOS/a-C selectivity, surface properties, and optical response in advanced patterning.

9:30am **PS1-TuM-7 Characterizing Spontaneous Etching of Si_3N_4 Sidewalls in Ar/Fluorinated Precursor Plasmas Using a Small-Gap Structure: Role of Precursor and Substrate Temperature**, ***Md Intaqer Arafat,*** University of Maryland College Park*; Pierre Ricou, Behnaz Ghaffari, Jessica DeMott,* Arkema Inc*; Gottlieb S. Oehrlein,* University of Maryland College Park

High-aspect-ratio (HAR) etching of ONO stacks for 3D–NAND is challenging due to profile defects and non-uniform selectivity; fluorinated precursors control etch and passivation, but the underlying plasma–surface mechanisms remain unclear. This study investigates a series of $C_2H_{5-x}F_{1+x}$ precursor candidates in low-pressure plasma, focusing on their deposition behavior and impact on isotropic etching (sidewall) of HAR structures. Key parameters include hydrofluorocarbon (HFC) film deposition rate, film properties, etch rate, and the degree of sidewall etching of silicon nitride (Si_3N_4), all evaluated as functions of precursor composition. To mimic HAR conditions, horizontal trench structures with aspect ratios (AR) up to 30 were used to examine the role of neutral radicals generated from $C_2H_{5-x}F_{1+x}$ plasmas. Nitride trenches were processed by inductively coupled plasma, with spatial analysis via ex situ ellipsometry and real-time ellipsometry on blanket films. Findings reveal systematic variations in the film deposition rate, refractive index, and sidewall etching behavior, with notable changes in spontaneous etching of Si_3N_4 observed for different $C_2H_{5-x}F_{1+x}$ precursors. Increasing fluorine content within the C_2 precursor family enhances deposition rates and reduces refractive index. At the same time, spontaneous etching of Si_3N_4 becomes more pronounced, particularly near trench entrances. For fluorine-rich precursors with H/F < 1, this etching extends further into HAR features, suggesting deeper penetration of reactive species. Experiments were conducted at substrate temperatures of 10 °C and –45 °C to examine sidewall etching. Lowering the substrate temperature from 10 °C to −45 °C significantly reduces Si_3N_4 sidewall etching. This reduction is accompanied by decreases in both HFC deposition rate and refractive index compared to 10 °C, indicating modified film growth characteristics. Additionally, operation at −45 °C limits the penetration of fluorine and carbon species into HAR structures and reduces the formation of fluorinated nitride. These results suggest viable strategies in which the chemical characteristics of the precursor are leveraged to control the balance between protective passivation and chemical removal on vertical surfaces during HAR etching, enabling improved precision in etching processes.

This material is based upon work supported by Arkema, USA.

9:45am **PS1-TuM-8 Effect of Substrate Temperature on Neutral Species Transport in High-Aspect-Ratio Holes During Plasma Etching** , ***Yusuke Imai,*** *Takayoshi Tsutsumi, Sekine Makoto, Kenichi Inoue, Kenji Ishikawa,* Nagoya University, Japan

The continued scaling and three-dimensional integration of semiconductor devices have significantly increased the complexity of plasma etching processes. In advanced device fabrication, such as high-aspect-ratio (HAR) patterning for 3D NAND structures, highly anisotropic and precisely controlled etching is required. Substrate temperature is one of the key parameters governing etching characteristics and is carefully controlled during the etching process. Recently, it has been reported that lowering the substrate temperature enables faster and deeper etching in HAR processing for 3D NAND fabrication compared with conventional processes. [1] Substrate temperature is considered to play an important role not only in surface reactions during etching but also in neutral species transport [2]; however, its influence has not yet been fully understood.

In this study, we investigated the effect of substrate temperature on neutral species transport in HAR holes using a quadrupole mass spectrometer (QMS). A cylindrical orifice mimicking a HAR hole was installed at the inlet of the QMS, enabling aspect-ratio-resolved mass spectrometry (ARMS). In addition, a temperature-controlled assembly was mounted around the orifice to control the orifice temperature during measurements. Neutral species transport through the HAR hole was investigated while varying the orifice temperature. The experiments were performed using a capacitively coupled plasma (CCP) reactor. RF power at 13.56 MHz was applied to the upper electrode, while argon and fluorocarbon gases were introduced into the reactor, where the pressure was maintained at 2 Pa.

As the orifice temperature decreased, the measured Ar intensity increased. This behavior is considered to originate from a reduction in the local gas temperature near the cooled structure, resulting in an increase in neutral gas density and flux into the orifice. These results suggest that low-temperature conditions during plasma etching may enhance the neutral species flux entering HAR features.

[1] R. Suda et al., J. Vac. Sci. Technol. B 43, 062210 (2025).[2] T. Lill et al., J. Vac. Sci. Technol. A 41, 023005 (2023).

Plasma Science and Technology
Room 315 - Session PS2-TuM

High Aspect Ratio and Cryogenic Etching II

Moderators: Dr. Hisataka Hayashi, Daikin Industries, Ltd., **Dr. Pingshan Luan**, TEL Technology Center America

11:00am **PS2-TuM-13 Plasma-Material Interactions in Cryogenic Hydrogen-Fluoride Plasma Etching**, ***Shih-Nan Hsiao,*** *Yusuke Imai, Makoto Sekine,* Nagoya University, Japan*; Ryutaro Suda, Yoshihide Kihara,* Tokyo Electron Miyagi Limited, Japan*; Masaru Hori,* Nagoya University, Japan **INVITED**

For more than half a century, reactive ion etching (RIE) has served as a cornerstone of semiconductor manufacturing, facilitating the high-throughput production of silicon wafers. Its success is fundamentally rooted in the ion-neutral synergy—the collaborative interaction between reactive chemical species and high-energy ions—which has been pivotal to the evolution of microelectronics [1]. However, as device architectures transition toward sub-nanometer scales and complex high-aspect-ratio (HAR) 3D structures, conventional RIE processes encounter significant physical and chemical bottlenecks. Specifically, the degradation of traditional ion-chemical synergy in these advanced regimes often leads to diminished etching efficiency and reduced production yields. To address these limitations, cryogenic plasma etching utilizing hydrogen fluoride (HF)-based chemistries has emerged as a sophisticated alternative [2]. This approach exploits a distinct interplay between incident ions, physisorbed surface layers, and the substrate. Despite its potential, the underlying etching mechanisms of cryogenic HF plasma remain partially obscured [3-5]. In this work, we elucidate the plasma-material interactions during the cryogenic etching of dielectric materials. By employing in-situ diagnostics, including spectroscopic ellipsometry and attenuated total reflectance Fourier transform infrared spectroscopy (ATR-FTIR), we systematically characterize the influence of bias voltage, substrate temperature, and HF

partial pressure on the etching behavior of SiO_2 and SiN. Based on our findings, we propose a comprehensive mechanistic framework for dielectric etching in cryogenic HF plasmas. Furthermore, we extend this discussion to the synergistic interactions governing plasma-assisted atomic layer processes using HF chemistries for nanofabrication.

References

[1] J. W. Coburn and H. F. Winters, J. Appl. Phys. 50, 3189 (1979)

[2] Y. Kihara et al., VLSI symposium T3-2 (2023).

[3] S. N. Hsiao et al., Small Methods, 8, 2400090 (2024).

[4] S. N. Hsiao et al., Chem. Eng. J., 522, 167517 (2025)

[5] S. N. Hsiao et al., Small Methods, 10, e01744 (2026).

11:30am **PS2-TuM-15 Investigation of Surface Reactions of SiO_2 and SiN Films Under Cryogenic Etching Process via in-Line/Situ Analysis***, **Hiroyuki Fukumizu,*** Kioxia Corporation, Japan **INVITED**

This study explores cryogenic etching processes for SiO_2 and SiN films, which are essential for high aspect ratio hole etching in 3D Flash Memory. The blanket SiO_2 films were etched by $H_2/F_2/Ar$ gas mixture plasma over a temperature range from 25 to −200 °C, examining the mechanisms involved in cryogenic conditions via in-situ FT-IR analysis. The etch rate at −100 °C is about 3.2 times higher than at 25 °C due to co-adsorption of H_2O and HF. However, below −100 °C, the solidification of H_2O decreases etching efficiency. In addition to SiO_2, the study addresses the etching behavior of SiN films, where cryogenic etching using HF/PF_3 gas mixtures was investigated. To clarify the factors influencing SiN etch rates, we employed a plasma beam irradiation apparatus equipped with low-temperature in-line XPS analysis to examine surface reactions in detail. Additionally, findings show that the ammonium salt NH_4F forms on the SiN surface under cryogenic conditions, enhancing etch rates. The introduction of PF_3 promotes the formation of NH_4PF_6, which can be decomposed by energetic ion irradiation to further boost etching efficiency. These insights contribute significantly to optimizing cryogenic etching processes.

12:00pm **PS2-TuM-17 Dynamics of Charge Conduction in Water Layers Formed During Cryogenic Etching of HAR SiO_2 Features***, **Chenyao Huang,** Yeon Geun Yook, Yifan Gui,* University of Michigan*; Steven Shannon,* North Carolina State University*; Mark J. Kushner,* University of Michigan

During the fluorocarbon plasma etching of dielectric materials, differential charging within features arises from the disparity between the arrival onto the wafer of energetic ions with narrow angular spread and low-energy electrons with broad angular distributions. The resulting intra-feature electric fields can deflect particle trajectories, leading to defect formation and reduced etch rates. Cryogenic plasma etching (CPE) is being investigated as an alternative due to its high etch rate and attractive sidewall profile control for high aspect ratio (HAR) features. During cryogenic etching of dielectrics using HF containing gas mixtures, water layers containing solvated HF form along the feature sidewalls in addition to charge deposition from incident charged particle fluxes. These liquid layers may have significant conductivity due to the ionic solute concentrations (e.g., H_3O^+ and F- when solvating HF in water). This conductivity can alter the potential distributions within the feature by conducting externally deposited charges and facilitating self-polarization.

In this work, we computationally investigated charging dynamics including conductive layers for pre-formed SiO_2 features, and during plasma etching of HAR SiO_2 features using Ar/HF gas mixtures in multi-frequency capacitively coupled plasmas. Feature evolution is modeled and using the 3D voxel-based Monte Carlo Feature Profile Model (MCFPM). Fluxes and energy angular distributions (EADs) of incident species are produced by the reactor-scale Hybrid Plasma Equipment Model (HPEM). The MCFPM samples incident fluxes to statistically launch pseudoparticles representing charged and neutral species, which are tracked until they interact with solid materials. We have developed and integrated modules into the MCFPM to account for charge conduction and redistribution within conductive water layers during etching. Our results indicate that these highly conductive, thin layers transform local maxima of electric potential into a broadened profile with lower peak potentials within the features. During SiO_2 etching, the water layer counteracts externally deposited charges through the redistribution of external and intrinsic charges, resulting in a reduced electric potential that correlates inversely with the intrinsic charge densities represented by the dissolved ions.

This work was supported by the Department of Energy Office of Fusion Energy Sciences (DE-SC0024545) and Samsung Electronics.

Quantum Science and Technology
Room 304 - Session QS-TuM

Quantum Sensing, Simulation, and Emerging Quantum Applications

Moderators: Dr. Suman Bhaumik, TEL Technology Center, America, LLC, **Dr. Walid Redjem**, University at Albany State University of New York, **Dr. Simon Seymour**, UIUC

8:00am **QS-TuM-1 Opportunities for Quantum Sensing and Computing for Energy and Infrastructure Security Applications***, **Hari P. Paudel,** Yuhua Duan,* National Energy Technology Laboratory **INVITED**

Quantum information science (QIS) harnesses quantum mechanics to solve problems that are beyond the reach of traditional methods and devices. The rapid advances of quantum sensing and computing are creating promising pathways to improve energy production, distribution, and consumption, and minimizing security challenges. However, applying emerging technologies in quantum information science to real-world systems remains challenging. The National Energy Technology (NETL) is actively leveraging both experimental and computational tools to strengthen the nation's energy and security competitiveness.

This presentation will highlight recent advances in quantum sensing for energy and infrastructure security applications. Examples of mineral detection and exploration will be discussed, and possibilities for the deployment of quantum tools will be examined. The presentation will also showcase opportunities for materials chemistry and complex optimization problems in areas such as energy storage, fluid dynamics, and grid operations. This presentation will review quantum simulations of ground state and vibrational properties of small molecules, benchmarking current algorithms against qubit counts, basis sizes, and memory demands. The presentation will conclude by identifying high-value application pathways for addressing major challenges in the energy sector.

8:30am **QS-TuM-3 Can NISQ-era Quantum Computing drive the design of new DFT Functionals?***, **Simon Seymour**, Andre Schleife,* University of Illinois, Urbana-Champaign

This work aims at comparing the epistemic uncertainty stemming from the lack of knowledge on the universal functional to the various uncertainty sources inherent to NISQ era quantum computing (QC). Three variational quantum subroutines with varying degrees of Quantum ErrorMitigations are implemented to estimate the total energies of quantum chemistry systems. Notably, one of the subroutines is novel and uses a Riemannian preconditioned Crank-Nicolson Markov Chain Monte-Carlo solver to infer the 2-Reduced Density Matrix (2RDM) of chemistry systems from sparse shadow tomography data. This construction was motivated to bypass both the limited quantum computational resources as well as to improve the scaling of previous 2RDM solvers based on Semi-Definite Programming. Finally, a dual Bayesian-Bootstrapping framework is established to identify the relevant sources of uncertainty within the QC workflow. This will help find strategies for improving QC performance and further the development of 2RDM tomography whose data we hope can eventually be used in the training stage of new Exchange-Correlation functionals.

8:45am **QS-TuM-4 Linearly Uncoupled Silicon Photonic Cavities for Quantum State Generation***, **Prabha Prasad Nair,*** University at Albany-SUNY

Quantum sensing leverages quantum mechanical resources to surpass classical limits of measurement precision. A key pathway is the use of squeezed states of light, which suppress quantum noise below the shot-noise limit and enable enhanced sensitivity in low-signal environments. In this work, we investigate the integration of squeezed light within silicon photonic circuits as a scalable platform for quantum-enhanced sensing. By embedding nonlinear optical processes into CMOS-compatible waveguides, we outline strategies for the on-chip generation and manipulation of squeezed states. To address the challenges associated with state-of-the-art squeezed-state generation, we propose a novel architecture consisting of two ring resonator cavities coupled through a Mach–Zehnder interferometer, enabling enhanced stability and control.

In addition to their applications in sensing, squeezed states play a crucial role in continuous-variable (CV) quantum information processing, underpinning protocols for universal quantum computation, quantum teleportation, quantum error correction, quantum secret sharing, and quantum key distribution. By combining compact nonlinear waveguides, interferometric architectures, and low-loss photonic integration, this work establishes a pathway toward fully integrated quantum sensors with sub-

shot-noise performance, while simultaneously contributing to the broader development of scalable CV quantum technologies.

Our theoretical modeling and circuit-level simulations demonstrate the potential for significant noise reduction and improved detection sensitivity across applications such as biosensing, navigation, and precision metrology. This work lays the foundation for the experimental realization of integrated squeezed-light sources, advancing the development of compact, high-performance quantum sensors for real-world applications.

9:00am **QS-TuM-5 High Precision Fiber-Integrated Micro-Optics for Quantum Photonic Interfaces***, **Raman Kumar**, Sebastian Will,* Brookhaven National Laboratory

Scalable quantum photonic technologies require efficient light matter interfaces that are compact, alignment stable, and compatible with optical fiber infrastructure. Here, we report the nanofabrication of high precision micro-optical elements directly on the end facets of single mode fibers. Our approach is based on focused ion beam nano-machining, enabling a new class of fiber integrated quantum photonic components. We fabricate and characterize multiple classes of fiber-integrated optics, including micro-concave and micro-convex spherical elements, spiral phase plates, and axicons, using focused-ion beam (FIB) to define three-dimensional optical profiles directly on the fiber core [1].

Precise alignment to the guided optical mode is achieved by selectively etching the fiber facet, which reveals the doped core as an alignment marker before FIB machining. Atomic force microscopy shows that the spherical surfaces achieve subwavelength form accuracy. Surface roughness analysis further shows no measurable degradation after optimized FIB processing, with roughness remaining in the sub nanometer range establishing quantum grade optical performance.

Optical characterization with visible laser illumination confirms the intended functionality of the fabricated elements. Axial imaging demonstrates fiber-integrated focusing from spherical micro-optics with radii of curvature in the range of hundreds of microns, while Mach-Zehnder interferometry verifies the azimuthal and radial phase structures generated by spiral and axicon fibers, respectively. The resulting far field patterns and interferometric signatures confirm deterministic phase control.

These results establish FIB-fabricated fiber micro-optics as a compact, alignment free, and quantum-grade platform for quantum photonic interfaces, with applications in fiber coupled atom cavity QED, and structured light generation for high dimensional quantum information processing.

References:

[1] Kumar, R., & Will, S., “High precision micro-optical elements on fiber facets via focused-ion beam machining.” *arXiv:2604.18426* (2026).

9:15am **QS-TuM-6 The Role of QED-C in Growing the Quantum Industry***, **Sebastian Engelmann**,* QEDC, United States Minor Outlying Islands (the)

The Quantum Industry has gathered lots of interest and is on track to surpass 3B market size by 2028. While many advances in the scientific community are highlighted, commercial success is still not a given.

In the US, an Industry led consortium called QED-C has formed, which collects input from industry, academia and Government agencies. I will introducte QED-C, its mission and services to its members. In particular I will showcase the emerging Technologies TAC (technical advisory committee) and our recent activites.

In this talk I would like to highlight the items that are important for community, specifically what QED-C is doing in regards to testbeds, standards and foundry pathways.

9:30am **QS-TuM-7 Rejuvenating Photonic Quantum Sensing by Replacing Traditional Beamsplitters with Higher-Dimensional Gauge-Invariant Multiports***, **Alexander Sergienko,*** Boston University **INVITED**

Photonics quantum sensors are among the central areas of quantum technologies. The optical Michelson or Mach-Zehnder interferometers are core elements of many photonics sensors. Introducing entangled and noise-squeezed quantum states in such interferometers boosts their sensitivity and resolution beyond classical limits. The original resolution of all conventional Michelson or Mach-Zehnder interferometers is limited by the maximum attainable slope of the intensity interference pattern as a function of the phase shift. The (cos^2) shape of all existing interferograms is determined by the physical properties of the optical beamsplitter - a traditional device that introduces an optical superposition and governs the operation of many known optical devices.

We introduced a novel concept of higher-dimensional gauge-invariant multiports. The directionally unbiased four-port Grover coin can be considered a higher-dimensional generalization of beam splitters, in which inputs to the four available ports have equal probability of exiting any of the four ports, including back reflection. *This offers direct access to a greater number of degrees of freedom* [1] (Fig.1).

We demonstrated that traditional interferometers acquire novel features and offer a dramatically ***enhanced resolution in phase measurement when directionally unbiased Grover multi-ports replace traditional beam splitters*** (Fig. 2). We demonstrated experimentally that the Grover-based counterpart of the conventional Michelson interferometer can substantially improve the phase measurement resolution due to a new feature of increasing the intensity-phase slope by 10X÷20X times instead of a traditional (cos^2) profile limited to 1 (Fig. 3). This converts any Michelson or Mach-Zehnder interferometer into a super-resolution sensor [2,3].

This novel approach dramatically elevates the baseline for optical interferometric measurements, even before quantum states of light are involved, thereby rejuvenating the field of high-resolution sensing. The introduction of quantum light (such as entangled or squeezed states) into new Grover-Mach-Zehnder or Grover-Michelson interferometers will increase the photonic measurement resolution even further.

[1] C. R. Schwarze, A. D. Manni, David S. Simon, A. Ndao, and A. V. Sergienko ''Next-Generation Interferometry with Gauge-Invariant Linear Optical Scatterers, '' Metrology, **v. 5**, 5040065 (2025).

[2] C. R. Schwarze, D. S. Simon, and A. V. Sergienko, Phys. Rev. A 106, 052615 (2023).

[3] C. R. Schwarze, D. S. Simon, A. D. Manni, A. Ndao, and A. V. Sergienko, ''Experimental demonstration of a Grover-Michelson interferometer'', Optics Express, v.32, p. 34116-34127 (2024).

Surface Science
Room 305 - Session SS-TuM
Dynamics

Moderators: Sara Mason, Brookhaven National Laboratory, **Dr. Zbynek Novotny**, Pacific Northwest National Laboratory

8:00am **SS-TuM-1 Hyperthermal Atomic-Oxygen Scattering Dynamics on Representative Satellite Surfaces***, **Timothy Minton**, Pedro Jorge,* University of Colorado Boulder **INVITED**

There is intense interest in the utilization of very low Earth orbit (VLEO, 100 – 350 km in altitude); a few missions in this region have been flown and more are planned. Despite the advantages of VLEO satellite operation (e.g., enhanced image resolution, faster data transfer rates, reduced development and launch costs, and straightforward demise scenarios), VLEO altitudes have long been avoided because of the high density and harsh oxidizing environment of the residual atmosphere. VLEO environments contain predominantly oxygen atoms and nitrogen molecules, which collide with ram surfaces on spacecraft at relative velocities of ~7.5 km s^{-1}. Momentum exchange between these atmospheric atoms/molecules and satellite surfaces results in an aerodynamic drag force on the vehicle. For VLEO operation, the drag is significant enough to require propulsion to counteract drag and maintain orbit, resulting in increased energy and also size (typically from solar panels and propellant storage) to operate the propulsion system. Increased size results in increased drag forces and the need for more energy and propellant, creating a vicious cycle. Beyond the clear necessity of minimizing drag for feasible flight in VLEO, the quantification of drag allows for orbital path determination and collision avoidance. Thus, minimizing and predicting drag are crucial for proliferated VLEO operation.

We have conducted molecular beam-surface scattering experiments with O atoms, traveling at orbital velocities of ~8 km s^{-1}, to investigate their inelastic scattering dynamics on several realistic and ideal material surfaces as a function of both polar (q) and azimuthal (f) scattering angles. The velocity and angular distributions of scattered O atoms depend strongly on the incident angle of the impinging atoms and the roughness of the surface in ways that are not *a priori* predictable. Using on the scattering dynamics data, a new gas-surface scattering model has been formulated, based on a washboard approach which uses a gamma function roughness model and a coupled Cercignani-Lampis (CL) model to describe the local atom-surface scattering dynamics. When parametrized to give the optimum fit to the molecular beam-surface scattering data, the model may be used for the

determination of overall energy and momentum accommodation and for simulations of satellite drag.

8:30am **SS-TuM-3 Beyond the Binary Collision Approximation: Approximate Modeling of Low-Energy Impingement Events Using Classical Molecular Dynamics**, ***Carson Mize***, *Jörg Meyer,* Leiden University, Netherlands

Since their development in the 1970s, Binary Collision Approximation (BCA) models are widely applied tools to help validate ion and atom implantation processes on materials, such as deposition, diffusion, and damage in good agreement with experimental data at high incidence energies (> 1 MeV). BCA codes are practical and useful due to their computational efficiency to account for nuclear and electronic contributions to the stopping of the impinging particles, however, the approximations are expected to break down completely within the low energy regime (< 1 keV). Considering recent advances in molecular dynamic (MD) models commonly used in gas-surface dynamics, we aspire to answer the following two questions: 1) Do BCA models have any validity in the low energy regime? 2) Can we develop a classical-MD based model that still is computationally inexpensive for common applications with considerably improved accuracy?

To this end, we focus on bombarding a tungsten surface with low energy hydrogen atoms (5 – 100 eV) as a showcase system due to the availability of an EAM potential designed to model H absorption in W and the associated defects caused by H.[1] While our dynamical models based on a "grand-canonical"-like MD are still a work in progress due to the modeling challenge of accounting for energy dissipation to electrons and phonons, here, we mimic the respective approximations inherent to the BCA to reduce the model comparison into the respective binary and many-body approaches. Our additive MC calculations provide us with high resolution snapshots, allowing us to capture surface evolution effects like implantation and damage, which are typically neglected in BCA models. Additionally, the model establishes a framework for future improvements such as replacing electronic stopping with a more robust electronic friction description or additional ability to describe the evolution of the surface at increasing exposure.

References

[1] D. R. Mason, D. Nguyen-Manh, V. W. Linblad, F. G. Granberg, M. Y. Lavrentiev J. Phys.: Condens. Matter 2023, *35*, 495901.

8:45am **SS-TuM-4 Influence of Subsurface Oxygen on the Energetics of CO Oxidation on Planar and Stepped Rhodium Surfaces**, ***Dan Killelea***, Loyola University Chicago*; Tim Schäfer,* Georg-August Universität, Göttingen, Germany

The ability to obtain velocity distributions of molecules desorbing from surfaces with both high temporal precision and angular resolution provide newfound insight into both the kinetics and the dynamics of recombinative desorption and subsurface emergence.

I will discuss our observations of the influence of subsurface oxygen on CO oxidation on both Rh(111) and Rh(332) and how the velocity distributions of the product CO_2 shifts when O_{sub} is present. I will discuss these observations and their potential impacts in oxidation reactions in heterogeneously catalyzed reactions over transition metal surfaces.

9:00am **SS-TuM-5 Unexpectedly Weak Vibrational Energy Transfer in O_2/Au(111) Collisions**, ***Igor Rahinov***, The Open University of Israel*; Itai Kallos,* Ben Gurion University Be'er Sheva, Israel*; Kerim Benfreha,* University of Goettingen, Germany*; Joshua Baraban,* Ben Gurion Uni. Be'er Sheva, Israel*; Tim Schäfer,* University of Goettingen, Germany*; Alexander Kandratsenka, Alec Wodtke,* Max Planck Institute for Multidisciplinary Sciences, Germany

Vibrationally inelastic scattering of molecules from metal surfaces provides a sensitive probe of electronically nonadiabatic energy transfer accompanying breakdown of the Born–Oppenheimer approximation. Previous studies established an intuitive semi-quantitative framework in which vibrational excitation and relaxation probabilities approximately scale with the energetic accessibility of transient electron transfer between molecule and metal. Within this framework, O_2 has long been an intriguing missing case: because of its high electron affinity, and the relatively small image-charge stabilization energy required for transient-anion-formation-driven vibrational energy transfer upon collision with Au(111), it should be among the strongest electronically nonadiabatic scatterers [1]. Yet this expectation could not be tested directly because effective quantum-state-resolved detection schemes for O_2 were not available.

Here we report quantum-state-resolved measurements of vibrational excitation in O_2(v = 0-->1) scattering from Au(111), enabled by a recently developed REMPI detection scheme for vibrationally excited O_2 [2]. Rotationally resolved detection of scattered O_2(v = 1) was achieved via two-color REMPI through the 3dπ Rydberg states, allowing direct determination of O_2(v = 0 → 1) vibrational excitation probabilities under direct scattering conditions.

Contrary to expectations based on electron affinity/work function considerations and trends established for NO, CO, and HCl scattering from noble metals [1], the measured vibrational excitation probabilities for O2/Au(111) are remarkably low. We discuss a physical picture in which O_2/Au(111) represents a frustrated strong-coupling system: although only modest image-charge stabilization is required to transiently access the anion formation, the repulsive interaction potential prevents the molecule from approaching sufficiently close to the surface for efficient electron-transfer-mediated vibrational energy uptake.

[1] I. Rahinov et al., Phys. Chem. Chem. Phys. 26, 15090 (2024).
[2] I.S. Kallos et al., J. Chem. Phys. 162, 051103 (2025).

9:15am **SS-TuM-6 High Temperature Annealing Dynamics and Surface Recovery of (3x1)-O Nb(100) Elucidated by Helium Atom Scattering**, ***Michael Van Duinen***, University of Chicago*; Cristobal Mendez, Tomas Arias,* Cornell University*; Steven Sibener,* University of Chicago

Superconducting radio frequency (SRF) cavities are the fundamental accelerating components of linear particle accelerators. Niobium is the material of choice for SRF cavities due to its high malleability, thermal conductivity, and superconducting critical temperature (T_C). Despite Nb having a T_C of ~9 K, the practical operating temperature of a Nb SRF cavity is ~2 K, below the boiling point of He and consequently quite expensive to operate. The improvement of Nb SRF cavities and the lowering of operating costs has focused primarily on the development of new materials on the Nb surface. One of the primary limitations to both Nb SRF cavities and the new materials under study is the presence of a thermally stable and robust oxide. Understanding the formation, stability, and dynamics of the oxide and its effects on the operation of Nb SRF cavities requires study of atomic-scale surface material chemistry. Helium atom scattering (HAS) is a surface diffraction technique that has the ability to probe surface structure, bonding, and dynamics. The chemically inert He and an ultra-high vacuum (UHV) environment make HAS an ideal probe for the chemically reactive and sensitive Nb surface. High-temperature HAS studies have revealed that the (3x1)-O NbO phase that forms readily on Nb(100) is stable and intact for surface temperatures as high as 1100 K. This phase of the oxide forms readily from high-temperature dissolution of the Nb_2O_5 pentoxide phase and forms optimally when annealed at 1900 K. However, little is known about the dynamics of the formation of the (3x1)-O, annealing timescales, or the effectiveness of annealing temperatures below 1900 K. The studies presented seek to take an in-depth look at the recovery of (3x1)-O surfaces that have been sputtered to disorder. High-surface-temperature helium diffraction allows for a closer look in to the temperatures relevant to the recovery of the (3x1)-O surface from sputtered defects. High-temperature diffraction also reveals the kinetics and activation energy of (3x1)-O recovery. Auger and LEED further explore the extent that elemental composition and structure influence (3x1)-O recovery from sputtering. These studies overall strengthen our understanding of the dynamics of oxides on the Nb surface that will assist in the development of new materials formed on Nb SRF cavity surfaces.

9:30am **SS-TuM-7 Isotopic, Structural, and Surface Dependencies in Non-Equilibrium Gaseous Condensation**, ***Francisco Lizano***, *Elizabeth Jamka, Steven Sibener,* University of Chicago

Gas-surface interactions mediated by adsorption dynamics are key to many necessary formation reactions in both astrophysical and terrestrial environments. This dynamic process of gas molecules colliding with a surface and losing energy through adiabatic and non-adiabatic interactions, however, remains poorly understood, especially regarding the mechanisms that govern the energy exchange between the impinging molecules and the interface. Factors such as the kinematics of the incident molecules, molecular structure, and surface phonon density of states can affect the rate of condensation and molecular formation efficiencies. This is especially important within the interstellar medium (ISM), where reactions between gaseous species and dust grains or ice mantles are necessary to explain the chemical evolution and formation of molecules in the ISM. Accurate simulations of the chemical evolution of ISM environments require accurate binding energies and adsorption probabilities from experimental data. Discrepancies in the $^{12}C/^{13}C$ abundance ratio between the solar system and

the ISM can possibly be attributed to mass-dependent adsorption or desorption of CO that leads to isotope fractionation. It has been shown that CO molecules are known precursors to many complex organic molecules detected in the ISM, the formation of which requires both gaseous CO and solid CO adsorbed onto a dust grain. Our work employs molecular beams to study the dynamics of gas-surface interactions and adsorption probabilities of a wide range of systems. In situ spectroscopic characterization of the surface via reflection-absorption infrared spectroscopy (RAIRS) coupled with the King and Wells mass spectrometry technique allows us to determine sticking probabilities of impinging molecules onto a well-characterized surface. This has allowed for the investigation of isotopic dependencies in non-equilibrium gaseous condensation for systems such as $^{12}CO_2/^{13}CO_2$ and $^{12}CO/^{13}CO$, as well as structural dependencies using isomers of butene, at a wide range of incident energies. Ongoing work is investigating the impact surface phonon modes have on the sticking of these molecules. Understanding the factors that influence the propensity of a gas molecule to adsorb to the surface will improve models of interstellar events and further our knowledge of non-equilibrium condensation in fields such as heterogeneous catalysis, thin film growth, and aircraft icing in cold environments.

9:45am **SS-TuM-8 Effects of Subtle Temperature Fluctuations on Surface Mobility of Atomic Steps and Oxidation Dynamics in High-Temperature Alloys**, ***Shyam Patel***, Brookhaven National Laboratory; *Chaoran Li,* Binghamton University; *Abdullah Al-Mahboob, Jerzy Sadowski,* Brookhaven National Laboratory; *Guangwen Zhou,* Binghamton University

In contrast to the traditional perspective that minute thermal fluctuations are inconsequential in surface dynamics, here we report the remarkable impact of subtle temperature changes on altering surface oxidation behavior. Using real-time low-energy electron microscopy imaging of the initial-stage oxidation process on NiAl(100), we investigate the interplay between minute temperature variations and surface reaction dynamics at the atomic scale. Our findings reveal that even minor fluctuations in temperature can exert significant influence on the dynamic process of oxide formation and surface mobility of atomic steps. Specifically, these nuanced temperature changes induce the nucleation of oxide islands, which subsequently locally pin the surface migration of atomic steps, leading to the lengthening of surface steps. Furthermore, our results demonstrate that persistent temperature variations have the ability to counteract the pinning effect imposed by oxides on the migration of atomic steps. These results underscore the profound effect of minute temperature changes in inducing significant alternations to surface reaction dynamics and highlight the critical importance of considering thermal fluctuations in understanding and dynamically manipulating surface processes.

11:00am **SS-TuM-13 Theoretical Investigation of the Adsorption and Diffusion of Co and Ni on Ceria**, *Nusrat Jahan Rifat, Md. Saeedur Rahman,* ***Ye Xu***, Louisiana State University **INVITED**

Transition metal nanoparticles supported on ceria are widely studied to catalyze technologically important reactions such as three-way catalysis, water-gas shift, and hydrocarbon reforming. There is ample evidence in the literature that base metals such as Co and Ni exhibit unique, superior catalytic activity when supported on ceria compared to other oxides. This is generally explained in terms of bifunctionality, interfacial effects involving metal-oxygen and metal-vacancy sites as well as charge transfer, and spillover / reverse spillover of surface species between the metals and oxide. Understanding the configuration and stability of nanoparticles of these catalytic metals on ceria is therefore of importance in heterogeneous catalysis.

We theoretically study and analyze the energy, geometry, and electronic configuration of Co and Ni clusters of up to several dozen atoms adsorbed on the CeO_2(111) surface based on density functional theory (DFT) calculations. Furthermore, potential diffusion mechanisms of small Co and Ni species up to tetramers on CeO_2(111) are investigated, and additional factors that enhance or hinder the diffusion of these metals on ceria are explored. The broad similarities and subtle differences between the two metals are revealed and discussed. The implications of the stability and diffusivity of the clusters to particle size distribution, stability, and growth are discussed in the context of mathematical and kinetic models. The totality of these findings is used to rationalize the findings of recent surface science studies, including STM and XPS, of Co and Ni deposited on model ceria thin film surfaces. Our work provides fundamental insights to the understanding of ceria-supported Co- and Ni-catalyzed reactions and guidance to improved catalyst design based on the Co- and Ni-ceria materials systems.

11:30am **SS-TuM-15 Stimulus-Driven Catalysis: Surface Reactions under Oscillatory Pressure Conditions**, *Esteban Fornero,* Instituto de Desarrollo Tecnológico para la Industria Química, Argentina; *Gengnan Li,* Brookhaven National Laboratory; *Zubin Darbari, Eliseo Perez Gomez, Jay Shukla, Ignacio Vargas,* Brookhaven National Laboratory and State University of New York at Stony Brook; *Dario Stacchiola, Qin Wu,* ***J. Anibal Boscoboinik***, Brookhaven National Laboratory

Periodic external stimuli provide a promising route for manipulating catalytic activity and accessing reaction pathways unavailable under steady-state conditions. Here, I present an in-situ experimental approach that combines synchronized pressure-wave perturbations with fast time-resolved spectroscopy to investigate catalytic dynamics on well-defined surfaces. Using CO oxidation on Pt(111) as a model system, we demonstrate how square-wave modulation of the CO partial pressure drives periodic changes in surface coverages and reaction kinetics. Infrared reflection absorption spectroscopy (IRRAS) and online mass spectrometry with millisecond time resolution directly track transient CO_2 production and reveal how controlled perturbations of the reaction environment can dynamically overcome CO poisoning. The measurements expose the formation of non-equilibrium surface states associated with enhanced catalytic turnover and provide direct insight into the coupling between gas-phase forcing and surface reaction dynamics. Beyond CO oxidation, this methodology is readily extendable to other catalytic systems and operando spectroscopic techniques, particularly to reactions governed by competitive adsorption processes where dynamic modulation of surface populations can strongly influence catalytic performance, reactivity, and selectivity.

11:45am **SS-TuM-16 Dynamic Metal–Support and Bimetallic Interactions in Ru Catalysts during Ammonia Decomposition**, ***Soomin Kim***, Korea Advanced Institute of Science and Technology, Republic of Korea; *Yujin Jeon,* Korea Advanced Institute of Science and Technology (KAIST) & Institute for Basic Science (IBS), Republic of Korea; *Kwangjin An,* Ulsan National Institute of Science and Technology, Republic of Korea; *Mu-Hyun Baik,* Korea Advanced Institute of Science and Technology (KAIST) & Institute for Basic Science (IBS), Republic of Korea; *Jeong Young Park,* Korea Advanced Institute of Science and Technology, Republic of Korea

Ammonia decomposition is a cornerstone of the green hydrogen economy, requiring highly active and durable catalysts. Ruthenium (Ru) is recognized as the most efficient catalytic candidate; however, its high cost, scarcity, and sensitivity to surface electronic structure necessitate precise optimization of Ru-based systems. To achieve this, fine-tuning the metal-support interface and surface composition is paramount. In this study, we investigate two distinct surface engineering strategies: leveraging facet-dependent Strong Metal-Support Interactions (SMSI) in Ru/TiO_2 and exploring bimetallic synergy in RuCo/MgO catalyst.

For Ru/TiO_2 catalysts, anatase TiO_2 supports exposing predominantly (101) or (001) facets were employed to regulate SMSI during ammonia decomposition. In situ ambient-pressure X-ray photoelectron spectroscopy (AP-XPS) and in situ DRIFTS reveal that NH_3 induces temperature-dependent formation of a TiO_x overlayer on Ru nanoparticles, accompanied by substantial modulation of Ru electronic states. The Ru/bipyramid-TiO_2 forms a thinner and partial TiO_x overlayer that preserves accessible Ru surface sites while generating an electron-rich Ru–TiO_x interfacial structure favorable for NH_3 dehydrogenation and N≡N recombination. In contrast, the Ru/nanosheet-TiO_2 undergoes more extensive encapsulation, resulting in reduced surface accessibility and lower catalytic activity. Complementary DFT calculations demonstrate that the oxide–metal interfacial sites lower the activation barriers for N–H bond cleavage through oxygen-assisted dehydrogenation pathways. In parallel, RuCo/MgO catalysts exhibit enhanced catalytic stability and reactivity arising from dynamic bimetallic surface interactions. The incorporation of Co modifies the electronic environment of Ru, stabilizing the surface ensembles under ammonia decomposition conditions and suppressing sintering while promoting NH_x activation and nitrogen recombination.

Our findings reveal that ammonia decomposition relies on dynamic surface and interfacial changes in Ru-based catalysts. In situ techniques uncover SMSI evolution, interfacial charge transfer, and bimetallic synergy, providing actionable design principles to optimize Ru-based catalyst efficiency for hydrogen production from ammonia.

12:00pm **SS-TuM-17 Vibrational Excitation in Plasma Catalysis: How Important Are Dynamical Effects?**, ***Floris van den Bosch***, *Jörg Meyer,* Leiden University, Netherlands

Plasma catalysis offers to be a promising alternative to current ammonia production processes, due to the combination of high selectivity of

heterogeneous catalysis and efficient activation of nitrogen in the plasma. However, the theoretical understanding of how various plasma processes contribute to efficiency improvements remains limited. The pioneering work of Metha et al. [1] extended the standard formulation of transition state theory by making it vibrational state-specific through the use of the Fridman-Macheret α model [2]. The resulting microkinetic model accounted for vibrational contributions under the non-equilibrium conditions of a plasma reactor. In this work, we critically examine the prototypical chemical process of activated N_2 reactivity on ruthenium through explicit rate coefficient calculations using state-of-the-art molecular dynamics, based on a potential energy surface previously validated against molecular beam experiments. Our findings reveal that vibrational activation is significantly more effective in promoting surface reactivity than predicted by the Fridman-Macheret α model, which fails to capture the full complexity of state-specific contributions. Furthermore, our calculations indicate that vibrational activation is also the primary driver of highly activated thermal catalytic reactions. These results provide a valuable benchmark to guide the development of future state-specific microkinetic models for heterogeneous and plasma catalysis.

[1] Metha, P., et al. Nat. Catal., 2018. 1: p. 269-275
[2] Fridman, A. Plasma Chemistry. Cambridge University Press, 2008. ISBN: 978-0-521-84735-3

Thin Films
Room 317 - Session TF-TuM
Fundamentals of TF II & Flash Session

Moderators: Prof. Elton Graugnard, Boise State University, **Dr. Richard Vanfleet**, Brigham Young University

8:00am **TF-TuM-1 Argon and Nitrogen Background Atmospheres as Growth Modulators in RIR-MAPLE Deposited $MAPbI_3$ Thin Films**, ***Joshua Ayeni***, *Adrienne Stiff-Roberts,* Duke University

Controlling material delivery during pulsed laser deposition (PLD) is critical for hybrid perovskites, where volatile organic components make film growth highly sensitive to deposition conditions [1]. Resonant infrared matrix-assisted pulsed laser evaporation (RIR-MAPLE) provides a solvent-mediated, low-damage deposition route for delicate hybrid materials. During RIR-MAPLE, inert background gases can alter plume expansion through collisional scattering and thermalization, affecting precursor transport and crystallization. Although RIR-MAPLE has been applied to diverse material systems [2,3], the comparative effects of inert gases on three-dimensional perovskite growth remain largely unexplored.

In this study, methylammonium lead iodide ($MAPbI_3$) thin films were deposited under controlled argon (Ar) and nitrogen (N_2) environments to investigate how inert atmospheres regulate plume propagation, precursor incorporation, and film evolution during RIR-MAPLE growth. $MAPbI_3$ possesses strong optical absorption, long carrier diffusion length, high mobility, and tunable bandgap energy, making it promising for photovoltaic and optoelectronic applications [4,5].

Depositions were performed using a resonant 2.94 μm Er:YAG laser, enabling gentle matrix sublimation and transfer of intact material toward the substrate for nucleation and crystallization. By varying gas species and pressure, distinct growth behaviors emerged due to atmosphere-dependent plume scattering and thermalization. Structural characterization revealed differences in crystallinity, orientation, and crystallite development between Ar- and N_2-grown films, indicating that the background atmosphere strongly influences growth kinetics.

Compared to Ar, N_2 environments promoted improved crystalline evolution (~35–43 nm) and increased film thickness (~150–260 nm), consistent with enhanced precursor retention and reduced loss of volatile species near the substrate. In contrast, Ar atmospheres produced thinner films (~100–147 nm) and stronger evidence of scattering-induced disruption of precursor transport. Optical measurements showed preservation of the characteristic $MAPbI_3$ absorption edge and photoluminescence response across both atmospheres, while subtle spectral shifts reflected atmosphere-dependent variations in structural order and defect-mediated recombination pathways.

Overall, the results demonstrate that inert background environments in RIR-MAPLE act as active growth regulators rather than passive chamber conditions. These findings establish the role of inert gases and pressure in tuning growth dynamics and support scalable RIR-MAPLE deposition of high-quality hybrid perovskite thin films.

8:15am **TF-TuM-2 High Throughput Thin-Film Ion Kinetic Testing Enabled Through Atmospheric-Pressure Spatial ALD**, ***Daniel MacAyeal***, *Ellen Owens, Kaydence Delgado, Alexander Kozen,* University of Vermont

Research in atmospheric pressure spatial atomic layer deposition (AP-SALD) has enabled new capabilities in quickly manufacturing thin metal-oxide coatings for photovoltaics, electrochemical interfaces, and low-cost transparent conductors for flexible electronic devices. Spatial ALD can also be used for rapid materials testing and processing through deposition of high-throughput combinatorial libraries. Here, we utilize this approach to investigate AP-SALD of Nb_2O_5 / TiO_2 mixed metal oxide (MMO) bronzes, which are known to exhibit fast ion transport. Discrete regions of each mixed metal oxide can be varied by an arbitrary material property or manufacturing parameter of our choosing. We construct TiO_2 / Nb_2O_5 bronze test structures with varied alloy composition, precursor flow parameters, nanolaminate thickness, and overall region composition. We use spectroscopic ellipsometry, Raman spectroscopy, AFM, and XRD to evaluate materials structure, composition, and morphology as a function of the aforementioned parameters. We demonstrate the capabilities of AP-SALD and highlight new accelerated methods for high-throughput complex oxide materials development.

8:30am **TF-TuM-3 Accelerated Approaches to Atmospheric Pressure ALD Process Development Using Predefined Test Structures**, ***Ellen Owens***, *Holly Wilson, Dan MacAyeal, Alex Zaccardi, Drew Ledger, Alexander Kozen,* University of Vermont

Process development and associated materials screening for atomic layer deposition (ALD) processes can be long and arduous, particularly for compositionally complex ternary quaternary, and pentanary films. Beyond conventional ALD, Atmospheric pressure spatial ALD (AP-SALD) is an emerging and powerful tool that can produce discrete arrays of deposited material on a single wafer to increase the rate of material optimization of thin-film materials. In this talk, we discuss strategies to dramatically decrease process development and materials characterization timelines for ALD films using atmospheric pressure spatial ALD (AP-SALD) onto prepatterned arrays of test structures and devices.

We use TiO2as a prototype material to demonstrate the high throughput capabilities of AP-SALD process by deposition onto interdigitated electrodes and evaluate the electrical, optical, and structural properties of these films.

We vary combinatorial parameters including precursor, carrier, and sheath gas flow rates, nozzle to substrate gaps, deposition temperatures, and post deposition processes, allowing us to quickly access a wide parameter space on a single substrate.

We evaluate the spatially-resolved deposition characteristics of TiO2 using profilometry, spectroscopic ellipsometry, and electrical measurements including IV, CV, linear& nonlinear impedance, and Hall effect measurements.

8:45am **TF-TuM-4 Facile Optimization of Combinatorial Sputtering Processes with Arbitrary Numbers of Components for Targeted Compositions**, ***Shelby Fields***, U.S. Naval Research Laboratory

Combinatorial thin films and coatings, which display analogue compositions that vary as a function of position, enable high-throughput materials discovery and optimization. For example, when paired with mappable characterization, whole explorations of composition effects on materials properties may be contained within a single synthesis step. However, the applicability of combinatorial films and coatings to many materials challenges is hindered by irreproducibility and constrained processing spaces, which reduce the extent to which these experiments map on to end-use technology. To address this deficiency, this presentation introduces a process development method that enables the reproducible synthesis of *n*-component sputtered combinatorial thin films with targeted compositions at specific coordinates. It is determined that areal mass density profiles of individually sputtered species are well described by two-dimensional Gaussian peak shapes, the amplitude of which possesses a strongly linear relationship with applied target power. In addition, areal mass density profiles are shown to be noncovariant during co-deposition. Based upon these characteristics, an optimization expression is derived that computes the power required to obtain a targeted atomic concentration at a specific coordinate. It is shown that a minimum of two depositions at different powers are sufficient produce an optimized process model, which is subsequently enabled to suggest powers to obtain any composition at a targeted coordinate, permitting the high throughput exploration of entire composition spaces. Furthermore, this optimized process allows for the substitution of substrates of different diameter and material following calibration, is compatible with both direct current and radio-frequency

magnetron sputtering, and can suggest powers to obtain identical compositions at different growth rates. As a proof-of-concept, a $Cr_vFe_wMo_xNb_yTa_z$ alloy thin film is synthesized on a 6"-diameter Si wafer with an equiatomic composition at the center that matches well with simulation following calibration. This capability is further demonstrated through the synthesis of alloy combinatorial wafers using reactive and rf sputtering processes for separate materials exploration investigations. In total, this optimization method enables the rapid and reproducible synthesis of combinatorial films with arbitrary numbers of components, which better connects this high throughput experimental method with down-stream applications and technology.

9:00am **TF-TuM-5 Combining Pyroelectric Calorimetry and Multiscale Modeling to Untangle the Interplay of Precursor Delivery, Kinetics, and Byproducts in ALD ZrO2***, **Ashley Bielinski**, Anik Biswas, Cong Liu, Alex Martinson,* Argonne National Laboratory

Thermal atomic layer deposition (ALD) processes are typically described as alternating sequences of self-limiting surface reactions. When we inspect the dynamics of individual reactions as they approach saturation, we see that in addition to simple mechanisms of ligand exchange reactions, this self-limiting nature also depends on an interplay between precursor delivery, reaction kinetics, and the role of reaction byproducts.An investigation of these dynamic processes can provide insights into the results of ALD processes ranging from fundamental reaction thermodynamics and kinetics to reactor design. However, these reactions happen quickly, often at rates faster than the sampling frequency of common in situ measurement techniques.Pyroelectric calorimetry provides in situ measurements of the heat generated and transferred from surface reactions as well as precursor and byproduct flow with sufficient time resolution to measure these dynamics.Here we present how experimental calorimetry measurements can be combined with multiscale computational modeling to untangle the influence of precursor flow dynamics and reaction kinetics for the reaction between tetrakis(dimethylamido)zirconium(IV) (TDMAZr) and water to form ZrO_2. By combining experimental measurements that represent the true conditions of realistic samples surfaces, first principles modeling of reaction mechanisms, and reactor-scale modeling of precursor flow and byproduct generation, we provide insight into the complexities of ALD surface reactions, the non-idealities of which have broader implications for the development of site- and area-selective ALD.

9:15am **TF-TuM-6 Flow Imaging for Validated Mass Transport Models of an Atomic Layer Deposition Chamber***, **Berc Kalanyan**, Hyuenwoo Yang, Vladimir Khromchenko, James Maslar,* National Institute of Standards and Technology (NIST)

Digital twins of semiconductor unit processes could provide value in process development, optimization, and real-time control applications. For a vapor phase deposition process, a digital twin would entail multiple linked models representing reactive transport processes at disparate length scales from the process equipment level to the device structures on the wafer. However, widespread development and validation of such models require non-proprietary process data, which is not readily available. To address this need, NIST is generating process data and validated models for atomic layer deposition (ALD) processes. An important component of this effort is *in situ* metrology development to access key process parameters such as partial pressures, flow rates, temperature, and mass uptake as a function of space and time. In this talk we will focus on 1) mass transport measurements within a research-grade ALD reactor and 2) the use of transport data to validate flow simulations. To obtain the process data, we use absorption imaging of precursor flow as a function of process conditions, *e.g.*, gas flow rate, chamber pressure, and temperature. Two precursors selected for this investigation are molybdenum pentachloride ($MoCl_5$) and molybdenum oxytetrachloride ($MoOCl_4$). Precursor flow was visualized at about 100 frames per second in the ultraviolet-visible spectral region using a CMOS camera and a light emitting diode source. Simulations of flow in this chamber were performed using commercial computational fluid dynamics (CFD) packages. Simulations were validated using the time-dependent, pathlength-integrated precursor concentration obtained from the absorption imaging measurements and the time-dependent total pressure measured at selected locations in the deposition system. Carrier gas flow rates and system pressures that resulted in quiescent and recirculating flow regimes were simulated using a single model. The spatial distribution of precursor in the chamber was found to be driven by continuum flow of the carrier gas. Flow imaging collected from two orthogonal axes was used to assess asymmetry in flow fields resulting from injector geometry.

References

(1) Maslar, J. E.; Kalanyan, B. Visualizing Molybdenum Pentachloride Flow During Vapor Deposition Processes Using Absorption Imaging. *Appl Spectrosc* **2025**, *79* (10), 1487–1496. https://doi.org/10.1177/00037028251325565.

(2) Alghamdi, A.; Ou, F.; Kalanyan, B.; Maslar, J. E.; Christofides, P. D. A CFD-Based Digital Twin Framework for Transient $MoCl_5$ Transport in an Experimental Atomic Layer Deposition Process. *Digital Chemical Engineering* **2026**, *19*, 100304. https://doi.org/10.1016/j.dche.2026.100304.

9:30am **TF-TuM-7 Mgo ALD Coatings for Improvement of Secondary Electron Emission***, **Sun Gil Kim**, Min-Seop Song, Hyun-Mi Kim,* Korea Electronics Technology Institute, Republic of Korea*; Jeonggil Na, Kyunghwan Jeong,* JJ CNS, Republic of Korea*; Hyeongkeun Kim,* Korea Electronics Technology Institute, Republic of Korea

Microchannel Plates(MCP) are used to amplify photoelectron, ion, or electron signals in spectrometers, electron microscopes, and night vision devices. Conventional MCPs are fabricated from lead glass, where a SiO_2 emissive layer is formed during glass fabrication, facilitating electron multiplication. Despite materials such as MgO and Al_2O_3 exhibiting superior secondary electron emission(SEE) properties compared to SiO_2, conventional deposition techniques such as physical vapor deposition(PVD) and chemical vapor deposition(CVD) have limitations in achieving uniform coating inside MCP channels. In contrast, atomic layer deposition(ALD) enables uniform coating of materials with excellent SEE properties even within the narrow MCP channels, thereby enhancing MCP performance. In this study, we developed the ALD process to deposit Al_2O_3 as a resistive layer and MgO as an emissive layer inside MCP channels.

Film thickness and density were analyzed using an ellipsometer and X-ray reflectometry (XRR). Additionally, X-ray photoelectron spectroscopy (XPS) was employed to examine the elemental composition and Mg/O ratio across different film thicknesses. The crystal structure was characterized using X-ray diffraction (XRD), while high-resolution transmission electron microscopy (HR-TEM) was utilized to investigate the microstructure of the deposited films. Moreover, the SEE coefficient of MgO thin films under various process conditions was measured using a γ-focused ion beam (γ-FIB) system, and based on these results, the optimal process parameters and film thickness were determined.

This study is expected to serve as a key reference for material selection in emissive and resistive layers of MCP. Future research will explore various oxide thin-film combinations and novel materials, not only to enhance MCP gain but also to improve MCP lifetime and noise characteristics, thereby contributing to overall performance advancements. Moreover, the findings can be applied across various industrial and research fields, including time-of-flight mass spectrometry (ToF-MS) and image intensifiers.

9:45am **TF-TuM-8 Autodoping of Thin-Film Ionic Materials Using Atomic Layer Deposition (ALD)***, **Steven Douglass**, Daniela Fontecha, Gary Rubloff, Sang Bok Lee, Keith Gregorczyk,* University of Maryland, College Park

Recently, our group has shown that semiconductor manufacturing techniques can be leveraged to add electrochemical functionality and make devices outside of the traditional semiconductor portfolio. These devices include solid-state microbatteries and super capacitors, aswell as electrochemical random-access memory (ECRAM). In the production of these iontronic devices (devices where ions operate as the main carriers of charge), notable intermixing of ionic material layers has occurred between, for example, the vanadium pentoxide (V_2O_5) cathode and the lithium phosphorus oxynitride (LiPON) electrolyte in solid-state microbatteries. This autodoping has been termed "autolithiation" and is believed to occur in two stages: before LiPON film growth and during LiPON film growth. It was first observed as a physical process during sputtering of LiPON onto a V_2O_5 substrate.

Since, we have observed a similar phenomenon while depositing ALD LiPON onto V_2O_5, with the lithium source being lithium *tert*-butoxide (LiO^tBu). In this talk we discuss how autolithiation during ALD depends on temperature in its initial stage. At 300°C, there was no lithiation after 20 pulses of LiO^tBu. However, one pulse at 350°C and 400°C yielded lithiation, followed by a linear trend of increased lithiation state with increased pulsing. Figure 1 displays the trend of lithium inserted through LiO^tBu pulsing at different temperatures, calculated from electrochemical delithiation of the samples. XPS demonstrates that the V^{4+}:V^{5+} oxidation state ratio grows quicker with increased temperature. Raman spectroscopy shows evolution of the bulk away from α-V_2O_5 with higher temperatures and more LiO^tBu exposure.

This presentation discusses characterization and quantification of ALD autolithiation of V_2O_5 before film growth. Future work on the subject will be focused on deconstructing autolithiation after film growth.

11:00am **TF-TuM-13 Use of Xps-Crem for Detecting Hydration-Driven Changes in the Electrical Conductivity of $La_2Ce_2O_7$ Thin Films**, ***Ayelet Vilan***, Weizmann Institute of Science, Israel

Chemically Resolved Electrical Measurements (CREM)[1] harnesses the charging-like effects in X-ray Photoelectron Spectroscopy (XPS) to extract sample's electrical properties. Here, we apply CREM to investigate a novel proton-conducting material comprising hydrated $La_2Ce_2O_7$.[2] Conventional electrical measurements show that the activation energy for conductance decreases from ~1.07 eV in the as-deposited film to ~0.7 eV after hydration. We attribute this reduction to a change in the dominant transport carriers: electron conduction via oxygen vacancies in the as-deposited film and proton conduction in the hydrated film.

As temperature decreases from 473 to 360 K, both films become less conductive; however, hydrated $La_2Ce_2O_7$ exhibits weaker temperature dependence: At 360 K, its conductance is approximately five times higher than that of the as-deposited film. Measurements below this temperature failed, because the films become too resistive for conventional measurements, preventing reliable room-temperature characterization.

To overcome this limitation, we employed CREM within the XPS chamber to evaluate conductivity at room temperature under ultra-high vacuum. In brief, CREM modulates the electron flood gun while simultaneously measure (1) the net current through the sample and (2) the shifts in core-level binding energies, reflecting resistive potential drops. The ratio of current changes over energy shifts, provides an effective film's perpendicular conductivity.[1] CREM measurements (see figure) revealed that, at room temperature, hydrated $La_2Ce_2O_7$ was roughly three orders of magnitude more conductive than the as-deposited film, consistent with the expected exponential dependence on activation energy. Although XPS cannot directly detect hydrogen, the sustained high conductivity under vacuum supports stable proton incorporation within the lattice.

To directly probe proton transport, we deposited proton-sensitive WO_3, which turns from transparent to opaque upon proton insertion (H_xWO_3), accompanied by reduction of W(VI) to W(V). Devices comprising ITO/$La_2Ce_2O_7$/WO_3 exhibited bias-induced coloration only when $La_2Ce_2O_7$ was hydrated. Furthermore, CREM-driven proton injection revealed a significant shoulder of reduced-tungsten in the W 4f line, characteristic of W(V), only when the underlying $La_2Ce_2O_7$ was hydrated. These results confirm proton-mediated transport.

The presentation will outline the CREM methodology and its application to XPS under varying electronic conditions.

References:

[1] Cohen, H., J. Elect. Spect. Rel. Phen. 176 (2010) 24–34;

[2] Freidzon D. et al., Solid State Ionics 438 (2026) 117150;

11:15am **TF-TuM-14 Influence of Substrate Interactions on the Growth of MoO3 on Graphene/Ru(0001) and Highly-Oriented Pyrolytic Graphite**, ***Buddhika Alupothe Gedara***, *Zdenek Dohnalek, Zbynek Novotny,* Pacific Northwest National Laboratory

Two-dimensional transition-metal oxides (TMOs) are promising for electronic applications due to their stability and favorable electrical and optical properties. Among them, molybdenum trioxide (MoO_3) stands out for its high dielectric constant, wide band gap (2.9-3.2 eV), and catalytic activity, enabling diverse electronic and energy-related applications. In this work, we investigate the effects of substrate topography and charge transfer on MoO_3 growth on highly oriented pyrolytic graphite (HOPG) and graphene (Gr)/Ru(0001) using scanning tunneling microscopy and X-ray photoelectron spectroscopy (XPS).Small MoO_3 clusters formed on Gr/Ru(0001), whereas large, dendritic, and disordered MoO_3 clusters formed on HOPG following deposition at 300 K. Upon increasing the temperature to 500-700 K, more ordered, crystalline MoO_3 islands form on both substrates. Notably, a distinct height difference of MoO_3 is observed on these two substrates over the studied temperature range. The height of MoO_3 islands on Gr/Ru(0001) corresponds to a single layer of MoO_3 (3.9 ± 0.2 Å), whereas the height of the MoO_3 islands on HOPG is consistent with the previously reported double layer (6.8±0.1 Å) [1, 2]. Single-layer MoO_3 on Gr/Ru(0001) comprises a planar MoO_2 sheet aligned parallel to the Gr/Ru(0001) surface, with Mo atoms terminated by additional oxygen atoms. We observed a brick-style pattern on the MoO_3 islands on Gr/Ru(0001) substrate and the formation of this characteristic pattern is due to the ordered removal of terminal oxygen atoms. Double-layer MoO_3 islands grow on HOPG with a staggered arrangement of corner- and edge-sharing MoO_6 octahedra [1, 2]. XPS data show that Mo in the islands on HOPG are predominantly in (6+) oxidation state while on Gr/Ru(0001) at least half is reduced to (5+) over the temperature range of 500-700 K. The formation of lower oxidation states is attributed to charge transfer from the substrate due to the electron chemical potential difference at the interface, and the presence of oxygen vacancies. Our results demonstrate that substrate-induced interfacial interactions play a key role in controlling the nucleation, growth mode, and structure of MoO_3 on graphene-based supports, providing a pathway to tailor 2D TMO heterostructures for electronic and catalytic applications.

References

[1] D.A. Kowalczyk et al., ACS Appl. Mater. Interfaces, 14 (2022) 44506-44515.

[2] J.H. Kim et al., 2D Materials, 6 (2019) 015016.

11:30am **TF-TuM-15 Atomic Growth Mode of Capping Layers for Surface Passivation of Nb**, ***Van Do***, *Robert Burnley, Margaret Hall, Helena Lew-Kiedrowska, Sarah Willson, Steven Sibener,* University of Chicago

Nb is the standard material for superconducting radio-frequency (SRF) cavities, but the accelerating performance of these cavities is limited by the spontaneous growth of Nb oxides on the surface. These oxides are insulating and dielectric in nature, which can lead to hot spots and vortex penetration, ultimately degrading cavity performance. To address this challenge, we are improving Nb surface stability through the implementation of two types of capping layers: an inert capping layer and sacrificial capping layer. A chemically inert Au film can suppress oxidation by protecting the underlying Nb surface from environmental exposure. In contrast, a sacrificial Zr layer, owing to its higher oxidation affinity, preferentially oxidizes and thereby shields the underlying Nb. In addition, Zr can intermix with Nb to form a substitutional Zr–Nb alloy with a predicted superconducting transition temperature of 17.7 K. Using scanning tunneling microscopy, we have visualized Au capping layers ranging from sub-monolayer coverage to 10 monolayers, as well as Zr capping layers from initial adsorption through alloy formation on the (3×1)-O/Nb(100) surface. We further evaluated the passivation efficiency of these modified surfaces by leaking oxygen and observing the chemical evolution using x-ray photoelectron spectroscopy. These results provide atomic mechanistic insight into surface treatment methods for enhancing the oxidation resistance and superconducting performance of Nb-based SRF cavities.

11:45am **TF-TuM-16 Distal electrofabrication and Microfluidic Integration of Chitosan Anion-Exchange Membranes for Low-Cost Direct Methanol Fuel Cells**, ***Phuc Long Duong***, College of Engineering, Physics and Computing, Catholic University of America; *Xiaolong Luo,* Catholic University of America

Commercial adoption of hydrogen fuel cells remains limited by high material costs and the lack of a dedicated hydrogen infrastructure. Direct Methanol Fuel Cells (DMFCs) offer a compelling alternative by using an easily refuelable liquid fuel with high energy density. However, conventional DMFCs face significant economic and technical hurdles due to their reliance on expensive proton exchange membranes (e.g., Nafion) and noble-metal catalysts, as well as issues with methanol crossover and sluggish reaction kinetics.

This work demonstrates the design of a microfluidics DMFC (DMFC) that uses ultra-low-cost, non-platinum-group-metal (non-PGM) catalysts and a sustainable, biopolymer-based anion exchange membrane (AEM). We apply a patent-pending distal electrofabrication technique to deposit freestanding chitosan thin films directly within microfluidic channel networks. The electrofabrication provides precise control and utilizes the biopolymer's naturally low methanol permeability to significantly minimize fuel crossover.

Material characterization, including Atomic Force Microscopy (AFM), Scanning Electron Microscopy (SEM), and X-ray Diffraction (XRD), confirms our hypothesis that distal electrofabrication induces high molecular alignment and a distinct crystallographic ultrastructure compared to standard cast membranes. Furthermore, Electrochemical Impedance Spectroscopy (EIS) validates enhanced hydroxide-ion conductivity within the thin-film networks.

Initial device performance testing demonstrated a peak power density of 70 mW/cm^2, with structural and crosslinking optimizations promising commercial adoption at 5%-10% the cost of existing commercial fuel cells. The success of this project may open a cost-competitive pathway for portable zero-emission energy solutions.

2D Materials

Room 304 - Session 2D-TuA

Synthesis and Processing of 2D Materials

Moderators: Tiancong Zhu, Purdue University, **Rafik Addou**, The University of Texas at Dallas

2:15pm **2D-TuA-1 Advances in Synthesis, Transfer, and Magnetization Dynamics in van Der Waals Magnets**, ***Roland Kawakami,*** The Ohio State University **INVITED**

In this talk, I will discuss two of our recent results on 2D materials. First is the observation of a new way to excite magnetization dynamics via optical pump pulses in $WS_2/CrGeTe_3$ bilayers [1]. The key result is that absorption of a laser pulse results in charge transfer between 2D semiconductor WS_2 and 2D magnet $CrGeTe_3$, which results in an ultrafast change in the magnetic anisotropy and the subsequent generation of torque on the magnetization of $CrGeTe_3$. This is an optically-excited analog of the magnetoelectric effect, where the optical pulse generates a dynamic interfacial electric field and an ultrafast variation of the carrier density. This ultrafast spin-torque represents a new way to excite magnetization dynamics, beyond typical thermal excitation mechanisms. The second result is the full-film dry transfer of van der Waals films grown by molecular beam epitaxy (MBE). Although there has been much work on the transfer of 2D materials produced by exfoliation or chemical vapor deposition, it turns out that the transfer of MBE-grown films had not been achieved due to a stronger adhesion of MBE films to the growth substrate. We show that by using the polymer PCL and a solid roller with a large radius of curvature to limit the peel-off angle, the MBE film can be released from the growth substrate with minimal cracking and a large area yield (>90%) [2]. Further, the magnetic properties of 2D magnets remained largely preserved during the transfer process. This provides a route for a layer-by-layer fabrication strategy for scalable, CMOS-compatible device arrays and applications.

[1] Wenyi Zhou, Ravi Kumar Bandapelli, Hari Paudyal, Bangzheng Han, I-Hsuan Kao, Ziling Li, Yuqing Zhu, Durga Paudyal, Jyoti Katoch, Simranjeet Singh, Roland K. Kawakami, "Ultrafast Light-Induced Magnetoelectric Effect in van der Waals Magnetic Semiconductor Heterostructures" arXiv:2604.19080

[2] Ziling Li, Wenyi Zhou, Matthew Swann, Vika Vorona, Haley Scott, Roland K. Kawakami, "Full-film dry transfer of MBE-grown van der Waals materials," 2D Materials 12, 035003 (2025).

2:45pm **2D-TuA-3 Approaching Synthesis of Large-Area Monolayer SnSe by Multi-Stage Growth and Bayesian-MBE (BaMBE)**, ***Eric Welp,*** *Qihua Zhang, Stephanie Law,* Pennsylvania State University

The outstanding piezoelectric and electronic properties of 2D SnSe has attracted significant interest with a wide range of applications such as efficient solar cells, ferroelectric memory devices, and more. While SnSe nanocrystals and large-area, 3-4 layer-thick deposited crystals have been grown in recent years, the growth of monolayer SnSe at large areas has not been reached due to poor substrate wetting. At the monolayer limit, the centrosymmetry present in multilayer films is removed resulting in strong ferroelectric and piezoelectric properties. Furthermore, SnSe stands out from the currently prominent piezoelectrics which employ lead (PZT, PMN-PT, etc.) in its lack of toxic constituents. This work develops a pathway towards large-area monolayer SnSe by molecular beam epitaxy (MBE) with multi-step growths and reconstruction of the monolayer, guided by recently developed methods in Bayesian optimization for MBE (BaMBE). The reconstruction of a deposited monolayer at high substrate temperature by supplied flux equal to the desorption rate allows small misoriented domains to desorb from the surface and preferentially grow large well-oriented grains that may coalesce into large films. To complete the efficient analysis of the multi-stage growth and reconstruction parameters with supervised machine learning, we implement Bayesian optimization to guide further synthesis by this novel method and approach large-area monolayer films of SnSe for the next generation of ferroelectric and piezoelectric devices.

3:00pm **2D-TuA-4 Plasma Enhanced Atomic Layer Deposition of Layered 2D $ZnIn_2S_4$ Thin Films: Toward Large-Area Synthesis of a Ternary 2D Chalcogenide**, ***Sudipta Mondal,*** *Ryan Weiland, Hamidur Rahman, Ageeth Bol,* University of Michigan, Ann Arbor

Ternary 2D layered chalcogenides have emerged as a promising class of n-type semiconductors for next-generation optoelectronic and energy conversion technologies due to their tunable electronic structure and strong light-matter interaction. Among them, $ZnIn_2S_4$ (ZIS), a wide-band-gap ternary chalcogenide, has attracted significant interest for photoelectrochemical (PEC) conversion, photocatalysis, and photodetector applications. Yet, scalable large-area synthesis routes, especially thin-film deposition techniques for the ZIS system, remain largely unexplored. In this work, we report the first atomic layer deposition (ALD) growth of ternary 2D $ZnIn_2S_4$ thin films. $ZnIn_xS_y$ thin films were deposited by plasma-enhanced atomic layer deposition (PEALD) using supercycles composed of ZnS and In_2S_3 subcycles, with growth monitored by in-situ ellipsometry. β-diketonate indium and zinc precursors, chosen for their thermal stability over a wide temperature window, were combined with H_2S plasma to develop the individual ZnS and In_2S_3 processes and, subsequently, the ternary ZIS process. Crystalline films were obtained at 500 °C, and the supercycle ratio was carefully tuned to approach the target $ZnIn_2S_4$ stoichiometry. Among the conditions investigated, a 2 ZnS:8 In_2S_3 (2-8) supercycle led to the formation of $ZnIn_{2.29}S_{3.48}$ as determined by XPS, closest to the desired stoichiometry. GIXRD analysis revealed the presence of a $(00l_1)$ reflection, characteristic of a layered ZIS phase. The observation of only basal-plane ZIS reflections, with no non-basal peaks, indicates highly preferred c-axis-oriented growth, with the basal planes parallel to the substrate. An increase in the number of indium subcycles in the ALD supercycle structure, such as a 2-10 recipe, led to the formation of a mixed ZIS and tetragonal β-In_2S_3 phase with a stoichiometry of $ZnIn_{3.03}S_{4.27}$, highlighting the importance of cycle ratio control to achieve a pure ZIS phase. AFM and SEM analyses showed the presence of triangular and hexagonal layered 2D-platelet-like morphology, confirming the GIXRD results and consistent with layered 2D growth. UV-Vis measurements gave an optical band gap of 2.6 eV for the 2-8 ZIS film, in good agreement with reported values. Moreover, the 2-8 sample was annealed in a tube furnace at 700 °C under H_2S atmosphere, leading to a stoichiometric $ZnIn_{2.10}S_{4.02}$ sample with an additional low-angle $(00l_2)$ reflection appearing, indicating a more crystalline and layered ZIS film formation. This study establishes a thin film deposition technique for layered $ZnIn_2S_4$ and provides insights into phase and defect engineering in ternary layered chalcogenide semiconductors.

3:15pm **2D-TuA-5 Two-Step Synthesis of MoSe2 from MoOx Thin Films by Low Temperature Thermal Atomic Layer Deposition**, ***Icelene Leong,*** Boise State University*; Brian Everhart, Drake Austin,* AFRL*; Steven M. Hues,* Boise State University*; Nicholas R. Glavin,* AFRL*; Elton Graugnard,* Boise State University

Two-dimensional (2D) semiconducting materials, including transition metal dichalcogenides (TMDs) and transition metal oxides, are of increasing interest for applications in microelectronics, photonics, catalysis, and energy technologies. Atomic layer deposition (ALD) provides a scalable route for synthesis of molybdenum oxide (MoO_x) thin films; however, the structural and functional properties of the resulting materials depend strongly on precursor chemistry, oxidation state, and post-deposition processing conditions. A two-step conversion approach offers a promising pathway to TMD formation from ALD metal oxides. Here, we report a laser-assisted two-step processing method for low-temperature ALD-grown MoO_x films for the conversion to $MoSe_2$. Laser annealing was employed to locally modify surface composition, crystallinity, and oxidation state under controlled environments, enabling systematic tuning of the intermediate oxide prior to selenization. High-throughput processing produced many distinct material conditions on a single sample by varying laser intensity and exposure time. Complementary high-throughput characterization using Raman spectroscopy, x-ray photoelectron spectroscopy (XPS), and x-ray diffraction, enabled rapid identification of processing conditions associated with high-quality $MoSe_2$ films. These results demonstrate new routes for processing ALD oxides to TMD that can be used in numerous applications.

4:00pm **2D-TuA-8 Epitaxy Growth of P-Type 2d Semiconductors**, ***Vincent Tung,*** The University of Tokyo, Japan **INVITED**

The rise of two-dimensional (2D) semiconductors represents the next wave of innovation in semiconductor technology, offering new opportunities for scaling channel materials and rethinking device architectures beyond the limits of bulk silicon CMOS. However, despite considerable progress in n-type 2D materials, such as MoS_2 and WS_2, the development of high-performance p-type counterparts remains significantly underdeveloped. This imbalance presents a critical bottleneck, as the lack of robust p-type 2D semiconductors hinders the realization of complementary logic circuits and limits the overall performance gain relative to silicon CMOS. A key challenge in identifying suitable p-type 2D semiconductors lies in the inherent difficulty of achieving stable valence band alignment, sufficient hole mobility, and reliable contact formation without introducing Fermi-level pinning or unintentional doping. Moreover, the performance of 2D devices is often compromised by degraded semiconductor/dielectric and

semiconductor/electrode interfaces, especially when harsh fabrication steps or transfer processes are involved. These interfaces, though only a few atoms thick, play a decisive role in governing charge transport, threshold voltage stability, and scalability. In this talk, I will present our recent efforts in addressing these challenges by focusing on the synthesis and integration of p-type 2D semiconductors, particularly under low-temperature conditions. Emphasis will be placed on strategies for the direct growth of these materials on insulating substrates, thereby preserving electronically clean and atomically well-defined interfaces. This approach offers a practical pathway toward realizing high-performance complementary 2D logic while maintaining compatibility with back-end-of-line (BEOL) process constraints.

4:30pm **2D-TuA-10 Repeatability and Reproducibility in the Chemical Vapor Deposition of 2D Films: A Physics-Driven Exploration of the Reactor Black Box**, ***Shahana Chatterjee***, Make Materials, Canada; *Thomas Abadie,* University of Birmingham, UK; *Meihui Wang,* IBS Center for Multidimensional Carbon Materials, Republic of Korea; *Omar Matar,* Imperial College London, UK; *Rodney Ruoff,* IBS Center for Multidimensional Carbon Materials, Republic of Korea

Chemical vapor deposition (CVD) on metal substrates is the method of choice for growing single-crystalline high-quality 2D films for various opto-electronic applications. Though one and a half decades have passed since the CVD synthesis of graphene was first reported (and followed by that of other 2D films), multiple problems remain, stemming from the fact that the CVD reactors are still virtual black-boxes with poorly understood reaction environments. For example, repeatability issues, such as an optimized growth condition changing over time in the same reactor, or reproducibility issues, such as the failure to reproduce the growth process in a different reactor (even in the same research laboratory), are well known. It is indeed quite difficult to (1) study process kinetics, (2) correlate experimental results to atomic level simulations, (3) build up from previous publications or test a new hypothesis, and, (4) scale-up and commercialize lab-scale processes. This presentation will explore what may be done to circumvent this complicated problem, as monitoring or measuring the reactor environment directly is challenging or even impossible. We will discuss how relevant external process and reactor parameters may first be identified with the help of the Computational Fluid Dynamics (CFD) toolbox OpenFOAM and then utilized to recreate the reaction environment. Finally, the critical importance of the reactor environment on such processes, and, a protocol for experimentalists to use while monitoring and reporting them will be discussed.

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2. Wang, M.; Kim, Y. C.; Meng, Y.; Chatterjee, S.; Bakharev, P.; Luo, D.; Gong, Y.; Abadie, T.; Kim, M. H.; Sitek, J.; Seong, W. K.; Lee, G.; Ruoff, R. S. *Growth Kinetics of Graphene on Cu(111) Foils from Methane, Ethyne, Ethylene, and Ethane*. Angewandte Chemie International Edition 2024, 63, e202412131.

4:45pm **2D-TuA-11 Topotactic Formation of 2D Ternary Single Crystals**, *Nitin Shinde, Shavit Ben David,* ***Ariel Ismach***, Tel Aviv University, Israel

The growth of 2D materials has advanced significantly in recent decades, enabling the synthesis of high-quality, epitaxial graphene, hexagonal boron nitride (h-BN), and transition metal dichalcogenides (TMDs). Beyond these mono- and binary systems, a vast number of 2D ternary compounds offer compelling physical and chemical properties. However, the growth of such ternary thin films and crystals *via* methods like chemical vapor deposition (CVD) remains largely unexplored.

In this talk, I will present our approach for synthesizing oriented ternary compounds of the type $MePS_3$, where Me represents a transition metal (*e.g.*, Ni, Fe, *etc.*). We propose a two-step methodology in which it begins with the growth of an epitaxial transition metal thin film, which is subsequently transformed into a ternary compound via a topotactic reaction. Because topotaxy is a solid-state reaction that maintains structural correlation with the initial film, oriented thin crystals form on the substrate, a methodology well-suited for large-scale growth and integration. I will detail the underlying growth mechanism and discuss the resulting crystal structure and magnetic properties. This work introduces a viable pathway for the scalable synthesis of complex 2D ternary compounds with tailored chemical compositions.

5:00pm **2D-TuA-12 Spatial Doping of CVD-Grown WSe2 for Lateral Junction and Optoelectronic Applications**, ***Utsab Kafley***, *Anupama Kaul,* University of North Texas

Two-dimensional (2D) transition metal dichalcogenides (TMDCs), particularly tungsten diselenide (WSe_2), have emerged as promising materials for next-generation electronic and optoelectronic applications due to their tunable electrical and optical properties. Here, we investigate localized chemical modification of chemical vapor deposition (CVD)-grown WSe_2 using a methylammonium based dopant to achieve selective carrier modulation and lateral junction engineering. The influence of selective chemical doping on the electronic, structural, and optical response of WSe_2 is systematically explored to understand charge-transfer-induced modulation in atomically thin semiconductors. The localized doping process leads to measurable variations in carrier transport, field-effect mobility, surface morphology, vibrational response, excitonic emission, rectification characteristics, and light sensitivity, indicating effective tuning of material properties through spatial carrier engineering. The formation of laterally modulated regions further enables investigation of junction-like transport behavior and optoelectronic response within single CVD-grown WSe_2 membranes.

5:15pm **2D-TuA-13 Interface-Engineered Epitaxial Growth of Two-Dimensional Materials and Heterostructures: Mechanisms and Scalable Strategies**, ***Asma Zaka,*** Gachon University, South Korea

The emergence of two-dimensional (2D) materials has opened new pathways for next-generation electronic, optoelectronic, and energy applications due to their unique layer-dependent properties and tunable electronic structures. However, the scalable synthesis of high-quality 2D materials and heterostructures remains a critical challenge, governed by complex interfacial phenomena during epitaxial growth.

In this work, we present a comprehensive analysis of interface-driven growth mechanisms in 2D material systems, with particular focus on transition metal dichalcogenides (e.g., MoS_2, WS_2), hexagonal boron nitride, and related layered materials. The roles of lattice mismatch, strain relaxation, interfacial charge transfer, and band alignment are systematically examined in relation to nucleation behavior, domain evolution, and crystallographic orientation.

Furthermore, advanced epitaxial strategies tailored for 2D materials, including van der Waals epitaxy, remote epitaxy mediated by graphene interlayers, and step-guided growth on vicinal substrates are critically analyzed as effective routes to overcome conventional lattice constraints. These approaches enable controlled nucleation, improved domain alignment, and reduced defect densities, even in highly mismatched systems.

By establishing a unified framework linking interface energetics with growth dynamics, this work provides key insights into the controlled synthesis of high-quality 2D materials and heterostructures. The results have important implications for scalable device integration in nanoelectronics and energy technologies.

Keywords

2D materials

- epitaxial growth
- heterostructures
- interface engineering
- van der Waals epitaxy
- thin films

5:30pm **2D-TuA-14 Controlled Synthesis and Precision Doping of 2D Materials by Nonequilibrium Approaches**, ***Kai Xiao***, *Daniel Yimam, Sumner Harris, Alexander Puretzky, Mina Yoon,* Oak Ridge National Laboratory; *Gerd Duscher,* University of Tennessee Knoxville; *Christopher Rouleau,* Oak Ridge National Laboratory; *David Geohegan,* University of Tennessee Knoxville

Atomically thin 2D materials offer exceptional tunability for optoelectronics, but scalable synthesis with precise control of phase, uniformity, and doping remains a central challenge. I will present our recent work in laser-based synthesis, characterization, and processing of atomically thin two-dimensional (2D) materials under nonequilibrium conditions. Using *in situ* diagnostics across multiple length scales, we probe crystallization pathways and phase transformations during growth and processing, which enables to link deposition conditions to resulting structure and optical properties. Then, I will discuss precision doping and the deliberate introduction of controlled heterogeneities—defects, dopants, and strain—during synthesis and post-growth processing. By tuning the type and distribution of these features, we modulate excitonic properties and dynamics in 2D materials,

providing a practical route to tailoring functionality for optoelectronic applications.

This work was supported by the U.S. DOE, Office of Science, Materials Sciences and Engineering Division and the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.

Atomic Scale Processing Mini-Symposium
Room 316 - Session AP1+EL+MS+PS+TF-TuA

Advanced Atomic Scale Processing through Modeling and Simulation

Moderators: Prof. Dr. David Graves, Princeton University, **Prof. Dr. Satoshi Hamaguchi**, Osaka University, Japan

2:15pm **AP1+EL+MS+PS+TF-TuA-1 Design and performance of AI agents interfacing with atomic layer deposition tools*, Angel Yanguas-Gil,*** Argonne National Laboratory **INVITED**

In recent years there has been an increased interest in exploring the integration of generative AI in combination with experimental tools to create multipurpose autonomous systems that can solve complex research problems. This vision relies on AI agents based on LLMs that can autonomously interact with experiments to solve multiple tasks (e.g. "Grow 20 nm of tin oxide" or "selectively grow 10 nm of Cu on Co but not on silicon oxide"). However, in order to be useful, these systems have to be compatible with state of the art manufacturing tools and they have to perform reliably well in a broad enough set of materials synthesis tasks.

In this presentation, I will focus on these two aspects in the context of atomic scale processing. First, I will describe how we have augmented an existing ALD tool so that it can be integrated with generative AI models. Our approach relies on defining a Python interface and API that abstract all the specific details of the hardware from the AI agent, while making it compatible with standard approaches for tool use with LLMs. I will also describe how we have implemented AI agents that can communicate with this ALD tool as well as with existing data, such as data logs and background data on ALD and area selective deposition.

In the second part of the presentation, I will introduce a general methodology to evaluate the performance of AI agents on atomic scale processing tasks. We have applied it to evaluate the performance of state of the art models in instruction, process discovery, and materials discovery challenges in the context of atomic scale processing, primarily ALD and selective growth. In all these cases the output of the challenge is a specific instruction to run one or more processes in an ALD tool. Our results show that state of the art models excel at instruction tasks, but they struggle on process and materials discovery tasks where they involve processes and materials that are underrepresented in the literature, pointing to potential limitations and areas of improvement for for future AI models specialized in materials synthesis and atomic scale processing.

This research is based upon work supported by Laboratory Directed Research and Development (LDRD) funding from Argonne National Laboratory, provided by the Director, Office of Science, of the U.S. Department of Energy under Contract No. DE-AC02-06CH11357.

2:45pm **AP1+EL+MS+PS+TF-TuA-3 A Multiscale Framework for ALD/ALE Process and Precursor Development Using Neural-Network-Potential Atomistic Simulations and COSMO-SAC Thermodynamic Modeling*, Yukihiro Shimogaki,*** The University of Tokyo, Japan

Atomic layer deposition (ALD) is indispensable for gate-all-around transistors, high-aspect-ratio DRAM capacitors, and 3D NAND, where conformality and precise thickness control are both required. Atomic layer etching (ALE), the reverse of ALD, matters for low-damage, selective integration, while area-selective deposition (ASD) is attractive but suffers "selectivity loss": unwanted nuclei form on non-growth areas and degrade selectivity over time. We present a multiscale framework coupling COSMO-SAC thermodynamic modeling for precursor down-selection with neural-network-potential (NNP) atomistic simulations for reaction-mechanism analysis; an integrated ALD+ALE scheme designed within it enables highly selective, robust ASD.

An ideal precursor reaches saturation adsorption and is delivered stably; a vapor pressure >=100 Pa below 100 C, preferably ~1000 Pa, broadens the process window. Conventional COSMO-SAC is often inaccurate for metal-containing organometallics. By tuning dispersion-related parameters we obtained good agreement between predicted and measured vapor pressures, enabling efficient down-selection. For Co precursors the framework predicted a high vapor pressure for CpCoCOTFE; the synthesized compound showed ~1060 Pa at 85 C. The same volatility prediction directly guides ALE, where formation and removal of volatile products are central.

Surface-reaction analysis has long been limited by the cost of reaction-path and vibrational searches. NNP-based simulations (e.g., Matlantis) now provide near-DFT accuracy at large scale, making ALD/ALE surface mechanisms tractable. For the Co precursor, NNP indicated that controlling surface hydrogen coverage prior to dosing suppresses carbon incorporation from side reactions; this was confirmed experimentally, showing precursor design (vapor pressure) and reaction design (surface state) must be co-optimized.

For ASD with CCTBA, NNP molecular dynamics showed facile reaction on Cu but low reactivity on SiO_2, and selective growth on Cu was experimentally confirmed. Residual Co nuclei on SiO_2 degrade selectivity; we designed an ALE path in which Co is chlorinated by SO_2Cl_2 and reacts with Hfac to form volatile products whose volatility is supported by COSMO-SAC. The resulting ALD (growth) + ALE (nuclei removal) scheme restores robust selectivity. Finally, sub-monolayer growth per cycle (~0.1 ML) is rationalized by steric hindrance, and NNP-MD with kinetic Monte Carlo captures these collective adsorption dynamics. This COSMO-SAC + NNP framework offers a unified route to co-develop ALD/ALE processes (Atomic Layer Process, ALP) and precursors and to overcome ASD selectivity loss.

3:00pm **AP1+EL+MS+PS+TF-TuA-4 Re-designing ALD Experiments for AI-ready Data: The IGZO Case Study*, Eleni Poupaki,*** *Cas Visser, Freek Klabbers, Adrie Mackus, Erwin Kessels,* Eindhoven University of Technology, The Netherlands

The AtomicLimits ALD database [1] is a community-driven repository of ALD processes from the literature. The next step is to populate it with more data suitable for artificial intelligence (AI) and machine learning (ML) models. [2] Recent efforts have used large language models for structured data extraction from publications. [3] However, literature data remains fundamentally limited for data-driven modeling: it is incomplete, often missing key process parameters, biased toward successful experiments, and inconsistently reported. ML can accelerate ALD development by predicting film properties, guiding experiment design, and identifying optimal recipes. Unlocking this potential requires not only more data, but experiments designed to produce data suitable for ML. We address this challenge using ALD of InGaZnO (IGZO) as a case study. IGZO is a quaternary oxide semiconductor that has emerged as an alternative to crystalline silicon channels, used in displays and increasingly explored for DRAM. Amorphous IGZO exhibits high electron mobility, ultralow leakage, and a low thermal budget. [4,5] ALD is well-suited for IGZO, due to its sequential, self-limiting surface reactions, enabling precise control of thickness and composition. [6] For multicomponent materials like IGZO, composition is controlled via the supercycle approach, with subcycles of In_2O_3, Ga_2O_3, and ZnO. Their relative ratios and sequence strongly influence the resulting film properties [7], creating a vast, interdependent parameter space. In this work, we develop a protocol for generating AI-ready ALD experimental data, demonstrated on IGZO. The protocol proceeds stepwise from binary to ternary to quaternary processes, with explicit criteria at each stage: binary processes are characterized for saturation and nucleation, and the ternaries (GaZnO, InZnO, InGaO) are screened to identify supercycle criteria. Using these findings, we explore the supercycle parameter space, focusing on cycle ratio and mixing, with consistent characterization. We discuss preliminary trends in crystallinity and electrical properties across the explored space, contrasting with conventional optimization-driven experimentation. Finally, we outline how the resulting datasets enable ML-guided exploration of the IGZO supercycle space, paving the way toward AI-assisted ALD process optimization and a richer experimental foundation for community resources such as AtomicLimits.

[1] 10.6100/alddatabase

[2] Westermayr et al., Chem. Mater. 2026.

[3] Saddrudin, Poupaki et al., JVSTA 2026.

[4] Song et al., Nat. Electron. 2025.

[5] Okajima et al., IEDM 2025.

[6] Sheng et al., ACS AMI 2019.

[7] Oh et al., Ceram. Int. 2025.

3:15pm **AP1+EL+MS+PS+TF-TuA-5 Atomistic Modeling of Atomic Layer Etching and Deposition: HF/SiO2 ALE and TMA/Al2O3 ALD**, ***Fedor Goumans***, Software for Chemistry & Materials, Netherlands

Atomic layer processes rely on surface reactions that are sequential, self-limiting, and highly sensitive to local chemical structure. Understanding these reactions at the atomistic level is essential for improving atomic layer deposition, atomic layer etching, and area-selective processing, but many key reaction steps occur at buried, transient, or chemically heterogeneous interfaces that are difficult to characterize directly. In this presentation, we discuss how reactive atomistic simulations can support the interpretation and design of atomic layer processes, with examples from HF-based SiO_2 etching and TMA/Al_2O_3 deposition.

Reactive force fields and machine-learned interatomic potentials provide complementary routes for exploring surface chemistry over length and time scales beyond conventional first-principles molecular dynamics. Using these approaches, one can follow bond breaking and formation, surface hydroxylation, ligand exchange, fluorination, densification, and volatile product formation under process-relevant conditions. For SiO_2 etching, simulations can help identify how HF exposure modifies hydroxylated and strained oxide surfaces, how local bonding environments influence fluorination and material removal, and which surface motifs may control etch initiation. For Al_2O_3 deposition, simulations of TMA reactions with hydroxylated alumina surfaces can reveal the molecular origin of saturation behavior, steric effects, methane elimination, and the evolution of reactive surface sites across ALD cycles.

The broader goal is to connect the relevant calculated parameters such as sticking rate, thermal accommodation coefficients, and atomistic reaction mechanisms with experimentally observable trends in growth, etch rate, selectivity, and film quality. We highlight practical considerations for building reliable reactive models, including training data selection, validation against quantum chemical calculations, and the use of accelerated workflows. These examples illustrate how atomistic modeling can complement experiments by exposing reaction pathways, identifying limiting surface structures, and guiding the development of more predictive models for ALD and ALE process optimization.

4:00pm **AP1+EL+MS+PS+TF-TuA-8 Characterizing Directionality, Energy and Spatial Uniformity of Plasma Generated Neutral Beams for Low-Damage Material Processing**, ***Gonçalo A. Cardoso***, *Mark J. Kushner,* University of Michigan, Ann Arbor

Ion bombardment onto biased wafers during plasma etching can result in charge buildup within features that can deflect incoming ion trajectories, resulting in feature defects such as bowing or notching, or lead to device damage. UV photons emitted from the plasma might also cause surface defects such as dangling bonds [1]. These issues are exacerbated as device dimensions are scaled down, due to larger electric fields for a given charging potential and increased surface-to-volume ratio. This is particularly the case for the fabrication of 2-dimensional materials consisting of nearly monolayer thickness. Energetic neutral beams have been proposed as an alternative, low-damage and charge-free technique for etching and deposition, and particularly so for 2D materials. Such beams can be produced through ion acceleration and subsequent neutralization, either through charge-exchange collisions (volume neutralization) or by reflection from surfaces (surface neutralization) [2, 3]. The primary technical challenges for neutral beam sources involve optimization of directionality, energy and spatial uniformity of the energetic neutral fluxes striking the substrate.

In this paper, we discuss the results of a computational investigation of a neutral beam source consisting of an inductively coupled plasma separated from the wafer by a radio frequency (RF) biased grid powered at 10 MHz. Typical conditions for this source are pressures of tens of mTorr, gas mixtures containing Ar, O_2 and Cl_2 and biases on the grid of hundreds of volts. This source has been simulated using the Hybrid Plasma Equipment Model (HPEM).The Plasma Chemistry Monte Carlo Module (PCMCM) in the HPEM tracks the motion of ions (and neutrals) as they are accelerated by electric fields, collide with background gas particles and neutralize by reflecting from the grid. The PCMCM records the resulting neutral energy and angular distributions (NEADs) at the wafer. This work investigates the characteristics of these NEADs and how they are influenced by grid surface roughness (non-specular scattering), inelastic scattering from the grid, gas-phase charge-exchange reactions and pressure gradients across the grid.

This work was supported by the US Department of Energy, Office of Science, Fusion Energy Sciences (FES) and Basic Energy Sciences (BES) as part of the Extreme Lithography & Materials Innovation Center (ELMIC), a Microelectronics Science Research Center (MSRC), through the Plasma-enabled 2D Materials project (DEAC02-09CH11466); and by FES (SC-00274510).

4:15pm **AP1+EL+MS+PS+TF-TuA-9 Plasma Etching of Diamond: Molecular Dynamics Studies and Comparison to Experiments**, ***Louis Hoffenberg***, Princeton University; *Justin Boles,* University of Houston; *Jack Draney,* Princeton University; *Igor Kaganovich,* Princeton Plasma Physics Laboratory; *Vincent Donnelly,* University of Houston; *David Graves,* Princeton University

Nitrogen-vacancy (NV) centers in diamond are promising for multiple applications in quantum information processing and sensing, including in the fields of high-power/high-frequency electronics, quantum computing, and quantum sensing.[1] Diamond NV centers near surfaces can locally detect and measure physical quantities such as magnetic and electric fields with unprecedented sensitivity. However, these devices are currently limited by near-surface (<10 nm) defects that compromise charge stability and spin coherence.[2] Plasma etching of diamond has been widely employed to process and pattern diamond, but there is limited understanding of the mechanisms of plasma etching. In this work, classical molecular dynamics (MD) simulations are used to simulate O_2/Ar plasma etching of diamond, with comparisons to experiment. We explore both conventional reactive ion etching (RIE) and atomic layer etching (ALE) conditions. The experimentally validated MD simulations are used to identify fundamental etch mechanisms. Based on the MD simulations, we propose a parameterized reduced order model of diamond plasma etching that relates etch yield to ion flux, ion energy, and ion composition, as well as neutral O• radical to ion flux ratio.

References:

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4:30pm **AP1+EL+MS+PS+TF-TuA-10 Predictive Screening of Sustainable Etchants via DFT Thermodynamics, Machine-Learned Vapour Pressures, and Infrared Spectra**, ***Christopher Pashartis***, *Philippe Bezard, Konstantina Philippidou, Geoffrey Pourtois,* IMEC Belgium; *Hideharu Shimizu, Yoshiki Nakoyama,* NSC, Belgium

Fluorinated etchants are heavily used in semiconductor processes for their high etch rates and material selectivity. Typical etchants such as CF_4 and c-C_4F_8 have global-warming potentials in the range of 7,400-13,900 over 100 years and atmospheric lifetimes exceeding hundreds of years, raising concern about the by-products of such processes. While abatement downstream is standard practice, it runs continuously and is never fully effective. Therefore, a more impactful path to reducing the climate footprint of fabrication is to identify replacement etchants that are intrinsically more sustainable while remaining competitive in performance.

Experimentally screening new etchants includes sourcing gases, fine-tuning reactor conditions, characterising effluent; it can be very slow and time consuming. We present a predictive screening workflow built on Density Functional Theory (DFT) rather than specialised plasma simulations: DFT-derived Gibbs free energies are used to solve the closed-system equilibrium for each etchant-substrate pair, giving both the predicted etch capability and the by-product distribution as a function of temperature, pressure, and stoichiometry. To translate predicted species into global warming potential, we couple this with two further ingredients: a graph neural network trained on open-source vapourpressure data to determine which by-products are most likely to be gaseous, and DFT-computed infrared spectra to estimate their radiative efficiency. We will present results aggregated across more than ten candidate etchants and three substrates (Si, SiO_2, Si_3N_4), demonstrating how the combined thermodynamics-volatility-impact screen can rank chemistries by their projected greenhousegas burden.

Atomic Scale Processing Mini-Symposium
Room 316 - Session AP2+EL+PS+TF-TuA

Advancing X-Ray Photoelectron Spectroscopy to enable Atomic Scale Processing

Moderators: Dr. Robert Bruce, IBM Research, T. J. Watson Research Center, **Dr. Eric Joseph**, IBM T.J. Watson Research Center

4:45pm **AP2+EL+PS+TF-TuA-11 Understanding the Chemical Reaction Mechanisms of Oxide, Nitride and Metal ALD: Insights from Operando X-Ray Photoelectron Spectroscopy***, Joachim Schnadt,* Lund University, Sweden **INVITED**

Over the past decades, atomic layer deposition (ALD) has emerged as a leading thin-film deposition technique, particularly within semiconductor technology. The reason is that ALD provides excellent thickness control down to the atomic scale, as a result of the use of sequences of self-limiting surface reactions. However, continued device miniaturization imposes more and more stringent demands on process control. Interfaces need to be engineered with extremely high precision, and lateral dimension control grows in importance. This implies that the exact surface chemistry underlying ALD – and this chemistry is both process and surface specific – needs to be understood in true detail. Experimental *operando* techniques provide an avenue towards the monitoring and characterization of the ALD surface chemistry in a time-resolved manner; these techniques can be applied during the deposition and at measurement rates that allow to resolve the time evolution of surface species and surface structure. Ambient pressure X-ray photoelectron spectroscopy (APXPS) is such an *operando* tool. In contrast to conventional X-ray photoelectron spectroscopy, it is carried out at pressures up to the millibar range, i.e. exactly the operational pressure regime of ALD. Time-resolved APXPS provides precise insight into the occurrence and time evolution of surface and subsurface species and their chemical state and provides information that can be used to formulate chemical reaction mechanisms in the different stages of deposition. In my presentation, I will discuss the capabilities of *operando* APXPS for research into ALD, using examples of research into the ALD of metal oxides and nitrides from transition metal amido or metal tetraisopropoxide complexes and water or ammonia. I will also highlight the first APXPS study into Pt metal ALD. Due attention will be given to instrumental aspects, foreseen future developments and a discussion of what can and what cannot be learned from APXPS.

5:15pm **AP2+EL+PS+TF-TuA-13 In vacuo XPS for Studying ALD Processes***, Matthias Minjauw, Tippi Verhelle, Jin Li, Jolien Dendooven,* ***Christophe Detavernier,*** Ghent University, Belgium **INVITED**

X-ray photoelectron spectroscopy (XPS) is a well-established technique for probing near-surface composition and chemistry. When employed as an in vacuo technique—i.e., without intermittent air exposure—it becomes a powerful tool for investigating surface chemistry during atomic layer deposition (ALD) processes. Three case studies will be presented: (1) the well-known TMA-based chemistry for ALD of alumina, (2) metal ALD with a focus on Pt growth (as reported by Li et al., J. Phys. Chem. C 2024, doi:10.1021/acs.jpcc.3c07568), and (3) ALD on lithium foil substrates (as reported by Verhelle et al., J. Mater. Chem. A 2026, doi:10.1039/D6TA00751A).

Applied Surface Science
Room 319 - Session AS-TuA

Applied Surface Science in Action II

Moderators: Dr. Hong Piao, FUJIFILM Electronic Materials USA., Inc., **Dr. Jeffrey Terry**, Illinois Institute of Technology

2:15pm **AS-TuA-1 Quantification of Surface Functional Groups on Nano- and 2D Materials***, Jörg Radnik,* Federal Institute for Material Research and Testing (BAM), Germany **INVITED**

Surface chemistry plays a crucial role in determining the properties of nanoforms. Incorporation into a matrix, solubility, and dispersibility are all strongly influenced by their surface. Therefore, measurements of surface functionalization are essential for nanoforms, both in terms of applicability and regarding safety and sustainability. Despite this importance, the reliable quantification of functional groups on nanoforms remains a challenge. Documentary standards have recently been published or are currently under development, proposing X-ray photoelectron spectroscopy (XPS) as one of the key methods.[1]

In developing protocols for the quantification of surface functionalities, we chose two approaches: (i) correlative measurements, in which the same samples were analyzed using at least two different methods, and (ii) interlaboratory comparisons (ILCs) carried out across multiple laboratories. Both approaches were successfully applied to functionalized graphene nanoplatelets. The comparison of XPS and energy-dispersive X-ray spectroscopy (EDS@SEM) results shows good agreement between the two methods when the different analysis volumes are considered.[2] The international ILC with XPS as method revealed a pronounced influence of excessively high humidity and sample preparation on the results.

XPS and quantitative nuclear magnetic resonance (qNMR) measurements were carried out on aminated silica nanoparticles, enabling a correlation between the N/Si ratio determined by XPS and the amine coverage on the nanoparticle surface derived from NMR.[3] Comparative measurements performed in two laboratories yielded comparable results. Based on the results obtained, uncertainty budgets could also be established.

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2:45pm **AS-TuA-3 Compositional Analysis of Al1-XScXN Thin Films***, Jeffrey Shallenberger, Saeed Almishal, Jon-Paul Maria,* Penn State University*; G. Bruce Rayner,* Kurt J. Lesker Company

Aluminum scandium nitride ($Al_{1-x}Sc_xN$) has received a lot of attention because of its ferroelectric properties and ability to be integrated on silicon. It has been synthesized over a wide compositional range by a variety of growth and deposition techniques including sputtering, molecular beam epitaxy (MBE) and atomic layer deposition (ALD). Determination of the composition of $Al_{1-x}Sc_xN$ thin films has been done by a variety of techniques including: SEM-EDS, XRF, RBS, SIMS and XPS. This talk will focus on the use of XPS to characterize both thin (~30 nm) and thick (300 nm) films produced by ALD and sputtering, respectively. XPS offers depth-resolved compositional information which is important as these films frequently have AlN layers to improve epitaxial growth or are grown on sapphire substrates. EDS, XRF and RBS have relatively poor depth resolution making it difficult or impossible to determine the stoichiometry in these cases, particularly on very thin films. Accurate measurement of oxygen content is also important as high levels of oxygen can degrade the ferroelectric properties.

We utilize Rutherford backscattering (RBS) to help calibrate the XPS-derived stoichiometry of a series of $Al_{1-x}Sc_xN$ films ($0.58<x<0.15$). This talk will also discuss the relative advantages and disadvantages of the commonly utilized thin film compositional techniques with a goal of providing guidance to users when selecting an analytical tool.

3:00pm **AS-TuA-4 Surface-Engineered Nanostructures for Wastewater Contaminants Sensing and Its Treatment by Thermocatalysts***, Zong-Hong Lin,* National Taiwan University, Taiwan*; **Jinn P. Chu,*** National Taiwan University of Science and Technology, Taiwan

Ensuring access to clean water is a critical global health challenge, yet the energy required for contaminant monitoring and treatment intensifies resource pressures. Self-powered sensing and remediation systems offer a sustainable path forward. This study introduces multifunctional surface-engineered metallic nanotube arrays (MeNTAs) as a tunable platform for both pollutant detection and degradation. By tailoring composition and structure, we controlled surface wettability across a wide range (5°–144°) to suit specific functions.For detection, a Ni-W-Ni MeNTA with optimal triboelectric output was integrated into a droplet-mode liquid-solid triboelectric nanosensor (DLS-TENS). Modified with ion-selective membranes, it rapidly (20 ms) and sensitively detected heavy-metal ions (Cr^{6+}, Pb^{2+}, Hg^{2+}). For bacterial sensing and thermocatalytic treatment, W-SS MeNTAs were employed. Their hydrophilic stainless-steel nanoparticles

enabled in-situ synthesis of aptamer-functionalized gold nanoparticles for highly sensitive E. coli detection (163 mV/decade). Simultaneously, surface Fe^{2+} ions catalyzed •OH radical generation via the Fenton reaction, while adhered Bi_2Te_3 nanoflakes generated H_2O_2 under a small thermal gradient (10 °C). This system achieved significant bacterial inactivation (E. coli: 97%; S. aureus: 95%) and 95% Cr^{6+} reduction.To demonstrate practical utility, we constructed a wireless sensing bottle for real-time wastewater analysis and integrated it with a treatment module for on-site, simultaneous monitoring and purification. This work presents a cost-effective, portable, and self-powered platform, highlighting the strong real-world potential of multifunctional MeNTAs for advanced water purification.

3:15pm **AS-TuA-5 Multi-Technique Structural and Chemical Characterization of Native Oxide Evolution on Niobium Thin Films for Nasa Astrophysics Detectors**, ***FEMI AKINRINOLA***, *Robbyn Trappen, Nethmi Loku Kankanamge, Tap Raj Bhandari,* West Virginia University, USA*; Thomas Stevenson, Emily Barrentine,* NASA Goddard Space Flight Center*; Mikel Holcomb,* West Virginia University, USA

Niobium-based superconducting detectors, including microwave kinetic inductance detectors (MKIDs) and transition-edge sensors (TESs), are critical for future NASA astrophysics missions operating in the far-infrared to microwave spectral range. Their performance can be strongly influenced by native oxide formation and surface chemical modifications introduced during fabrication and post-processing. Building on our previous X-ray absorption spectroscopy (XAS) investigation of niobium oxide formation in superconducting device structures, we present an expanded study combining XAS with grazing-incidence X-ray diffraction (GIXRD) and X-ray reflectivity (XRR) to obtain complementary chemical and structural information from the near-surface region of Nb thin films.

This work examines Nb films subjected to multiple surface-processing conditions relevant to superconducting device fabrication, including pristine films, buffered oxide etch (BOE) treatments, unbuffered HF treatments, and hydrogen-exposure conditions. Oxygen K-edge XAS is used to probe changes in the local electronic structure and bonding environment associated with oxide evolution, while GIXRD measurements at multiple incidence angles are used to evaluate crystalline phase formation and structural changes near the film surface. XRR measurements provide additional information on film thickness, interface quality, density, and surface roughness. Preliminary XRR analysis indicates that the films remain structurally dense after processing while supporting thin oxide-like surface layers, whereas GIXRD measurements show that crystalline metallic Nb remains the dominant phase in the films studied thus far.

Rather than relying on a single characterization technique, this combined approach is intended to provide a more complete understanding of how different fabrication and surface-treatment conditions influence oxide evolution, crystallinity, and near-surface structure in Nb-based superconducting materials. Ongoing analysis is focused on correlating spectroscopic trends observed in XAS with structural information obtained from GIXRD and XRR across the different processing conditions. These results contribute to NASA's broader effort to better understand and optimize superconducting detector fabrication processes for future space-based astrophysics missions.

We acknowledge support from NASA 80NSSC22M0173 and NSF 2417349.

4:00pm **AS-TuA-8 Interfacial Solution Structure Impacts Crystal Growth, Ice Nucleation, and Particle Aggregation**, ***Elias Nakouzi,*** Pacific Northwest National Laboratory*; Mingyi Zhang,* University of Oklahoma*; Kuan-Ting Liu, Dong June Jang,* Cornell University*; Philip Brahana, Bhuvnesh Bharti,* Louisiana State University*; Jaehun Chun,* Pacific Northwest National Laboratory*; Ulrich Wiesner, Lara Estroff,* Cornell University **INVITED**

Solution structure at solid-liquid interfaces creates inter-particle forces and chemical potential gradients that influence particle stability, reactivity, and aggregation. However, despite this relevance to a variety of research fields, significant knowledge gaps remain in our understanding of solid-liquid interfaces at the molecular scale. Using a combination of atomic force microscopy, confocal fluorescence microscopy, colloidal theory, and atomistic simulations, we present three case studies examining the effect of interfacial solution structure on particle aggregation, crystal growth, and heterogeneous nucleation. Firstly, we determined that extreme salt concentrations enhance ion correlations at the surface of boehmite nanoparticles, resulting in strong repulsive forces at short particle separations that decrease the rate of particle aggregation. In the second study, we investigated the incorporation of ligand-coated nanoparticles in growing calcite crystals. This process is governed by the interactions experienced by an incoming particle as it penetrates the interfacial hydration layers, as well as the binding energy upon adsorption to the growing crystal surface. Thirdly, we determined that oxidizing a polymer surface results in the assembly of hydration layers at the polymer-water interface, which increase the surface hydrophilicity and the propensity for nucleating ice. We anticipate that these studies will provide insights into the molecular nature of solid-liquid interfaces with important implications on relevant problems in geochemistry, electrochemistry, and materials synthesis.

4:30pm **AS-TuA-10 Surface Distribution, and Thermal Evolution in Nuclear Graphite: What We Can Learn Using XPS**, ***Jonathan Counsell,*** Kratos Analytical Limited, UK*; Chris Moffitt,* Kratos Analytical Inc.

Analysis of material samples related to nuclear industry remains an important research area considering the rapid evolution of new nuclear power plants planned for the coming century. Critical in these systems is the neutron moderator material graphite. Understanding the interaction of high-energy particles radiation and these effects on structure and chemistry of the graphitic lattice.

XPS is used to analyse the changes in sp2/sp3 character under high-energy Cs ion bombardment and the relationship between dose and depth of change for impinging ions. We will discuss not just structural changes but also chemical relationships between the ions present in the near-surface region and the constituent graphite. We will show how HAXPES can be used to gain insight also.

The life cycle of a graphitic rods in a reactor involves withstanding harsh environments, therefore, considering the operating environment, we explore the effects of heating to determine possible thermal effects from thermal cycling. Here we will exploit different options for analysis including in-situ thermal treatments of the surface to understand the processes occurring in the surface and the stabilisation of incorporated ions. We will introduce best practices and experimental design considerations to optimise and probe the process taking place.

4:45pm **AS-TuA-11 Energy Materials and the Importance of Cryo-XPS**, ***Liam Soomary,*** Kratos Analytical Limited, UK*; Chris Moffitt,* Kratos Analytical Inc.

The development of advanced energy storage materials is crucial for the transition to sustainable energy solutions. Cryogenic X-ray Photoelectron Spectroscopy (cryo-XPS) plays a pivotal role in understanding the surface chemistry and electronic properties of these materials under extreme conditions. This study focuses on vitrification techniques to preserve the transient states of energy storage materials, allowing for accurate characterization before degradation occurs.

Using cryo-XPS, we investigate the surface distribution and chemical composition of various energy storage materials, capturing transient states and reducing beam damage through optimized sample preparation and analysis protocols. Software workflows, developed for specific sample types are utilized to streamline the data acquisition and post-processing steps, ensuring reproducibility and reliability of the results. Additionally, vacuum damage is minimized by employing cryo conditions, which are critical for maintaining the integrity of the sample during analysis.

This work highlights the importance of cryo-XPS in providing detailed insights into the surface properties of energy storage materials, enabling the identification of key mechanisms governing their performance. By integrating vitrification, software workflows, and vacuum optimization, we aim to advance the understanding and development of next-generation energy storage technologies.

5:00pm **AS-TuA-12 In-Vacuo Detection of Ti Hydride Using Advanced XPS Technique**, ***Ravi Prakash***, *Jacqueline van Veldhoven,* Semicon Equipment Lifetime, TNO, the Netherlands Organisation for Applied Scientific Research, Netherlands*; Herman Bekman, Leon Arkesteijn,* Semicon Equipment Metrology, TNO, the Netherlands Organisation for Applied Scientific Research, Netherlands*; Ronald Hultermans, Violeta Navarro Paredes, Mark van de Kerkhof,* ASML, Veldhoven, Netherlands

Titanium has an outstanding strength-to-density ratio, high tensile strength, and is naturally resistant to chemical corrosion. Due to the favourable mechanical properties in harsh environments, titanium is widely used in chemical processing equipment, aerospace structures and marine systems. However, when it is exposed to environments with H_2-gas/H-radicals/H-ions, hydrogen may diffuse into the bulk titanium and start forming hydrides which leads to embrittlement, posing a significant risk under extreme conditions.

To measure hydride formation in titanium in-vacuo is crucial. ToF-SIMS and EBSD are ideal techniques to detect the hydrides, but using these techniques requires a very specific combination of exposure and analysis techniques which is not very common. If a hydride containing Ti sample is exposed to air, the surface state may alter, which limits the ability to detect early stage hydride formation on the surface. Also, our investigation shows that titanium oxidizes rapidly even under UHV conditions.

This work introduces a novel in-situ methodology for detecting titanium hydride using X-ray photoelectron spectroscopy (XPS) focused on valence band measurements. A plasma/radical exposure tool attached to an XPS setup enables in-vacuum sample transfer, which allows to study hydrogen ingress in a controlled environment during exposure to H-plasma/H-radicals/H_2-gas. The approach uses a peak fitting model to isolate the overlapping oxygen and titanium hydride signals in the valence band region. Correlating this signal with the oxygen O 1s content enables the identification of hydride formation. This method reliably differentiates between hydride-containing and hydride-free samples, allowing for the early-stage detection of embrittlement precursors after hydrogen exposure. This method not only improves detection sensitivity but also streamlines the experimental workflow by eliminating the need for additional ex-situ measurements. This allows for quicker testing of more representative samples that could contribute to enhancing lifetime.

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5:15pm **AS-TuA-13 Chemical Mapping of sub-Monolayer Oxygen Functionalities on Acid Treated HOPG Surfaces Through Photo-Induced Force Microscopy*, David Morgan,*** Cardiff University, UK

Carbon is widely used as a support for heterogeneous catalysts because of their relatively low cost, high surface area and the ease with which precious metals can be reclaimed from the support at the end of the catalyst's active life [1]. In most cases, these carbons are acid washed, before the adsorption of the active component. The wash serves two purposes; it removes unwanted inorganic contaminants present in the carbon; and it introduces oxygenated functionalities that modify the behaviour of the carbon towards the adsorption of the active component and the reaction solvent [2].

Our previous work using HOPG as a model substrate has shown HCl and HNO_3 has a significant impact on the surface topography through intrusion by the acid into the graphite, causing weakening and breakage of the interplanar bonds [3]. Chemical derivatisation studies via XPS, has shown that depending on the acid, the surface forms hydroxyl, carbonyl and nitrate containing functions, however, to date the location of these features, especially with relation to the protrusions are unknown [4].

Herein, we present the first Photo-Induced Force Microscopy (PiFM) studies of acid treated HOPG surfaces allowing the unambiguous correlation of surface topography with sub-monolayer oxygen functionalities through chemically distinct vibrational spectra.

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5:30pm **AS-TuA-14 The XPS of Azines: Relationship to Chemical Bonding*, Paul S. Bagus,*** University Of North Texas, United States Minor Outlying Islands (the)*; Connie J. Nelin,* Cosultant

The properties of several azine molecules, particularly their XPS spectra, are examined. These molecules contain one, two, or three nitrogen atoms positioned in either equivalent or inequivalent sites within the benzene ring, where N replaces a C–H unit. The primary objective is to determine the extent to which C(1s) and N(1s) XPS can be used to identify specific molecular species and whether these spectra can be directly related to chemical bonding. The analysis focuses on binding energies (BEs) and relative intensities, I_{rel}. Interpretation of the spectra requires theoretical input because the observed XPS features include contributions from inequivalent atoms whose energy splittings, often on the order of ~1 eV, are near or below the resolution limit of standard measurements. To address this, Dirac Hartree-Fock calculations are used to obtain wavefunctions for both initial states and core-hole final states, providing reliable estimates of BE shifts and relative intensities. While our results are specifically for the azines whose spectra are analyzed, they have important implications for the interpretation of the XPS of other compounds. A key question is whether final-state effects are approximately constant across different atoms and molecules. If so, Koopmans' Theorem. which neglects relaxation, may be sufficient to relate XPS to chemical bonding; otherwise, explicit treatment of relaxation effects is required. Additional factors such as bond length variations and environmental effects are also considered. The focus will be on the main XPS features but excitations that would lead to satellite features are also considered. Pyrazine ($C_4N_2H_4$), which has only one inequivalent nitrogen and one inequivalent carbon atom, serves as a reference system. Its relatively simple spectrum aids in interpreting more complex molecules such as pyridine and pyrimidine, each of which contains three inequivalent carbon atoms and Triazines, with additional inequivalent atoms.

Biomaterial Interfaces
Room 321 - Session BI-TuA
Functional Materials and Biosensing

Moderators: Dr. Kenan Fears, U.S. Naval Research Laboratory, **Prof. Morgan Hawker**, California State University, Fresno

2:15pm **BI-TuA-1 Fibronectin and ECM-Mediated Regulation of Synovial Fluid Film Formation and Nanomechanics*, Roberto Andresen Eguiluz,*** University of California Merced **INVITED**

Film formation is critical during locomotion to lubricate and protect the surface of articulated joints. The molecular components of the cartilage extracellular matrix (ECM) provide anchoring sites for lubricating molecules, thus serving as a platform for the assembly of the load/energy-dissipative films. The role of the collagen family in mediating the adsorption of lubricating and wear-protecting molecules, such as lubricin or hyaluronan, has been studied. However, the role of fibronectin (Fn) and its various conformations in regulating the adsorption of synovial fluid (SF) components and the wear-protecting properties of SF has been overlooked. During this talk, I will present our research efforts to understand the roles of various ECM components in controlling the supramolecular assembly of SF-derived films and SF components, and to gain insights into the synergies that regulate synovial joint surface nanomechanics. For this end, we employ experimental tools that include the surface forces apparatus (SFA), quartz crystal microbalance with dissipation (QCM-D), and atomic force microscopy, which I will briefly introduce.

2:45pm **BI-TuA-3 Magnetic Microparticle Biointerfaces for Fluorescence-Based Detection of C-Reactive Protein in Biological Fluids***, Pegah Jamali, Zia Syed, **Umer Hassan,*** Rutgers, The State University of New Jersey

Biofunctionalized particle surfaces are useful model interfaces for studying biomolecular recognition while also enabling compact biosensing formats. In this work, we developed an antibody-presenting magnetic microparticle interface for fluorescence-based detection of C-reactive protein (CRP), an inflammatory biomarker associated with infection. The study focuses on the design and characterization of the bead–biomolecule interface, including antibody immobilization, target capture, fluorescence signal generation, and matrix-dependent assay response in biological fluids.

Carboxylated magnetic microparticles were chemically activated using EDC/NHS chemistry to create reactive surface groups for covalent antibody attachment. Anti-human CRP antibodies were then immobilized on the particle surface to form a biomolecular capture interface. The

functionalized particles were incubated with FITC-labeled recombinant human CRP prepared across a concentration range of 0.5–100 µg/mL. After magnetic washing, bead-associated fluorescence was measured by optical microscopy, and image-based quantification was performed using background-corrected mean intensity analysis. This workflow links the surface density and stability of antibody-functionalized microparticles with the resulting optical response from captured protein.

The particle biointerface produced a concentration-dependent fluorescence signal in PBS buffer, human serum, and human urine. Calibration curves showed strong analytical linearity in all three matrices, with regression fits of $y = 54.10 + 1.12x$, $R^2 = 0.98$ in PBS; $y = 58.95 + 1.35x$, $R^2 = 0.98$ in serum; and $y = 13.0 + 0.32x$, $R^2 = 0.95$ in urine. The assay achieved a limit of detection of 0.5 µg/mL across all matrices. Serum produced the strongest optical response, while urine showed reduced sensitivity, highlighting the role of fluid composition, ionic environment, and nonspecific matrix effects on antibody–antigen recognition at the bead surface. Surface-conjugation stability was also evaluated over 28 days at 4°C and room temperature, with approximately 90% of the initial fluorescence signal retained, supporting the robustness of the covalent antibody–particle interface.

These results demonstrate a functional magnetic microparticle biointerface for CRP capture and fluorescence microscopy readout in complex biological environments. The platform is relevant to biomaterial-interface engineering, optical characterization of biofunctional surfaces, and particle-based biosensing, with future potential for integration into microfluidic workflows for rapid inflammatory biomarker testing.

3:00pm **BI-TuA-4 Potassium-Selective Nanoelectrode Arrays for Single-Cell Profiling of human iPSC-Derived Cardiomyocytes***, **Dhivya Pushpa Meganathan**, Joseph Wang,* University of California San Diego*; Zeinab Jahed Zeinab Jahed,* University of California at San Diego

Potassium ion (K^+) dynamics are central to cardiac electrophysiology, with early disruptions in K^+ flux often preceding arrhythmia and contractile dysfunction. However, current sensing technologies, such as patch-clamp, Microelectrode arrays (MEAs), and fluorescent indicators, either lack chemical specificity for K^+ or are unsuitable for long-term, single-cell analysis. Conventional ion-selective electrodes (ISEs), while more selective, are limited by bulk-phase design and poor spatial resolution. To address these limitations, we present KINESIS (K^+-Ion Nano-Electrode Selective Interface System), a nanofabricated, cell-compliant platform that enables direct, label-free potentiometric measurement of K^+ gradients with subcellular precision. KINESIS features high-aspect-ratio nanopillars coated with a valinomycin-based K^+ recognition membrane, forming a stable, non-invasive interface with human induced pluripotent stem cell-derived cardiomyocytes (hiPSC-CMs). This architecture allows localized, Nernstian sensing of K^+ efflux or depletion without disrupting cell membranes. Pharmacological validation shows distinct potential shifts in response to caffeine and ouabain. KINESIS thus offers a highly selective, spatially resolved approach for studying K^+ handling in cardiotoxicity screening and patient-specific disease modeling.

3:15pm **BI-TuA-5 Peptide Biosensor for Pathological Tau Detection in Neurodegenerative Disease***, **Megan Pitz**, Rebecca Mickol, Hugo Miranda Quijada, Sean Brown, Kenan Fears, Maryssa Beasley,* US Naval Research Laboratory

Tauopathies are a class of neurodegenerative diseases that are characterized by an abnormal aggregation and accumulation of the tau protein. Included in this class are Alzheimer's disease (AD), chronic traumatic encephalopathy (CTE), corticobasal degeneration (CBD), and Pick's disease (PiD), among others. Definitive diagnosis of many of these diseases is limited to post-mortem analysis of brain tissue, due to a lack of medical technologies allowing diagnosis during the patient's lifetime. However, diagnosis of these diseases ante-mortem would allow for much more targeted care and treatment for these patients. Therefore, there is a compelling need for technologies that can identify tau accumulations ante-mortem with high specificity. Here, we present a peptide-based biosensor system with the goal of detecting pathological tau aggregations in biological samples ante-mortem. One limitation in developing tau biosensors is the difficulty in producing the tau protein in laboratory settings. Consequently, in this project, we first explored recombinant expression of dGAE, a truncated form of tau which is responsible for protein aggregation. This protein segment has been historically difficult to express due to its high propensity for aggregation, interfering with efficient recombinant expression and purification. We explored three different purification tags to decrease aggregation after protein expression and compared total protein yields across expression and purification conditions. The second aim of this project explored a detector peptide system for identifying tau aggregations. A de novo peptide sequence was designed and evaluated via molecular dynamic simulations for its ability to selectively identify tau aggregates using a molecular probe. Preliminary results show the detector peptide aligning and changing conformation in the presence of tau aggregates, suggesting a peptide system capable of acting as a biomolecular probe for identifying pathological tau accumulation.

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Electronic Materials and Photonics
Room 318 - Session EM-TuA

Pioneering Directions in Logic and Memory Devices and Materials: AI Hardware, Microelectronics, 2D Materials, Processing, Interconnect, Heterogeneous Integration, Energy Cooling

Moderators: Dr. M. David Henry, Sandia National Labs, **Prof. Dr. Haozhe "Harry" Wang**, Duke University, **Prof. Michelle Paquette**, University of Missouri-Kansas City, **Dr. Fei Zhou**, Sandisk Corp.

2:15pm **EM-TuA-1 Topography as a Design Knob to Create Exotic Electronic Phenomena in 2D Materials***, **Sunny Gupta**, Boris Yakobson,* Rice University **INVITED**

When atoms are confined to atomically thin two-dimensional (2D) lattices, they host many electronic behaviors that simply do not exist in bulk crystals, putting 2D materials at the heart of next-generation electronic and quantum technologies. Beyond their reduced dimensionality, 2D materials possess another remarkable feature: like a sheet of paper, they can bend, wrinkle, and undulate. These topographical deformations are not merely structural imperfections; they can act as powerful design knobs that generate new electronic phenomena absent in pristine flat systems. In this talk, I will present how quantum ab initio theoretical calculations can be used to explore **topography as a design principle** for discovering exotic electronic behavior in 2D materials. I will discuss how engineered undulations in monolayers generate pseudo-electric and pseudo-magnetic fields, enabling electron-optics effects [1], one-dimensional correlated electronic states [2], artificial quantum wells [3], and long-lived persistent spin-helix textures [4] relevant to spintronics. These examples show that controlled curvature and strain can transform simple 2D crystals into platforms for emergent quantum functionality. More broadly, this work points toward a new design paradigm, **curvatronics**, where geometry and topography are used as active ingredients for engineering quantum materials.

[1] Nano Lett. 22, 2934–2940 (2022)

[2] Nature Communications 13, 3103 (2022)

[3] Physical Review B 112, 115308 (2025)

[4] Matter 8,102378 (2025)

2:45pm **EM-TuA-3 Engineering Precursor Chemistry for Deterministic Growth of Two–Dimensional Semiconductors***, **Andrew Mannix**,* Stanford University

Atomically thin semiconductors are a leading platform for next-generation electronic, photonic, and quantum devices. Their promise depends on synthesis methods that deliver crystalline quality and uniformity rivaling exfoliated flakes, a standard that grown monolayers have historically failed to meet. In this talk, I will present advances in chemical vapor deposition (CVD) of transition metal dichalcogenides (TMDs) driven by deliberate control of the reactor environment: tuning precursor oxidation state, promoting salt-flux transport, and managing trace impurities to improve nucleation, reduce defect densities, and bring polytype and doping under direct control.

For solid-source CVD growth of WSe_2, uncontrolled oxyselenide formation and residual impurities can seed parasitic nucleation and degrade film quality. We address this with a targeted pre-annealing strategy that removes contaminant phases and yields a chemically more uniform, kinetically favorable precursor [1]. The resulting monolayer WSe_2 shows improved uniformity, grain sizes of ~10-30 µm, and charged defect densities below 10^{10} cm^{-2} as quantified by conductive AFM, enabling high-performance monolayer p-type transistors with on-state currents up to 888 µA/µm.

To extend these controls to wafer-scale synthesis and systematic chemical tuning of WS_2 and WSe_2, we employ metal-organic chemical vapor deposition (MOCVD) and a hybrid approach that uses solution-processed transition-metal salt precursors [2]. This route enables repeatable control of substitutional doping, alloy composition, and polytype, including selective formation of the ferroelectric 3R phase under confined-space growth conditions [3]. Across both platforms, machine-learning-enhanced hyperspectral reflectance microscopy provides rapid, spatially resolved feedback at high throughput [4]. We further implement locally engineered dopant gradients during MOCVD to program lateral carrier density profiles.

Together, these results advance oxidation-state control and precursor engineering as practical levers for making composition, defects, polytype, and doping more deterministic in two-dimensional semiconductors. [1] A. T. Hoang et al., arXiv, arXiv:2509.07299 (2025).[2] Z. Zhang*, L. Hoang* et al., ACS Nano, 18, 25414 (2024). doi:10.1021/acsnano.4c02164[3] Z. Zhang et al., Nano Letters, 24, 12775 (2024). doi:10.1021/acs.nanolett.4c02766[4] Z. Peng et al., 2D Materials, 13 (2), 025005, 2026. doi:10.48550/arXiv.2506.1834

3:00pm **EM-TuA-4 Natural Organic Fructose based Sustainable Resistive Switching Memory for Neuromorphic Computing**, *Md Shakil Jiban,* Missouri University of Science and Technology*; Zhigang Xiao,* Alabama A&M University*; **Feng Zhao**,* Missouri University of Science and Technology

The rapid expansion of AI and IoT demands computing systems capable of efficiently processing trillion–scale datasets. Conventional Von Neumann architectures, which separate memory and computation, suffer from severe energy inefficiencies due to frequent data transfer and raise sustainability concerns because of their reliance on inorganic, non–renewable materials. Neuromorphic computing offers a compelling alternative by mimicking the brain's ability to store and process information within the same physical structure. Resistive switching memory (RSM) is a key enabling technology, as they integrate memory and computation in a single device. When implemented using renewable and biodegradable natural organic materials, RSM can further advance environmentally sustainable neuromorphic systems.

In this work, we present an eco–friendly RSM based on fructose, a naturally abundant monosaccharide extracted from fruits and vegetables. The fructose-RSM is fabricated via a solution–based process to form a dried organic film sandwiched between an ITO bottom electrode and an Al top electrode, creating a metal–dielectric–metal structure analogous to biological neurons and synapses. The device exhibits reliable non–volatile memory characteristics, including resistive switching, endurance, and retention, as well as essential synaptic functions such as potentiation and depression, short– and long–term memory, and neural facilitation. These results represent an important step toward sustainable, energy–efficient neuromorphic computing systems based on natural organic materials.

3:15pm **EM-TuA-5 Read Transistor Engineering in Heterogeneous 2T0C DRAM for Multi-level Operation for Artificial Synapse Applications**, ***Minkook Kang**, Peter Hayoung Chung, Youngwook Kim, Jae-Gwan Park, Tae-Sik Yoon,* Ulsan National Institute of Science and Technology, Republic of Korea

Conventional 1T1C DRAM faces fundamental scaling limitations due to the use of capacitor, leading to challenges in maintaining sufficient charges as device dimension shrinks. To address this issue, capacitor-less memory architectures such as 2T0C DRAM have been proposed, offering improved scalability ($4F^2$) and longer retention characteristics. Amorphous oxide semiconductor thin film transistors (TFTs) are actively investigated for 2T0C DRAM due to their excellent uniformity, high mobility, low off-current, and back-end-of-line (BEOL) compatibility.

2T0C DRAM consists of two transistors, which are write transistor (W_{TR}) and read transistor (R_{TR}). Drain of the W_{TR} is connected to gate of the R_{TR}, and the connected line serves as the storage node (SN). During the write operation, gate voltage higher than the threshold voltage is applied to the W_{TR}, and the charge is stored in the SN by applied bias at the source of W_{TR}. Then, the electric field induced by the stored charges in the SN turns on the channel of the R_{TR}. Therefore, by reading the drain current of R_{TR}, whether charge is stored (memory state 1) or not (memory state 2) in the SN can be detected. Because the amount of stored charges in the SN controls the R_{TR} conductance, the multi-level operation (> 2 memory states) is thought to be feasible, dependent on the channel properties of R_{TR}. For this reason, employing the R_{TR} with higher subthreshold swing would increase the distinguishable state ranges, thereby enabling a greater number of multi-level states. Not just for the stand-alone memory applications, the multi-level memory states of 2T0C DRAM could be employed for processing-in-memory (PIM) operations by updating and inferring the conductance as synaptic weight.

In this work, multi-level operation characteristics of the IGZO homogeneous 2T0C, e.g., IGZO channel for both W_{TR} and R_{TR}, and heterogeneous 2T0C with IGZO channel for W_{TR} and ZnO channel for R_{TR}, were compared. IGZO channel exhibits a low off-current and low subthreshold swing (279 mV/dec), which enables a long retention time and clear binary memory application when used as W_{TR} and R_{TR}, respectively. For the R_{TR} of heterogeneous 2T0C, ZnO channel layer showed higher subthreshold swing (1455 mV/dec) than the IGZO. Adopting these multi-level conductance characteristics of R_{TR}, the pattern recognition accuracy for MNIST patterns was evaluated as benchmark for PIM applications.

4:00pm **EM-TuA-8 3D Flash Memory Word Line Metallization Evolution**, ***Fei Zhou**, Senaka Kanakamedala,* Sandisk Technologies **INVITED**

3D flash memory scaling continues to increase the structural and electrical demands on word line metallization, where film conformality, resistivity, void control, stress, and integration compatibility directly affect array performance and yield. Conventional tungsten-based word line schemes have provided manufacturable solutions for multiple generations; however, continued pitch scaling, higher aspect ratio structures, and longer replacement depth increasingly expose the limitations of traditional CVD tungsten processes, including nucleation-layer non-conformality, fluorine-related concerns, and resistance scaling. As a result, alternative deposition methods and metal systems are being actively evaluated to support future generations of 3D flash memory.

This presentation reviews the evolution of 3D flash memory word line metallization from CVD-dominated tungsten integration toward more advanced ALD-enabled metal fill approaches, with particular emphasis on the transition from tungsten to molybdenum. We compare key process and material considerations, including precursor chemistry, nucleation behavior, step coverage, impurity control, film continuity, and compatibility with high-aspect-ratio structures. The discussion highlights how ALD-based approaches can provide improved thickness control and conformality, while also introducing new challenges in productivity, stress management, and interface engineering.

In addition, we examine the motivation for molybdenum as an alternative word line metal, focusing on its potential benefits in resistance scaling, integration flexibility, and compatibility with future array architectures. Process tradeoffs between tungsten and molybdenum are discussed from both device and manufacturing perspectives, including metal resistivity, liner requirements, thermal stability, etch/clean compatibility. Case studies are used to illustrate how deposition methods and material selection jointly influence word line resistance, structural fill quality, and downstream integration margin.

Overall, this presentation summarizes the opportunities and challenges associated with next-generation word line metallization for 3D flash memory. By connecting process evolution from CVD to ALD with material evolution from tungsten to molybdenum, this work provides an integration-focused framework for evaluating future metallization schemes. These findings suggest that successful word line scaling will require co-optimization of metal selection, deposition chemistry, nucleation control, and array integration design to balance electrical performance, manufacturability, and long-term technology extendibility.

4:30pm **EM-TuA-10 Scalable Growth of Epitaxial Ferroelectric Oxides**, ***Peter Meisenheimer**,* Kepler Computing*; Tsung-Chi Wu,* UC Berkeley*; Vishantak Srikrishna,* Kepler Computing*; R Ramesh,* UC Berkeley

Computational technologies based on functional oxides have the potential to dramatically reduce energy consumption due to properties such as loss-free switching and nonvolatility. One of the primary challenges with these technologies, however, is that epitaxial deposition is often incompatible with silicon. Here, we demonstrate scalable, epitaxial deposition of ferroelectric oxides on silicon. We utilize magnetron sputtering to deposit high quality perovskite oxides on SrTiO3 buffered substrates. Electrical measurements show ferroelectric switching down to 100s of mV, firmly within the realm of potential CMOS integration, as well as the nonvolatility that is expected from high-quality ferroelectric materials. Additionally, the use of Si substrates allows for significantly more advanced device integration than what would be possible with the single crystalline oxide substates that are normally used for epitaxy.

4:45pm **EM-TuA-11 Electrically Tunable Remnant Polarization via Oxygen Vacancy Migration in Ferroelectric Al-doped HfO2-based MIFM structure**, ***Youngwook Kim***, *Jimin Han, Yong-Sang Cho, Tae-Sik Yoon,* Ulsan National Institute of Science and Technology, Republic of Korea

Ferroelectric hafnium oxide (HfO_2)-based FeFETs have attracted considerable attention for fast, low-power, and high-density non-volatile memory applications, with advantages of stable spontaneous polarization, non-volatility, and full CMOS compatibility. A single-transistor architecture modulates a threshold voltage (V_{th}) between two distinct polarization states via a ferroelectric gate, suitable for both high-density storage and neuromorphic computing. Nevertheless, conventional FeFETs are fundamentally constrained by the fixed remnant polarization (P_r), which limits the memory window (MW) and consequently narrows the read margins between discrete V_{th} states, posing a critical challenge for reliable Multi-Level Cell (MLC) operations.

In this study, we investigate electrically tunable remnant polarization via oxygen ion exchange in Al-doped HfO_2 (HAO) ferroelectric layer with ion reservoir layer, where polarization is enhanced by the increase of oxygen vacancy concentration in the HfO_2 lattice. To implement oxygen vacancy exchange with HAO, we propose a Metal-Insulator-Ferroelectric-Metal (MIFM) structure incorporating a low-temperature deposited HfO_{2-x} as a high defect-density reservoir layer of oxygen ions. The device exhibits a distinct and controllable $2P_r$ window of approximately 7 μC/cm², modulating between 21 and 28 μC/cm², enabling a tunable and broadened MW with V_{th} shift for stable multi-level operations. Specifically, the polarization state of the HAO layer remains stably upon low-voltage pulse application, whereas oxygen vacancy migration between the HAO and HfO_{2-x} reservoir layer occurs, tuning the polarization state under high-voltage or repetitive pulse application. This tunable remnant polarization is attributed to the changes in oxygen vacancy concentration in the ferroelectric layer, thereby modulating the fraction of the ferroelectric orthorhombic phase.

This tunable remnant polarization can be applied to the FeFETs by constructing MIFS(Metal-Insulator-Ferroelectric-Si) capacitor stack, where applying the gate bias induces the remnant polarization of HAO and consequently modulates V_{th} shift for memory operation. Moreover, the P_r values can be further increased by high voltage application, which enhances MW and enables more reliable MLC operation.

In conclusion, we propose a novel method for enhancing MW and V_{th} controllability via electrochemical ionic modulation in HAO-based ferroelectric devices. By incorporating a low-temperature HfO_{2-x} reservoir layer, oxygen vacancy migration is effectively facilitated, potentially providing a reliable and reversible pathway for MW expansion and precise multi-level ferroelectric tuning.

5:00pm **EM-TuA-12 Non-Volatile Charge-Trap Memory Characteristics Using Nanocrystal (HfO_2 or ZnO) Charge-Trap Layer Deposited by Atomic Layer Deposition**, ***Taeyun Noh***, *So-Young Lim, Jimin Han, Tae-Sik Yoon,* Ulsan National Institute of Science and Technology, Republic of Korea

Emerging non-volatile memory (NVM) devices have been attracting significant attention due to the increasing demand for data-driven applications.Among various NVMs, charge-trap flash memory (CTF), which operates by modulating the threshold voltage (V_T) via charge trapping, offers the highest storage density with the lowest bit cost. The bit density of CTF has been further increased by employing a three-dimensional structure, i.e., 3D NAND flash. However, as the dimensions of devices keep scaling down, several reliability challenges arise, including reduced memory window, electrostatic interference, and unintended V_T shifts. In particular, the lateral charge migration through the charge-trap layer (CTL) to adjacent cells becomessevere as the distance between cells decreases.

In this study, the improved NVM characteristics of CTF device are demonstrated by employingmulti-layered nanocrystal (NC) CTL deposited by atomic layer deposition (ALD), herein referred to as NC-CTL. The NC-CTL composed of physically and electrically isolated NCs enables potentially to store charges more reliably even in the highly scaled-down architecture bysuppressinglateral charge migration, unlike a continuous layer-type CTL. In addition to geometric modulation, NC material engineering could control NVM characteristics by modifying the energy-band structure of the devices. Notably, the discrete HfO_2 and ZnO NCs were uniformly deposited with high density by controlling the number of ALD cycles. In the device with ALD-HfO_2 NCs, the wider bandgap of HfO_2 reduces the kinetic energy of injected electrons during programming, leading to more uniform charge trapping throughout the NC-CTL and enabling a wide memory window. For comparison, the device with ZnO NC-CTL having a narrower bandgap exhibits a smaller memory window, attributed to the existence of a dead zone in the NC-CTL near the tunneling oxide, where high-energy electrons injected into the NC-CTL are less likely to be trapped. It highlights the impact of energy-band structure of CTL to achieve a wide memory window. Moreover, memory performance such as programming efficiency and reliability properties could be enhanced by adopting SiO_2/Al_2O_3 bi-layered blocking oxide and rapid thermal annealing processing, achieving a memory window of >7 V at programming voltage of +20 V and retention of ~91 % after 12 hours. These results demonstrate that the use of multi-layered NC-CTL is a promising strategy to simultaneously enlarge a memory window and achieve stable retention, thereby enhancing the reliability of highly scaled 3D NAND flash.

Acknowledgement

This work was supported by Samsung Electronics Co., Ltd(IO260312-15875-01)

5:15pm **EM-TuA-13 A Scalable Approach to Bioinspired Films for Passive Daytime Radiative Cooling**, ***Emily McGuinness***, *Joshua Goetze, Christopher Ellison, Vivian Ferry,* University of Minnesota

Cooling of people and places consumes massive amounts of energy and is anticipated to rise 45 % by year 2050 (IEA 2023). Passive daytime radiative cooling (PDRC) is an emerging net-zero energy cooling method where warm surfaces emit radiation to the cold of deep space (4 K) through the atmospheric transmission window (wavelengths of 8-13 micron). By virtue of their chemical structure, polymeric materials naturally emit in this region. However, to reach a net-cooling effect, materials must simultaneously prevent heat gain from the absorption of solar radiation. In polymers, this is commonly achieved via scattering from pores where pore length scales are designed to correspond to the wavelengths of the solar spectrum. While multiple methods have emerged to created porous polymers for PDRC, most lack interconnected pores which impacts mechanical properties and reduces moisture vapor transport. Mirroring the network structure observed in the Cyphochilus beetle, we have developed a scalable method to create porous polymer films with broadband solar rejection (R_{solar} > 96 %), high levels of moisture vapor transport, and durable optical properties. In this talk, we will explore how polymer processing influences characteristic length scales in these materials and their resultant optical performance. Through process optimization, this scalable structure is found to be particularly attractive for rugged use PDRC applications where movement and moisture transport are key.

Materials and Innovations for Fusion Energy
Room 321 - Session FUS-TuA

Materials and Innovations for Fusion Energy

Moderators: Dr. Eric Dombrowski, Commonwealth Fusion Systems, **Dr. Zachary Robinson**, Laboratory for Laser Energetics, The University of Rochester

4:00pm **FUS-TuA-8 Challenges in Tritium Surface Characterisation: From Memory Effects to Fusion byproducts management**, ***Florian Priester***, *Dominic Batzler, Robin Größle, Michael Sturm, Simon Niemes, Alexander Marsteller,* Karlsruhe Institute of Technology - Tritium Laboratory, Germany

INVITED

The characterisation of tritium (T_2) in materials presents a set of unique challenges that distinguish it significantly from its stable isotopes, hydrogen (H_2) and deuterium (D_2). In vacuum environments and analytical devices, tritium's radioactive nature and high mobility lead to a so-called "memory effect"—the adsorption and diffusion of tritium into system surfaces—which complicates maintenance protocols, degrades analytical precision, and artificially raises the Limit of Detection (LoD).

This presentation evaluates the current suite of measurement technologies utilised for tritium quantification, including calorimetry, Beta-Induced X-ray Spectroscopy (BIXS) for (near-) surface analysis, and liquid scintillation counting. A critical bottleneck in the field remains the sound determination of decontamination factors across these methodologies.

Furthermore, we explore some examples to assess material properties with regard to tritium sticking and decontamination possibilities. Beyond the technical hurdles, there is a burgeoning economic demand for "cheap" and accessible detection methods. In the absence of reliable, cost-effective quantification, facilities are forced into the conservative—and significantly more expensive—declaration of byproducts as intermediate-level waste. This work underscores the necessity of advancing surface characterisation

techniques to enable the economic declassification of materials and streamline future fusion and nuclear waste management.

4:30pm **FUS-TuA-10 Evaluating the Performance of Next Generation Plasma-Facing Materials**, ***Robert Kolasinski***, Sandia National Laboratories; *Kent Christian,* Stony Brook University; *Jonathan Coburn, Antonio Cruz, Feng-Jen Chang, Mary Alice Cusentino,* Sandia National Laboratories; *Lance Snead, Jason Trelewicz, David Sprouster,* Stony Brook University **INVITED**

The science of plasma-material interactions (PMI) is fundamental to the realization of magnetic fusion as an energy source, and predicting how materials behave in the extreme environments of fusion devices remains one of the most daunting challenges in materials science. Surfaces directly exposed to intense plasmas will be continually reconfigured over their operational lifetime. This evolving surface structure governs material degradation and is also intimately coupled to neutral and impurity recycling and edge turbulence in the core plasma.

This presentation will provide an overview of recent laboratory testing and surface characterization of advanced tungsten alloys and ceramics that are among the leading candidate plasma-facing materials for fusion devices. The work combines experiments and modeling to better understand the effects of high-flux plasma exposure on these materials. Although they offer promising thermomechanical properties and microstructural stability, important gaps remain in our understanding of their response, including erosion/redeposition, near-surface defect nucleation and growth, and tritium uptake. Recent efforts have focused on evaluating these materials in a high-flux steady-state plasma source, coupled with in situ and post-mortem diagnostics to track the evolution of surface composition and structure. Initial studies of doped and dispersoid-strengthened tungsten have yielded promising results, including improved resistance to recrystallization and plasma-induced surface morphology changes. Likewise, ultra-high-temperature ceramics are emerging as attractive alternatives to tungsten, with the potential for greater resilience to neutron damage. These laboratory studies have motivated recent experiments at tokamak facilities, where tungsten and ceramic microstructures are exposed to reactor-relevant heat and particle fluxes. Such experiments enable systematic evaluation of how compositional and microstructural variations improve surface resilience under combined loading. Together with complementary modeling across multiple length scales, these results help identify promising pathways for further materials optimization.

SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

5:00pm **FUS-TuA-12 Optimised Variable-Temperature Cryocooler Design for Reduced Tritium Inventory and Operational Risk**, *Pankaj Sharma, Robert Buchanan, Adam Bruce,* ***William Schofield***, UKAEA, UK

Thermal conducting materials (TCMs) are commonly used at cryogenic interfaces to improve heat transfer between a cryocooler cold head and a sample cell. However, in tritium-handling systems, conventional TCMs may introduce hydrogen-containing materials that contribute to isotope exchange, tritium retention, and increased operational complexity. This study evaluates whether TCMs are essential for achieving the required thermal performance of a cryogenic adsorption system, or whether their function can be replaced through optimised mechanical interface design. Controlled heat transfer experiments were performed at four target temperatures (75, 150, 200, and 323 K), representing the operating range of planned adsorption studies. Baseline experiments were conducted using the original cold head-sample cell assembly, both with and without a Type 120 silicone TCM interface. Cold head and sample cell temperatures were monitored under steady-state conditions to assess thermal coupling efficiency. Results showed that the TCM-assisted configuration provided effective thermal coupling, with sample cell temperatures closely matching cold head temperatures across the full operating range. The temperature deviation between the cold head and sample cell remained minimal, with variations of approximately 0.3 K at 150, 200, and 323 K, and ~0.75 K at 75 K. In contrast, removal of the TCM introduced significant interfacial thermal resistance, resulting in substantially larger temperature deviations (up to ~38.2 K) and slower thermal response, particularly under cryogenic conditions at 75 K. To eliminate TCM usage, alternative mechanical interface designs were developed and tested. Through optimisation, a modified assembly achieved the required improved thermal performance without the use of TCMs.

5:15pm **FUS-TuA-13 Pellet Flight Path Design Challenges and Solutions for ITER**, ***Matt Williamson***, *Sarah Smith, Steven Meitner, Eileen Sibley, Oscar Martinez,* Oak Ridge National Laboratory

The ITER Fuelling Pellet Injection System (FPIS) will provide hydrogenic, cylindrical pellets for steady-state plasma core fueling and control of Edge Localized Mode instabilities. ITER will be the world's largest tokamak, a magnetic confinement fusion device with the primary mission to demonstrate the scientific and technological feasibility of fusion energy. In the final ITER machine configuration FPIS injectors will be housed in three secondary tritium containment casks, with one cask allocated to each of three lower-level ports positioned 120° apart. For each cask, there will be three pellet flight lines with penetrations through the cryostat and vacuum vessel (VV). Pellets will be extruded, sized, propelled through the flight line selector, and guided to the plasma injection points located in the VV via flight lines.

The pellet flight path for ITER presents a variety of design challenges. Pellets are required to survive gap jumps through isolation valves, propellant removal pumping stages, diagnostic cavities, and mechanical connections required to permit phased installation of the FPIS. Pellet-facing flight path components adjacent to these gap jumps have been designed to minimize impact on pellet survivability while allowing for manufacturability, assembly, and removal. Portions of the flight path must also accommodate radial displacement of the VV during machine operation while maintaining fuel confinement and containment. Known displacements and as-built misalignments must be absorbed by the design while maintaining a robust pellet flight path and secondary vacuum containment. The pellet flight path must endure high temperatures, electromagnetic displacements, and pass through several interfacing ITER subsystems.

The ITER pellet flight path design must provide reliable pellet delivery while allowing flexibility for machine as-built installation, complying with material requirements for plasma purity and high-vacuum environments, and withstanding harsh environmental conditions for decades of machine operation. These key design challenges must be resolved to successfully fuel ITER and inform practical fueling systems deployed at future fusion plants.

This work was supported by the U.S. Department of Energy contract DE-AC05-00OR22725. The views and opinions expressed herein do not necessarily reflect those of the ITER Organization.

5:30pm **FUS-TuA-14 Westinghouse'S Experience in the Fabrication and Welding of ITER'S Vacuum Vessel Sectors**, *Stefano Batticci,* Westinghouse Italy; *Simon Roche,* Westinghouse Electric France; ***Paolo Ferroni***, Westinghouse Electric Company

Westinghouse is most often known as a world leader in the development of nuclear fission power plants, including manufacturing of nuclear fuel and major equipment required to best exploit energy from nuclear fission. However, for several years Westinghouse has not only been following advances in fusion energy – while being agnostic to the type of fusion technology being pursued – but has also been involved in fusion technology development as Service Provider. This role has found its most notable example in the manufacturing, together with Ansaldo Nucleare and Walter Tosto (collectively known as the AMW Consortium), of five out of the nine sectors comprising the ITER's Vacuum Vessel (VV) (see Figures 1 and 2), and in the welding of all nine sectors which is an operation currently in qualification phase. In this presentation, Westinghouse will describe the manufacturing strategy utilized for the ITER's VV sectors, including:

- Review of the Conceptual Design received from the ITER Organization and suggesting several changes to improve manufacturability;
- Development of the Detailed Manufacturing Design (fabrication models and drawings) and manufacturing engineering (i.e., assembly sequence, , work sequences, development of dedicated jigs and tools needed for fabrication, re-verse engineering for CAM Computer Aided Machining purposes, NDE inspection plans, etc.) for the items to be fabricated;
- Development of the manufacturing engineering for the final assembly phase of all European Sectors, including the development of the Virtual Fitting process as main engineering tool for the assembly of extra large components.

In addition, information will be provided on the preparatory activities for the in-situ welding of all nine VV sectors. We will describe what Westinghouse proposed to the ITER Organization to weld the 9 VV Sectors in parallel at the same time. Accounting for the pre-qualification phase we

anticipate a 30 month welding sequence on-site inside the ITER Tokamak Pit:

- Phase 1-2-3 – Feasibility Study
- Phase 4 – Pre-qualification: Trials Mechanical, machining, reverse engineering, welding, NDT, RT Linac, logistics
- Phase 5 – Vacuum Vessel Sectors Welding. Welding preparation: qualification process, resource training, tooling procurement, anticipated operations. Welding phase: welding/machining operation, post welding NDE

Nanoscale Science and Technology
Room 320 - Session NS-TuA

Multimodal Techniques in Surface and Interface Engineering at the Nanoscale II

Moderators: Dr. Son Le, University of Maryland, **Dr. Taisuke Ohta**, Sandia National Laboratories

2:15pm **NS-TuA-1 Multimodal Investigation and Interface Engineering of Near-Surface Diamond Quantum Defects**, ***Nazar Delegan,*** Argonne National Laboratory **INVITED**

Solid-state spin defects, such as the nitrogen-vacancy (NV) center in diamond, are premier candidates for quantum sensing and information processing due to their long spin coherence times and robust room-temperature operation. However, when brought within nanometers of the surface to maximize coupling to external targets, their quantum properties degrade due to interface defects, uncontrolled surface terminations, and parasitic "dark" electron spins. Overcoming these challenges requires a multimodal approach that pairs sub-nanometer characterization with precise chemical control of the interface.

In this talk, we address this problem by leveraging atomic layer etching (ALE) and atomic layer deposition (ALD) as a dual framework for highly sensitive surface diagnostics and precise interface engineering. We show that sub-angstrom ALD nucleation profiles serve as an analytical probe capable of distinguishing between common diamond (001) surface terminations. Expanding on this capability, we deploy ALD-grown ultrathin titanium oxide (TiO_2) films to passivate the diamond interface, drastically reducing the background density of deleterious dark surface spins.

This controlled processing allows for the realization of pristine diamond surfaces. Enabled by this approach, we present direct atomic-scale imaging, spectroscopic characterization, and charge-state manipulation of individual near-surface NV centers using scanning tunneling microscopy (STM). By utilizing a conductive graphene capping layer to circumvent diamond's bulk insulating nature, we identify clear spectroscopic signatures of NV- defects. Critically, we demonstrate local control over the defect's electronic environment, dynamically tuning the charge state from NV^- to NV^0 via tip-induced gating. Together, these complementary nanoscale imaging and conformal engineering paradigms offer a robust toolkit for mitigating surface noise and optimizing diamond-based quantum architectures.

2:45pm **NS-TuA-3 Multi-Technique Nanoscale Probe Studies of Intercalated Phases of Pb, Gd and Dy Under Graphene on SiC**, ***Shen Chen,*** *Salma Khatun, Umamahesh Thupakula,* Ames National Laboratory*; Zhe Fei,* Iowa State University*; Marek Kolmer,* Ames National Laboratory*; Michael C. Tringides,* Iowa State University

Metal intercalation beneath epitaxial graphene on SiC (Gr/SiC) can host different subsurface phases, which is a way to control the band structure, subsurface superstructure, metal nucleation and charge transfer. Realizing and controlling these subsurface phases requires identifying the galleries occupied by the intercalants and the types of intercalated phases formed. Here, we use complementary techniques, including STM/STS, SPA-LEED, and ARPES to address the previous questions. Among Pb-intercalated phases, $(10\times10)_{gr}$ is of particular interest because the large supercell generates replica Dirac cones at the corners of mini-Brillouin zones. However, establishing reproducible growth conditions for the $(10\times10)_{gr}$ phase remains challenging. By monitoring deposition and annealing cycles, we quantitatively show that during growth the $(10\times10)_{gr}$ and Pb(10) intensities are correlated, suggesting that Pb(111) islands preferentially nucleate on $(10\times10)_{gr}$ domains[1]. For Gd intercalation, multiple phases with different gallery occupancies form, depending on growth conditions of coverage and annealing temperature, all of which have been comprehensively studied with the previously listed techniques. Multiprobe STM transport confirm the decoupling of the top graphene by the large displacement field generated by intercalated Gd[2]. Recent experiments show the formation of pre-designed Gd intercalated phases by kinetically controlling the Gd subsurface occupation[3]. Dy [4] intercalation shares similar intercalated phases and growth as Gd and both metals are ideal metals to control graphene magnetism. These experiments show that metal intercalation is a very promising approach for further engineering graphene's exceptional electronic properties. They establish a framework to identify metal intercalated phases in Gr/SiC heterostructures and to generate 2-d quantum materials with tunable electronic properties.

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3:00pm **NS-TuA-4 Multidimensional Characterizations of Pyrrolidine Dissociations on Cu(100) Surface with the Single-Bond Resolution**, ***Liya Bi,*** *Hao Zhou, Zihao Wang, Shaowei Li,* University of California San Diego

Here, we report the development of a multidimensional characterization platform for identifying surface adsorbents with the single-bond resolution. This platform is based on low-temperature scanning tunneling microscopy, encompassing the bond-resolved STM (BR-STM), STM-inelastic electron tunneling spectroscopy (STM-IETS) and infrared-integrated STM (IRiSTM). We demonstrated both its chemical sensitivity and spatial resolution through fully characterizing the dissociation products from a pyrrolidine (C_4H_9N) to a dehydrogenated pyrrole (C_4H_4N) on Cu(100) surfaces. We unambiguously assigned a series of products after step-by-step dehydrogenation to dehydrogenated pyrrolidine (C_4H_8N), 1-pyrroline (C_4H_7N), dehydrogenated 2-pyrroline (C_4H_6N), 3H-pyrrole (C_4H_5N) and dehydrogenated 1H-pyrrole (C_4H_4N), which was supported by bond-resolved topographic imaging and/or IETS mapping and/or single-molecule IR spectroscopy. Our experimental scheme is expected to aid in chemical identification in on-surface synthesis or catalysis with both structurally and vibrationally sensitive probes.

3:15pm **NS-TuA-5 Linking Sers Spectral Variability to Reliable Detection of Low-Affinity Analytes via Plasmonic Substrate Physics and Machine Learning**, ***Amit Kumar,*** *Fengbo MA,* University of Georgia*; Susu M. Zughaier,* Qatar University, Qatar*; Xianyan Chen, Yiping Zhao,* University of Georgia

Surface-enhanced Raman spectroscopy (SERS) provides ultrasensitive molecular detection through localized plasmonic field enhancement; however, reliable sensing of low-affinity analytes remains limited by spectral variability arising from heterogeneous electromagnetic enhancement and adsorption-orientation-dependent Raman tensor projections. In this work, we establish a physics-informed and machine-learning-assisted framework linking SERS spectral variability with sensing reliability on oblique-angle-deposited silver nanorod (AgNR) substrates. A comprehensive SERS dataset was constructed using 1,2-bis(4-pyridyl) ethylene (BPE) under six controlled experimental conditions, including defect mapping, batch-to-batch variation, nanorod-length variation (200-1000 nm), concentration-dependent drop-casting (10^{-3}-10^{-12} M), static immersion (10^{-3}-10^{-10} M), and real-time adsorption (10^{-5} M). Hierarchical cluster analysis (HCA) partitioned the spectra into seven reproducible spectral clusters spanning high- and low-SNR regimes, while principal component analysis (PCA) revealed that cluster separation originates from systematic redistribution of Raman modes rather than stochastic noise. The results show that geometry-dependent plasmonic enhancement redistributes Raman peak intensities through electromagnetic weighting, while tensor-based orientation analysis demonstrates orientation-selective enhancement governed by Raman polarizability anisotropy. Building on this spectral variability framework, HCA and PCA were further applied to concentration-dependent bacterial biomarker datasets to identify distinct spectral evolution regimes associated with adsorption affinity and concentration variation. Strongly adsorbing biomarkers, including 2,3-DHBA, 2,5-DHBA, and pyocyanin, produced stable high-intensity spectra, whereas weakly adsorbing biomarkers, including lipoteichoic acid (LTA), enterobactin, and β-carotene, exhibited weak enhancement and non-monotonic spectral evolution that limited conventional calibration-based quantification. Using HCA/PCA-derived spectral patterns, convolutional neural network (CNN) classification and regression models were implemented directly on the SERS spectra. The CNN classification model

achieved 99.99% classification accuracy, while regression models yielded concentration prediction performance exceeding R^2 >0.97 with MAE <0.27 despite substantial spectral variability. These results establish SERS spectral variability as a physically interpretable phenomenon governed by coupled plasmonic and molecular-orientation effects and demonstrate a scalable framework for robust nanoscale sensing in complex chemical and biological environments.

Plasma Science and Technology
Room 315 - Session PS1-TuA

Atmospheric and Liquid Plasmas

Moderators: Prof. Michael Gordon, University of California at Santa Barbara, **Prof. Dr. Mohan Sankaran**, University of Illinois at Urbana-Champaign

2:15pm **PS1-TuA-1 Synthesis of Organic and Inorganic Spatially Differentiated Coatings by Cold Atmospheric Plasma***, Marie Brabant, Celine Dergham,* ***Francois Reniers,*** Université libre de Bruxelles, Belgium

In earlier studies, we have shown that one could immobilize filaments in an atmospheric pressure dielectric barrier discharge (DBD). This setup allows to deposit coatings presenting spatially differentiated chemistries that lead to tunable surface properties, such as, for instance, coatings presenting simultaneously hydrophobic and hydrophilic areas [1].

In this talk will methyl metacrylate (MMA) and hexamethyl disiloxane (HMDSO) are used as precursor to deposit localized PMMA and SiOx coatings, respectively. The chemistry, roughness and thickness of the coatings obtained under the filaments and between the filaments is studied by XPS, FTIR, Raman, profilometry and SIMS. The effect of the nature and flow rate of the plasma gas and the power injection mode on the resulting coating is presented and discussed.

For PMMA deposit, a drastic influence of the plasma gas nature is evidenced: transparent, sticky coatings are obtained with Ar, with excellent preservation of the ester function, whereas well polymerized yellow – orange coatings are obtained with N_2. In these last coatings, nitrogen is incorporated.

SiOx coatings deposited under the filaments are much thicker than those deposited between the filaments, with a chemistry depending on the ratio HMDSO/O_2. Adhesion of such coatings on glass substrates is superior.

This study highlights the versatility of plasma polymerization for microscale patterning and surface functionalization. Localized AP-PACVD enables micron–scale deposition and controlled chemical tuning without vacuum infrastructure [2], making it a promising technique for advanced surface engineering. The ability to modulate plasma chemistry through gas composition opens new perspectives for designing functional polymer and inorganic coatings with spatially selective properties.

Acknowledgements :

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2:30pm **PS1-TuA-2 Atmospheric Plasma-Induced Surface Modification of Carbonaceous Thin Films***,* ***Thea Ferley,*** School of Physics, Clinical and Optometric Sciences, TU Dublin, Ireland*; Vladimir Milosavljevic,* School of Physics, Clinical and Optometric Sciences, TU Dublin, Ireland & Faculty of Physics, University of Belgrade, Serbia, Ireland

This study investigated the influence of operating conditions in a pulse resonance atmospheric pin plasma system on the surface modification of carbonaceous thin films representative of contaminant layers found in fusion environments. The work focused on the effects of applied voltage, pulse frequency, duty cycle, and working gas environment on the wettability, thickness, roughness, and void fraction of the films. Samples were exposed to controlled plasma conditions using ambient air, He and Ar as working gases and were characterised using contact angle measurements and ellipsometric analysis.The results demonstrated that plasma-induced surface modification strongly depends on both the electrical operating parameters and the gas environment. Among the investigated parameters, applied voltage produced the clearest effect on wettability, where increasing voltage resulted in larger reductions in contact angle, indicating an increase in surface energy. In contrast, duty cycle showed limited and inconsistent influence on the measured surface properties, while pulse frequency mainly affected structural properties such as roughness and void fraction through repeated plasma–surface interactions.Statistical analysis confirmed a highly significant effect of plasma exposure on contact angle (F=115.036, P<0.001), with gas type and the interaction between exposure and gas also being statistically significant (F=3.476, P=0.045). Ambient air produced a smaller reduction in contact angle (-10.32°), while Ar and He produced larger reductions of -19.30° and -17.27°, respectively, demonstrating stronger surface modification under inert gas conditions. Thickness measurements showed a slight increase in ambient air (+1.4 nm) and reductions for He (-4.3 nm) and Ar (-9.5 nm). Surface roughness decreased for all gases, with the largest separation of 17.5 nm observed between Ar and He conditions. Void fraction measurements further highlighted the differences between gas environments, with He producing the largest decrease (-6.8%) compared to Ar (-1.5%).The observed differences indicate that ambient air promotes chemically driven surface interactions through reactive O_2 and N_2 based species, whereas Ar and He primarily contribute through physical plasma mechanisms such as ion bombardment and momentum transfer. Overall, the results demonstrate that the pulse resonance atmospheric plasma pin system can produce controlled and measurable changes in surface properties. These findings support the potential of this system as a flexible atmospheric-pressure plasma technology for surface cleaning and conditioning applications in fusion-relevant environments.

2:45pm **PS1-TuA-3 Influence of Pulsed Power Parameters on the Properties of Submerged Argon Plasmas***,* ***Michael Johnson,*** US Naval Research Laboratory*; Mackenzie Meyer,* National Research Council*; David Boris, Scott Walton,* US Naval Research Laboratory

Atmospheric pressure plasmas create a unique chemical and electrical environment that is well-suited for liquid treatment applications, such as decontamination and remediation. These plasmas can operate in a nonthermal regime when driven by pulsed power of sufficiently short duration. However, the influence of pulse power parameters on plasma behavior in gas-liquid systems is challenging to understand given the strong spatial and temporal variations that can arise. In this work, we discuss the use of short duration (< 1 ms), high voltage (> 10 kV) pulses driven at frequencies between 100 Hz and 10 kHz to produce an argon plasma submerged in flowing water. Varying the pulse width, impacts the induced plasma chemistry since excitation of the argon feed is dominant early, while hydrogen emission increases over time as water vapor dissociates. Spatial profiles show uniform hydrogen emission, while argon emission is stronger near the negative electrode. Stark broadening analysis reveals that the lifetime of electrons after the pulse is strongly influenced by the pulse width, as electron density can persist for several microseconds post-pulse. Varying the repetition frequency reveals that higher frequencies decrease the breakdown voltage because residual reactive species facilitate easier plasma reignition. Discharge current rises with frequency until limited by power supply resistances, with energy delivered per pulse peaking near 500 Hz for the present system. Higher water flow rates increase the frequency required for consistent ignition, suggesting liquid dynamics influence the quenching of residual species. Electron density peaks between 800 Hz and 3 kHz, beyond which it decreases as molecular gases like H_2 and O_2 alter formation conditions. Optical emission spectroscopy also indicates greater electrode erosion at higher frequencies. The implications of these results are discussed in terms of water treatment applications. This work supported by the Naval Research Laboratory base program.

This work was partially supported by the U.S. Naval Research Laboratory Base Program.

3:00pm **PS1-TuA-4 Non-Invasive Short-Wave Infrared Imaging for High-Resolution Thermal Mapping of Graphene-Growth Atmospheric Plasmas***,* ***Logan Holler,*** *Mia Sawkik, Brenna Miller, Parker Hayes, Drhuval Patel, David Ruzic,* University of Illinois at Urbana-Champaign*; Michael Stowell,* Lyten*; Dren Qerimi,* University of Illinois at Urbana-Champaign

Atmospheric-pressure plasma synthesis of graphene has emerged as a promising route for scalable carbon nanomaterial production. While it is well established that graphene formation is highly temperature-dependent, the distinction between the formation of graphene flakes versus nodules remains insufficiently characterized within plasmas. A key step forward centers on better mapping the temperatures across our different plasma mixtures. However, conventional diagnostic tools often fall short: most diagnostic systems only provide one-dimensional snapshots, and physical probes degrade rapidly when exposed to atmospheric plasmas.

The development of Short-Wave Infrared (SWIR) imaging has allowed time-averaged spatially-resolved temperature profiles to be developed for these systems. SWIR imaging leverages thermal radiation emissions to determine temperature by integrating spectral radiance over the detectable range of our camera. Provided that the camera's solid angle to the plasma remains fixed, changes in the integrated spectral intensity can be used to derive temperature ratios emitted by heated graphite. By calibrating the system using a known temperature, SWIR snapshots can correlate image intensity with absolute temperature. Within the capacity of pure plasma imaging, this allows for dynamic temperature mapping throughout the plasma, which is limited only to the refresh rate of the SWIR Camera.

Graphite was chosen for these experiments due to its capacity to survive exposure in these plasmas, while also having a near-blackbody emissivity. Having developed a calibration curve for each rod, it is then possible to map the full temperature profile of the plasma by incrementally raising the rod through the plasma. A snapshot is taken at each point once the rod is in thermal equilibrium with the plasma. Stitching these images together forms a complete spatial map to better show thermal gradients across the plasma. A future development of this system aims for a plug-and-play plasma temperature profiling of unobstructed, in-situ plasma temperatures. This would allow for graphene growth modules to be better correlated to the different temperature profiles within the atmospheric plasma. This diagnostic provides a pathway toward in-situ, non-invasive plasma thermal profiling to better understand graphene growth morphology.

3:15pm **PS1-TuA-5 Spatially Resolved Spectroscopic Imaging of Plasma in Contact with a Liquid Interface***, **Robert Pierrard**,* University of Illinois at Urbana-Champaign*; Shurik Yatom,* Princeton Plasma Physics Laboratory*; Davide Curreli, Sean M. Peyres, Mohan Sankaran,* University of Illinois at Urbana-Champaign

Atmospheric-pressure plasmas (APPs) are highly effective at driving complex chemical reaction pathways. When coupled with a liquid interface, these plasmas deliver reactive species directly to a solution, enhancing chemical kinetics and enabling new reactions. Plasma-liquid systems have found applications across diverse fields, including nanomaterial synthesis, wound healing, environmental remediation, and sustainable agriculture via nitrogen fixation. Here we discuss the application of optical spectroscopy to provide deeper insight into plasma-based nitrogen fixation.

Our investigation focuses on a low-temperature APP formed in contact with liquid water, where gas-phase electrons are injected into solution to generate solvated electrons, the strongest known chemical reducing species, capable of reducing molecular nitrogen (N_2) to ammonia (NH_3). However, competing radicals are simultaneously created, yielding concurrent reduction and oxidation pathways and a wide range of chemical products.

To unravel this complex system, our work was divided into two phases. In the first, we constructed a simplified experiment without a liquid interface, introducing controlled concentrations of water vapor into a nitrogen plasma to isolate its effect on reaction pathways. Using optical emission spectroscopy (OES) with an argon actinometer and laser-induced fluorescence (LIF), we measured steady-state densities of intermediate species to validate a global chemical kinetic reaction network. We found that increasing water vapor dramatically suppresses atomic nitrogen density by quenching two key excited states of N_2. Moreover, the oxidative pathway toward NO and NO_2 was strongly favored over the reductive pathway toward NH_3 due to kinetic bottlenecks, explaining the enhanced oxidative species production commonly observed in the literature.

These findings informed our second phase, where we transitioned to the targeted plasma-liquid system. We extended our OES measurements to spatially resolve the plasma, enabling mapping of gas temperatures, electron temperatures, and key radical species. Measurements revealed striking variation in temperature and species profiles along the discharge, localized either near the metal electrode where the plasma emanates or near the liquid water surface. These results indicate that plasma properties are not uniform, and resolving the inhomogeneities is critical to understanding plasma-liquid processes.

Plasma Science and Technology
Room 315 - Session PS2+EUV-TuA

Plasma Processes for Feature Scaling

Moderators: Prof. Dr. Erwin Kessels, Eindhoven University of Technology, the Netherlands, **Dr. Pingshan Luan**, TEL Technology Center America

4:00pm **PS2+EUV-TuA-8 Advanced Logic Pitch Scaling in the High NA EUV Era***, Arame Thiam, **Yannick Feurprier**,* TEL Europe, Belgium **INVITED**

High NA (0.55 NA) EUV lithography enables the single exposure of critical layers for future generations of logic (14A and below) and DRAM (1d and below) devices. Its implementation, however, introduces challenges in meeting both technology and high-volume manufacturing requirements. We will review and discuss the challenges of certain processes for logic use cases (Place and Route and Tip-to-Tip CD control, random logic via) and for the memory cases (contact holes and pillar). Co-optimization of the lithography process (resist, source, mask and development method) together with the etch pattern transfer process and the defectivity assessment enables the demonstration of a failure free process window for Place and Route (PnR) logic clips at tight pitches (down to 18 nm pitch) and for 28 nm pitch pillars for the memory use case.

The stringent tip-to-tip (T2T) CD control required by the technology in the PnR also creates opportunities for directional etch techniques. Gas Cluster Beam (GCB) technology can complement high NA EUV lithography by providing precise T2T CD control, reducing LER and helping to mitigate defectivity. Finally, further validation of the high NA EUV and etch patterning transfer is presented through electrical test.

Keywords: High NA EUV, Etch patterning, PnR, DRAM, Defectivity, Directional etch, Electrical test

4:30pm **PS2+EUV-TuA-10 Dry Resist Patterning Solutions for High-NA EUV Lithography***, **Ali Haider**,* Lam Research Corp.*; Zhengtao Chen, Shruti Jambaldinni,* Lam Research Belgium BV, Belgium*; Anuja De Silva,* Lam Research*; Rich Wise,* Lam Research Corp. **INVITED**

High-NA EUV lithography patterning at increasingly tight pitches introduces significant challenges, including elevated defectivity, reduced depth of focus (DOF), shrinking process windows, and the need for dose reduction without degrading pattern quality. These challenges become increasingly severe near ultimate resolution at P18 L/S and limit the extendibility of conventional wet solution processed resists.

In this work, we demonstrate the performance of Lam's Aether® dry resist technology for dense P18 line/space patterning using high-NA EUV lithography. We address key challenges such as defectivity, DOF, and line wiggling through co-optimization of dry resist deposition, underlayer, post exposure bake (PEB), and dry development. We introduce next-generation dry resists based on novel precursor chemistries with enhanced EUV sensitivity, enabling reduced dose to size without compromising roughness, while expanding the defect-free process window through co-optimization with dry development. We further introduce new dry development schemes that increase the effective resist budget after development, resulting in improved defect performance and lower roughness.

To address the high NA EUV challenge of limited DOF and profile control, we have introduced 3D engineered dry resist films using multi layer deposition with controlled composition and tunable EUV sensitivity in the vertical direction.1,2 We show that 3D engineered resist provides lower dose to size, improved profile control, reduced line wiggling, and enhanced DOF.

Overall, we show that Aether dry resist and development solutions address key challenges in high-NA EUV P18 L/S through innovations in dry resist and development strategies with co optimization of process parameters.

[1]Gulati, Saumya, et al. "Evaluating three dimensionally engineered dry resist film performance for 0.33 NA and High-NA EUV patterning." Advances in Patterning Materials and Processes XLIII. Vol. 13983. SPIE, 2026.

[2]A. Haider et al., "Advances of dry resist towards next-generation lines-spaces patterning in high-NA EUV lithography," Proc. SPIE 13686, 1368608 (2025)

5:00pm **PS2+EUV-TuA-12 Study of Electron-Induced Etching Mechanisms for Chromium and Ruthenium** *, **Michael Hinshelwood**, Gottlieb S. Oehrlein,* University of Maryland, College Park*; Hubertus Marbach, Michael Remmel, Gerson Mette, Michael Budach, Daniel Rhinow, Klaus Edinger, Maik Szafarska,* Carl Zeiss SMT GmbH, Germany

Chromium (Cr) and ruthenium (Ru) are materials critical for semiconductor manufacturing, particularly as part of DUV and EUV photomasks,

respectively. Both can be effectively etched with plasmas containing both oxygen and a halogen. Cr can be etched through the formation of CrO_2Cl_2 or CrO_2F_2, while Ru is etched through the formation of RuO_4 or volatile RuO_xCl_y. To limit surface damage caused by ion bombardment during plasma etching, there is significant interest in isolating ions from the reaction system.

Y. Li et al. demonstrated rapid etching of Ru by combining a low-energy electron beam (EB) with a remote plasma (RP)-created flux of O_2/Cl_2-derived neutrals [1]. The combination of EB and RP resulted in a synergistic etch effect, while RP or EB alone caused either low-rate etching or growth. Here, we aim to describe the mechanism that leads to this synergistic effect and expand it to the etching of Cr, and also investigate how etching selectivity between the two materials may be achieved.

Using in-situ ellipsometry, we model the real-time etching and modification of the metal surfaces. This modelling is complemented by direct chemical characterization of the surface with X-ray photoelectron spectroscopy (XPS). In the case of Ru, we have found that the EB increases the uptake of Cl on the Ru surface, which in turn activates the Ru toward oxidation to volatile compounds. The growth rate and composition of this chlorinated layer formed by the EB are investigated via XPS measurements with increasing EB/Cl_2 exposure time. In the case of Cr, we find a stronger synergistic effect with F/O etch chemistry as opposed to Cl/O. The etch rate with RP alone is highly dependent on the oxygen percentage in the feed gas as well as the oxidation state of the Cr. With a fluorine-rich feed gas, the surface quickly forms a CrF_x passivation layer, preventing further etching. The EB can break through this passivation and continue the Cr etch process by forming vacancies that allow O radicals to diffuse into the surface and form volatile Cr–O–F compounds. By combining ellipsometric observations with chemical quantification from XPS, we obtained mechanistic insight for the development of low-damage etch processes for Cr and Ru, and insights on paths to high Cr hard mask and Ru capping layer selectivity.

[1] Y. Li *et al.*, "Investigation of ruthenium etching induced by electron beam irradiation and O_2/Cl_2 remote plasma-based neutral fluxes: Mechanistic insights and etching model," *J. Vac. Sci. Technol. A*, vol. 43, no. 2, p. 023005, Feb. 2025, doi: 10.1116/6.0004219.

5:15pm **PS2+EUV-TuA-13 3 Layers Dielectric Patterning in Grid Module for OSC 3DDRAM Application**, ***Yuchao Jiang***, *Jeongsoo Kim, Alejandro Fernandez Rodriguez, Hemant Kumar Raut, Nouredine Rassoul, Eren Canga, Robert Carpenter, Attilio Belmonte, Katia Devriendt,* IMEC, Belgium

3 layers dielectric patterning in Grid module for OSC 3DDRAM application

Yuchao. Jiang[1], Jeongsoo Kim[1], Alejandro Fernandez Rodriguez[1], Hemant Kumar Raut[1], Nouredine Rassoul[1], Eren Canga[1], Robert Carpenter[1], Attilio Belmonte[1] and Katia Devriendt[1]

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DRAM applications have reached a limiting point with 2D design (planar device) because of the process challenges for ~12nm nodes and scaling difficulty of density. Since 2011, monolithic 3DDRAM has been explored with different integration approaches (HBL, VBL, capacitorless etc), and recently it has experienced renewed interest by major players in memory market.

In this presentation, a dry–etch process for grid patterning in MOLD–based monolithic 3D DRAM was reported, the process enables robust isolation of active regions in vertical–bit–line architectures. The method addresses morphology degradation and sidewall profile asymmetry arising from pattern–loading effects and hard–mask facet evolution in multi–layer SiN/SiO_2 ONO stacks. By optimizing passivation balance, ion directionality, and process conditions, the approach achieves stable dielectric grid formation with controlled critical dimensions and near–vertical sidewalls. The demonstrated process provides reproducible grid patterning suitable for high–aspect–ratio 3D DRAM integrationIn monolithic 3DDRAM with MOLD–based vertical–bit–line (VBL) architecture, the Grid module (SINGRID) is the key dielectric–etch step that isolates active areas by etching through a multi–layer SiN/SiO_2 ONO structure (~355 nm). The grid lines have tight CD requirements and require near–vertical profiles (>87°) to ensure VBL alignment and prevent capacitor/gate shorts.

The grid exhibits major–axis vs. minor–axis HM (hard–mask) facet differences, caused by imbalanced ion/radical flux between dense vs. semi–dense regions. Consequences include:

- Unequal CD narrowing
- Facet tilt differences (leading to asymmetric top rounding)
- Risk of local bowing when ARDE.

For morphology improvements, a leaner DARC open step is applied (with reduced CHF3 and increased CF4/O2 flow) to reduce the morphological deformation.

For sidewall profile improvements, the process mitigates these effects through controlled anisotropic dry etching, combining directional ion bombardment with carefully tuned sidewall passivation.

5:30pm **PS2+EUV-TuA-14 Role of Interfacial Force Balance in Gap Filling of TEOS-based Flowable CVD: Insights from Molecular Dynamics**, ***Hu Li,*** Tokyo Electron America Inc.,*; Takeo Nakano, Nobuo Matsuki, Masaaki Matsukuma,* Tokyo Electron Ltd., Japan*; Raymond Joe, Anthony Dip,* Tokyo Electron America Inc.,

Achieving void-free gap filling in high-aspect-ratio structures is one of the key challenges in advanced semiconductor processing. Flowable chemical vapor deposition (CVD) has been widely studied as a promising approach, and its behavior is often interpreted in terms of wettability or viscosity. However, these conventional descriptors do not always explain the differences observed in gap-fill performance across various precursor chemistries and geometries.

In this work, we focus on the pre-cure stage of flowable CVD and investigate the transport-driven filling behavior using classical molecular dynamics simulations. By intentionally excluding chemical reactions, we isolate the role of intermolecular interactions and interfacial forces in confined geometries. The simulation system consists of siloxane-based liquids on SiO_2 substrates, with trench structures of varying aspect ratios.

To better understand the filling mechanism, we introduce a force-based analysis by decomposing the total force acting on liquid molecules into liquid-substrate and liquid-liquid contributions. This approach reveals a clear spatial variation in the driving forces within the trench. Near the sidewall, strong downward forces promote infiltration, while in the center region, the driving force is significantly reduced, which leads to incomplete filling and void formation.

We further show that increasing the aspect ratio enhances this imbalance in force distribution, making uniform filling more difficult. In addition, surface modification, such as Si-rich surface, can reduce the interfacial interaction strength and improve liquid mobility.

These results suggest that gap-fill behavior cannot be fully described by wettability alone, and that a force-based perspective provides more direct insight into the underlying mechanism. This study offers a more detailed understanding of pre-cure transport processes and may help guide the design of future flowable CVD processes.

Surface Science
Room 305 - Session SS-TuA
Chemical Reactions

Moderators: Fang Xu, The University of Texas at San Antonio, **Prof. Ye Xu**, Louisiana State University

2:15pm **SS-TuA-1 Atomic-Scale Insights Into Reactivity and Excitations at Oxide Surfaces**, ***Camilla Ferreira de Sá Codeço,*** Federal University of Rio de Janeiro, Brazil **INVITED**

Oxide surfaces exhibit a strong interplay between local electronic structures, chemical reactivity, and collective excitations, governing processes relevant for catalysis, energy conversion, and infrared nanophotonics. In this work, we investigate how oxidation state, structural disorder, and local coordination affect both surface reactivity and light–matter interactions in model oxide systems.

The reactivity of transition-metal oxide surfaces was investigated considering CO_2 hydrogenation and hydroxylation conditions. On α-Fe_2O_3(012), near-ambient-pressure X-ray photoelectron spectroscopy (NAP-XPS) and low-energy electron diffraction (LEED) were used to correlate surface structure and Fe charge state with CO_2 activation pathways. Exposure of the reconstructed (2×1) surface to CO_2 + H_2 induces partial surface reduction and the formation of electronically enriched Fe^{2+} sites, which stabilize activated CO_2^- intermediates. Complementary studies on MnO(001) and Mn_3O_4(001) surfaces show that hydroxylation by water strongly depends on the oxidation state of surface Mn cations, with Mn^{2+} sites acting as active centers for hydroxyl formation. Together, these results demonstrate that oxide surface reactivity is directly governed by local electronic structure and cation valence.

Beyond surface reactivity, oxide interfaces also support collective excitations that are highly sensitive to local chemical environments. Using synchrotron infrared nanospectroscopy (SINS), we investigated surface phonon polaritons (SPhPs) in amorphous SiO_2 films after fluorine-ion irradiation. The dominant SPhP associated with the asymmetric stretching mode exhibits a pronounced reduction in intensity, revealing modifications in the local dielectric response induced by ion-generated disorder. Finite dipole model calculations indicate that the measured response originates from an effective medium composed of mixed SiO_2 and SiO_x regions, demonstrating how nanoscale chemical heterogeneity modifies polaritonic excitations at oxide surfaces.

Together, these results show how local electronic structure and chemical heterogeneity govern both catalytic activation pathways and confined light–matter interactions at oxide interfaces.

2:45pm **SS-TuA-3 In Situ AP-STM and AP-XPS Studies of CO_2 Activation on Oxide-Tuned PdIn(111) Surfaces**, ***Jiwon Park,*** Korea Advanced Institute of Science and Technology (KAIST), Republic of Korea; *Jeongjin Kim,* Pohang Light Source II, Pohang University of Science and Technology (POSTECH), Republic of Korea; *Jeong Young Park,* Korea Advanced Institute of Science and Technology (KAIST), Republic of Korea

The catalytic conversion of CO_2 into value-added products, such as methanol, presents a promising strategy towards carbon neutrality. Palladium-Indium (Pd-In) intermetallic alloys have emerged as a highly selective and effective catalyst for CO_2 hydrogenation. However, their surface structures and interactions with CO_2 at the solid-gas interface require further understandings. In this study, the CO_2 activation pathways on the oxide-tuned PdIn(111) single crystal alloy surfaces were investigated in situ, using ambient pressure scanning tunneling microscopy (AP-STM) and synchrotron-based ambient pressure X-ray photoelectron spectroscopy (AP-XPS).

Under ultra-high vacuum (UHV), the metastable PdIn(111) surface adopts unique surface structure consisting of clusters, atomic protrusions and ordered superstructure domains. Exposure to ambient pressure O_2 or CO_2 drives dramatic morphological transformations, as dissociated atomic oxygen triggers indium-selective oxidation, and upward segregation of InO_x. Such surface restructuring generates interfacial Pd-In-O_x nanostructures with defect-rich oxygen vacancies, serving as highly active sites for CO_2 activation and the formation of carbonate intermediates. In contrast, the elevated O_2 pressure and temperatures accelerate the dealloying of the Pd-In lattice and the growth of passivating indium oxide overlayer with significantly lower CO_2 activation capabilities.

These in situ observations provide fundamental insights into the active role of the metastable PdIn(111) intermetallic alloys surface in CO_2 activation. Furthermore, they demonstrate that precisely tuning the PdIn(111) surface oxide structures to maintain active interfacial sites is essential for the rational design of robust Pd-In intermetallic catalyst for CO_2 conversion.

3:00pm **SS-TuA-4 Growth, structure and surface chemistry of Pd/In surface alloys and InOx thin films on Pd(111)**, ***Aditya Patidar,*** *Om Amar Zavare, Shubham Ravan, Jason F. Weaver,* University of Florida

Growth, structure and surface chemistry of Pd/In surface alloys and InO_x thin films on Pd(111)

Thermo-catalytic conversion of carbon dioxide (CO_2) to methanol (CH_3OH) is important for mitigating CO_2 emissions and producing fuels and value-added products. Indium oxide (In_2O_3) has emerged as a promising catalyst for activating CO_2 and selectively converting it to methanol while suppressing competing reactions. Adding transition metals (TMs), such as Pd, improves catalytic performance, presumably by promoting efficient H_2 dissociation. Under reducing conditions and during CO_2 hydrogenation, TMs supported on In_2O_3 can transform into TM-In intermetallic compounds, giving rise to complex couplings between surface chemistry and coexisting metal and metal-oxide structures. These effects motivate fundamental studies using model systems.

In this talk, I will first discuss the structural evolution of Pd-In alloys grown on Pd(111) as a function of In coverage and temperature. Temperature-programmed X-ray photoelectron spectroscopy (TP-XPS) demonstrates that Pd-In intermixing produces In-rich surface alloy phases at room temperature and that the surface In concentration decreases with increasing temperature as In dissolves into the bulk Pd. XPS fitting identifies distinct Pd 3d and In 3d components associated with In-poor and In-rich Pd-In phases, whose compositional regimes correlate with the extent of Pd-Pd connectivity within the intermetallic structures. We further show that an ordered ($\sqrt{3} \times \sqrt{3}$)R30° surface alloy (Pd_2In) forms upon heating 2 ML In/Pd(111) to 600 K, while InPd(110) domains develop on an initial 6 ML In/Pd(111) surface between ~400 and 525 K.

I will also discuss the formation and structure of InO_x thin films on Pd(111), characterized using low-energy electron diffraction (LEED) and scanning tunneling microscopy (STM). STM shows that InO_x film growth follows the Stranski–Krastanov mechanism, in which InO_x initially forms a well-connected wetting layer up to an oxide coverage of 1 ML (monolayer), after which multilayer InO_x islands develop. Both the wetting layer and thicker oxide islands exhibit (5 × 5) periodicity relative to Pd(111), characteristic of bixbyite In_2O_3(111). Lastly, I will discuss cooperative interactions between InO_x islands and the exposed Pd surface regions. XPS and TPD measurements show that H_2 dissociates readily on Pd domains, and that a substantial fraction of the resulting H-atoms migrates to neighboring InO_x domains, driving InO_x hydrogenation rather than recombinative H_2 desorption. These findings provide molecular-level insights into cooperative metal/oxide interactions to CO_2 hydrogenation chemistry.

3:15pm **SS-TuA-5 Activation and Selective Hydrogenation of CO_2 on Inverse MgO/Cu(111) Surface**, ***Arephin Islam,*** Brookhaven National Laboratory; *Jose Rodriguez,* Brookhaven National Laboratory and State University of New York at Stony Brook

Industrial CO_2 emissions remain a major driver of climate change, motivating the development of efficient capture and conversion materials. Magnesium oxide (MgO) is an earth–abundant, thermally stable oxide having the capacity of CO_2 capture and conversion, yet the role of nanoscale structure and metal–oxide interfaces in governing its reactivity remains insufficiently understood. Here, we investigate morphology–dependent CO_2 activation and hydrogenation pathways on MgO nanostructures supported on metal substrates using a combined experimental and theoretical approach. Scanning tunneling microscopy (STM), ambient–pressure X–ray photoelectron spectroscopy (AP–XPS), low–energy ion scattering (ISS), temperature–programmed desorption, and catalytic measurements reveal that sub–monolayer MgO clusters (0.3–1.8 nm) dispersed on CuO_x/Cu(111) are 4–5 times more reactive toward CO_2 than bulk MgO and enable selective hydrogenation to methanol at moderate temperatures (500–550 K). MgO forms nano–islands rich in low–coordinated sites at the oxide–metal interface, producing adsorption and activation patterns distinct from bulk MgO(001), Cu(111), or Cu_2O/Cu(111). Spectroscopy indicates hydroxyl formation during H_2 activation and carbonate–like CO_2 binding. Density functional theory (DFT) shows that while isolated MgO motifs enhance CO_2 and H_2 activation, they are limited in promoting complete $CO_2 \rightarrow CH_3OH$ conversion. In contrast, the MgO/Cu(111) inverse catalyst exhibits a substantially smoother reaction landscape, with a highest barrier of only 0.98 eV compared to 1.49 eV on unsupported MgO clusters. The MgO–Cu interface stabilizes CO_2–derived intermediates and lowers hydrogenation barriers, enabling both strong CO_2 trapping and selective conversion. Together, these findings demonstrate that MgO nanostructuring on Cu creates cooperative interfacial sites that integrate efficient CO_2 activation with tunable reactivity, offering a promising route for sustainable CO_2 utilization.

4:00pm **SS-TuA-8 Interpreting Composition-Dependent Oxygen Vacancy Mechanisms in Layered Oxides Through Machine Learning Residuals and Electronic Structure Analysis**, ***Sara E. Mason,*** Brookhaven National Laboratory **INVITED**

Layered transition metal oxides underpin a wide range of functional materials, including intercalation electrodes and oxide catalysts, where oxygen activity strongly influences stability, reactivity, and electronic behavior. Understanding oxygen vacancy formation across compositionally complex chemistries remains challenging due to the interplay between local coordination, electronic structure response, and redox behavior. Here, we investigate oxygen vacancy energetics across layered oxide chemistries using density functional theory (DFT), random forest tree (RFT) models, and electronic structure analysis.

RFT models successfully capture composition-dependent trends in pristine layered oxide formation enthalpies using physically motivated descriptors, demonstrating that bulk thermodynamic properties remain transferable across chemistries. In contrast, prediction accuracy decreases for oxygen vacancy formation energetics, where systematic residual patterns emerge as a function of both local coordination environment (LCE) and host composition. These structured residuals suggest that defect-driven redox behavior introduces mechanistic complexity not fully represented within generalized descriptor-based models.

To probe the origin of these deviations, we analyze charge redistribution following oxygen vacancy formation. Vacancy accommodation mechanisms

vary significantly with composition and extend beyond purely local bonding effects. Ni-rich environments preferentially stabilize vacancies through metal-centered reduction and localized electron accommodation, whereas Mn-rich systems exhibit more heterogeneous redistribution pathways. Co-rich and electronically inactive cation environments suppress conventional transition-metal redox, promoting increased oxygen-centered or delocalized compensation behavior.

Together, these results demonstrate that oxygen vacancy energetics in layered oxides arise from a continuum of composition-dependent electronic response mechanisms that are fundamentally more complex than the pristine-state properties used to describe the host lattice. More broadly, this work highlights an important limitation of transferable ML models for complex oxides: while generalized descriptors can successfully predict bulk thermodynamic properties, defect-mediated redox processes depend sensitively on emergent electronic structure effects that require more mechanistically informed representations. These findings demonstrate how structured ML residuals can serve as physically meaningful indicators of unresolved chemical complexity, providing a pathway for integrating interpretable machine learning with physics-based electronic structure analysis.

4:30pm **SS-TuA-10 Adsorption of Carbon Monoxide on the r-cut Hematite Fe_2O_3(012)-(1×1) Surface**, ***Moritz Eder***, *Johannes Filzmoser, Faith J Lewis, Adam Vavrecka, Maosheng Hao, Tun Sinner, Florian Kraushofer, Margareta Wagner, Christian Schäfer, Jiři Pavelec, Florian Libisch, Gareth S Parkinson,* TU Wien, Austria

Understanding CO adsorption on well-defined metal oxide surfaces provides critical benchmark data for interpreting catalytic processes and infrared spectroscopy on complex powder materials. We present a multi-technique study of CO on the Fe_2O_3(012)-(1×1) r-cut surface, which has a structurally homogeneous array of equivalent Fe^{3+} and O^{2-} sites. Nevertheless, temperature-programmed desorption (TPD) reveals three distinct desorption peaks (58, 100, 125 K) despite the homogeneous surface. We attribute this finding to lateral repulsive interactions between CO molecules. Infrared reflection absorption spectroscopy (IRAS) shows blue-shifted CO frequencies relative to the gas phase (>2143 cm^{-1}) at low coverage that red-shift with increasing coverage. This is consistent with electrostatic interaction between CO and cationic Fe^{3+} sites. Light polarization-dependent measurements provide direct evidence for tilted CO orientation. Non-contact atomic force microscopy (nc-AFM) reveals protrusions consistent with adsorption atop surface Fe^{3+} sites, with distinguishable static and mobile CO populations. Our multi-technique approach establishes adsorption energetics, vibrational signatures, spatial ordering, and bonding geometry, providing a molecular-level foundation for interpreting complex powder catalyst systems.

4:45pm **SS-TuA-11 A Closer Look at Oxygen Reconstructions of Rh Single Crystals** , ***Elizabeth Serna-Sanchez***, *Alexis Gonzalez, Dan Killelea,* Loyola University Chicago

Heavy transition metals such as Rh are commonly used for catalysis and have been heavily studied for oxidative reactions. The fundamental understanding of an oxidized Rh surface is widely investigated on low index single crystals however; limited information is available on the behavior of oxygen on high index surfaces. Using a bi-faceted Rh(111)/(322) crystal, we were able to analyze how oxidation of the two facets compared using scanning tunneling microscopy (STM) to characterize the reconstruction oxidation by surface defects and step width. Alongside with the STM, other techniques such as temperature programmed desorption, and low energy electron diffraction are used to identify the various species of oxygen present on the surface and the structures those oxygen species form.

5:00pm **SS-TuA-12 Desorption Characteristics of CO on Oxidized Rh Surfaces**, ***Alexis Gonzalez***, *Dan Killelea, Elizabeth Serna-Sanchez,* Loyola University Chicago

Heterogeneous catalysis plays an important role in energy production, environmental remediation, and chemical manufacturing, where reactions occur on solid surfaces. Understanding how oxygen interacts with catalytic metal surfaces is necessary for improving catalytic performance. In this study, we investigate oxygen adsorption on two Rh single-crystal surfaces: the flatRh(111) surface and a bifaceted surface with a flat (111) surface and a stepped (322) surface, which contains a high density of under-coordinated sites. Using Reflection Absorption Infrared Spectroscopy, different oxygen prepared surfaces were exposed to CO to examine how surface structure influences CO adsorption behavior. Comparisons between the two crystal single crystals revealed differences in CO vibrational peak positions, peak shifts, and relative intensities, suggesting the presence of distinct CO adsorption species. The results demonstrate that oxygen pre-coverage and surface morphology affect CO adsorption on Rh surfaces. This study provides understanding into structure sensitive adsorption behavior relevant to catalytic oxidation processes.

5:15pm **SS-TuA-13 CO on a Rh/Fe_3O_4 Single-Atom Catalyst: High-Resolution Infrared Spectroscopy and Near-Ambient-Pressure Scanning Tunnelling Microscopy**, ***Nail El Hocine Barama***, *Chunlei Wang, Panukorn Sombut, David Rath, Adam lagin,* Institute of Applied Physics, TU Wien, Austria*; Martin Ormos,* Department of Surface and Plasma Science, Charles University in Prague, Czechia*; Lena Puntscher, Faith Lewis,* Institute of Applied Physics, TU Wien, Austria*; Zdenek Jakub,* Central European Institute of Technology (CEITEC), Brno University of Technology, Czechia*; Florian Kraushofer, Moritz Eder,* Institute of Applied Physics, TU Wien, Austria*; Matthias Meier,* Faculty of Physics and Center for Computational Materials Science, University of Vienna, Austria*; Michael Schmid, Ulrike Diebold,* Institute of Applied Physics, TU Wien, Austria*; Cesare Franchini,* Dipartimento di Fisica e Astronomia, Università di Bologna, Italy*; Peter Matvija,* Department of Surface and Plasma Science, Charles University in Prague, Czechia*; Jiri Pavelec, Gareth Parkinson,* Institute of Applied Physics, TU Wien, Austria

Infrared (IR) spectroscopy is one of the most powerful techniques in heterogeneous catalysis and remains the most widely used optical spectroscopy in the field. Its various experimental modes enable the investigation of a broad range of samples, from powders studied by diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) to flat single crystals examined by infrared reflection–absorption spectroscopy (IRAS or IRRAS). Owing to this versatility, IR spectroscopy is widely regarded as a bridging technique that connects fundamental surface science with applied catalysis.

In this work, we use a newly developed IRAS setup optimised for dielectric single crystals to investigate CO adsorption on the model single-atom catalyst Rh/Fe_3O_4(001).[1] Our spectra resolve three distinct Rh–CO species: monocarbonyls on isolated twofold-coordinated Rh adatoms, monocarbonyls on fivefold-coordinated Rh atoms incorporated into the surface, and gem-dicarbonyls on isolated twofold-coordinated Rh adatoms.[2] These assignments are established unambiguously by combining isotope-substitution experiments (^{12}CO, ^{13}CO, and mixed $^{12}CO/^{13}CO$) with precise control of Rh coverage and surface preparation. The interpretation is further supported by our previous SPM, XPS, and TPD studies, as well as DFT calculations.[3]

Under UHV conditions, monocarbonyls at Rh adatom sites are the predominant species. Gem-dicarbonyl formation is kinetically hindered, occurring primarily through CO-induced dissociation of Rh dimers rather than sequential CO adsorption on isolated adatoms. However, NAP-STM shows that the sequential adsorption pathway becomes accessible at millibar CO pressures, linking the behaviour observed under UHV to that expected under realistic reaction conditions. Although DFT provides qualitative insights, it does not quantitatively reproduce the experimental frequencies and is highly sensitive to the computational parameters, underscoring the need for robust experimental benchmarks. The spectroscopic fingerprints established here provide benchmark reference spectra for oxide-supported single-atom catalysts and a reliable basis for assigning Rh coordination environments in practical catalysts and for evaluating theoretical predictions.

1 D. Rath, *et al.*, *Rev. Sci. Instrum.*, 2024, **95**, 065106.

2 N. E. H. Barama, *et al*., https://arxiv.org/abs/2512.15194v2,.

2 C. Wang, *et al.*, *Angew. Chem. Int. Ed.*, 2024, **63**, e202317347.

5:30pm **SS-TuA-14 Well-Defined Cu-Delafossite Catalysts**, ***Dario Stacchiola***, BNL

Cu-based catalysts are active for partial and full oxidation reactions. Deciphering the local atomic environment and oxidation state of active centers in supported copper catalysts, as well as the design of materials to control their stability under reaction conditions remains a great challenge. We show here that mixed-oxides of copper delafossites with gallium, aluminum or iron ($CuMO_2$, Cu^{1+} and M^{3+}; M: Ga, Al, Fe) in the form of porous nanoplates and films are promising materials as model catalysts to explore the activity and stability of Cu^{1+}-activated reactions. *In situ* experiments allow the observation of dynamic processes and phases under reaction conditions.

Thin Films

Room 317 - Session TF1-TuA

VSHOP Fundamentals

Moderators: Prof. Dr. Greg Parsons, North Carolina State University, **Dr. Junjie Zhao**, Zhejiang University

2:15pm **TF1-TuA-1 What Infiltrates What? An Experimental Survey of Precursor-Polymer Vapor Phase Infiltration Chemistries***, Mark Losego, Typher Yom,* Georgia Tech

Vapor phase infiltration (VPI) exposes polymers to gaseous inorganic precursors that dissolve into the polymer, become entrapped, and convert the polymer into an organic-inorganic hybrid material. VPI hybrids have unique mechanical, electrical, optical, and chemical properties that make them of interest for applications including EUV resists, membranes, and photocatalysts. However, fundamental predictions of which inorganic precursor chemistries will "successfully" infiltrate into which polymer chemistries is still elusive. Despite various systematic studies, no clear chemical "rules" have yet to be established to make these predictions. In this study, we conduct an experimental survey of "infiltration success" for a range of polymer chemistries, precursor chemistries, and infiltration temperatures to determine if any new insights for prediction can be gained. In total we study 12 different polymers, 3 different precursors, and 3 different infiltration temperatures. We include a range of different heteroatom functional groups on the polymers (e.g., nitrile, carboxylate, pyridine, etc.) as well as some differences in bending rigidity and free volume. Along the way, we note characterization tools best-suited for simple, fast detection and assessment of inorganic loading into polymer films, specifically SEM-EDX and XRF. This talk will show how analyzing the signal-to-noise ratio from these methods can then be used to provide a normalized assessment of inorganic loading. Broadly, the $TiCl_4$precursor is capable of successfully infiltrating into all the polymers that trimethylaluminum (TMA) can infiltrate, but just at a lower concentration, which is often not detectable with EDX alone. In contrast, the diethylzinc (DEZ) precursor does not successfully infiltrate many of the polymers that are successfully infiltrated with $TiCl_4$and TMA, like PMMA and P4VP. However, in certain instances, it appears that this lack of infiltration is not due to a lack of "dissolution" into the polymer, but rather a lack of permanent binding to the polymer. These insights along with efforts to train a machine learning model on this experimental data combined with other literature reports to better address the question of "What infiltrates what?" will be discussed.

2:30pm **TF1-TuA-2 Chemical Stability of Vapor-Phase-Infiltrated Poly(vinylpyrrolidone), Poly(4-vinylpyridine), and Polyacrylonitrile***, Alexandra Wnuk, Mark Losego, Typher Yom,* Georgia Institute of Technology

Vapor phase infiltration (VPI) of polymers to form organic-inorganic hybrid materials has been demonstrated to improve the material's chemical resistance to swelling and/or dissolution in organic solvents. Understanding the chemical stability of these hybrid organic-inorganic materials is important for developing new technologies, new membrane materials, and new photoresists. In this study, we examine the ability to use VPI of trimethylaluminum (TMA) and water (H2O) to alter the chemical stability of three different polymers: poly(vinylpyrrolidone) [PVP], poly(4-vinylpyridine) [P4VP], and polyacrylonitrile [PAN]. We find that all three of these polymers can be infiltrated with TMA, and we study their physicochemical structure and dissolution behavior after VPI at 70°C, 90°C, 120°C, and 150°C. For all polymers, the hybrids get thicker (swell) upon infiltration, indicative of inorganic loading into the film. This swollen thickness increases with VPI temperature, suggesting more inorganic loading at higher infiltration temperatures. This increased loading is further verified by combusting the hybrid at high temperatures (burn out) and measuring the residual inorganic layer's thickness. After burnout, the infiltrated P4VP and PAN had inorganic film thickness of 19.2% and 17.0%, respectively, of their original hybrid thickness compared to an inorganic burnout thickness of only 8.8% for PVP , suggesting significantly less inorganic loading in PVP than the other two polymers. When these hybrid materials are then tested for dissolution in solvents known to dissolve the parent polymer, infiltrated PVP films dissolve almost immediately, showing no change in dissolution behavior after VPI. In contrast, infiltrated P4VP shows resistance to dissolution at VPI temperatures of 120°C and 150°C, and infiltrated PAN shows resistance to dissolution at VPI temperatures of 90°C, 120°C, and 150°C. These differences suggest that inorganic loading is likely an important predictor for chemical stability in these systems, however we will also discuss chemical structure changes interrogated with infrared spectroscopy (FTIR) and X-ray photoelectron spectroscopy (XPS) to provide more insights for how the chemical differences also contribute to chemical stability in these hybrid materials.

2:45pm **TF1-TuA-3 Understanding the Vapor Phase Infiltration of Trimethyl Aluminum (TMA) into Polyethylene Terephthalate (PET)***, Mary Kate Broadway, Mark Losego,* Georgia Institute of Technology

Vapor phase infiltration allows for the creation of hybrid organic-inorganic polymers through co-reaction with gas-phase small molecules. During VPI, polymers are isolated under vacuum and exposed to gas phase metal-organic precursors, which sorb into the bulk polymer and create hybrid materials possessing qualities of both the original polymer and the infiltrated inorganic. Despite the utility of VPI, well-defined reaction pathways, processing conditions, and resultant properties remain undefined for some of the most common commercial polymers. Herein, vapor phase infiltration of polyethylene terephthalate (PET) films via trimethlyl aluminum (TMA), in co-reaction with water, is explored as a function of both precursor dose time and subsequent isolation before introduction of water, in order to elucidate the process mechanisms. The rapid sorption of TMA is found to be followed by a slower, time-dependent desorption process that critically influences the resultant hybrid structure, chemical stability, and mechanical properties. In the case of inadequate desorption time, outdiffusing TMA reacts with subsequently dosed water vapor to form a brittle, aluminum oxide "coating" layer. If a longer desorption time is implemented between the TMA dose and water dose, then a homogeneous organic-inorganic hybrid can be achieved, resulting in the retainment of the PET film's optical clarity and observed increases in the strength and resilience of the resultant surface when subjected to strain or bending. Between these extremes, however, we observe unusual transitory behavior with some hybrid character, but susceptibility to brittle cracking when exposed to certain levels of strain. This talk will examine this transitory behavior, and provide insights into how the physicochemical structure is changing at different levels of infiltration. Overall, this work elucidates new understanding of balancing reagent dosage and purge time in controlling the VPI process for infiltration of PET polymers.

3:00pm **TF1-TuA-4 Vapor-Phase Synthesis and Process Optimization of Porphyrin-Based Covalent Organic Framework Thin Films***, Mohammad Arham Khan, Hamidreza Mohajeri Khorasani, Syed Ibrahim Gnani Peer Mohamed, Mona Bavarian, Siamak Nejati,* University of Nebraska-Lincoln, USA

Porphyrin based organic-inorganic hybrid thin films are promising for catalysis, energy conversion, sensing, biomedicine, and environmental applications because of their tunable structures, rich coordination chemistry, and programmable functionality. Among them, porphyrin-based covalent organic frameworks (POR-COFs) are especially attractive due to their intrinsic porosity, ordered structure, and potential for electroactive and optoelectronic applications. However, the poor solubility and limited processability of many two- and three-dimensional covalent frameworks limit their direct integration onto technologically relevant substrates. Here, we investigate vapor-phase growth of POR-COF thin films using 5,10,15,20-tetra(4-aminophenyl)porphyrin (TAPP) as the molecular precursor. Sequential delivery of precursor and oxidant species into the reaction chamber, followed by argon purge steps, enables solvent-free film formation and controlled integration onto surfaces. Temperature, pressure, and precursor exposure time are systematically varied to understand how vapor transport, precursor adsorption, and surface reaction kinetics influence nucleation, surface coverage, film thickness, and deposition rate. Film growth is studied using quartz crystal microbalance (QCM), spectroscopic ellipsometry, atomic force microscopy (AFM), scanning electron microscopy (SEM), and residual gas analysis (RGA). QCM monitors in situ mass uptake during exposure and purge cycles, while ellipsometry tracks thickness evolution under different growth conditions. RGA is used to monitor volatile fragments and reaction byproducts during precursor and oxidant exposure, providing mechanistic insight into oxidant-driven TAPP activation. AFM and SEM provide complementary information on surface morphology, film continuity, roughness, and uniformity. By correlating vapor-phase processing conditions with mass uptake, thickness evolution, and surface morphology, this work identifies growth conditions that promote uniform POR-COF film formation and provides insight into transport-limited and surface-reaction-limited growth regimes. Overall, this study demonstrates vapor-phase synthesis as a versatile strategy for integrating conjugated porous organic frameworks into functional thin-film architectures.

3:15pm **TF1-TuA-5 Enhancing Metalized Polymers Disassembly Using Plasma Polymer Films as a Sacrificial Interlayer**, ***Alexandre Culot***, *Dariane Fadoras, Robin Dantinne,* UMons, Belgium*; Damien Cossement,* Materia Nova Research Center, Belgium*; Jean-Marie Raquez, Damien Thiry,* UMons, Belgium

Metal coatings on polymers are widely used in industries such as electronics, automotive, and packaging for their conductivity, barrier properties, and aesthetics. While strong adhesion between the metallic layer and the polymer is typically beneficial, it poses a significant challenge for their recycling. The separation of such composites is the critical step, requiring costly and limiting methods (e.g., shredding, pyrolysis, dissolving), often resulting in disposal of such waste, causing considerable environmental impact.

In this context, this study explores the use of sacrificial plasma polymer films (PPF) as intermediate layers between metals and polymers to improve the recyclability of the composite. The PPF would ensure strong adhesion with the metallic layer (i.e., Al) while embrittling the coating when exposed to a stimulus (e.g., water immersion, heating).

The PPFs are synthesized from acrylic acid, known to generate PPFs with a high content of carboxylic acid groups, ensuring a strong interaction with aluminum coatings.[1] The analysis of the XPS data reveals a higher retention of the carboxylic group at low plasma power (P_{RF}). ToF-SIMS analysis further shows that, at low P_{RF}, the reduced ionic bombardment during deposition, combined with the higher oxygen content in the PPFs, results in lower cross-linking density compared to PPF deposited at high P_{RF}. Consequently, low P_{RF} PPFs can be readily delaminated upon immersion in water, making them particularly suitable as sacrificial interlayers. Finally, aluminum thin film deposited by magnetron sputtering adheres well to this interlayer while its subsequent removal is significantly facilitated by water exposure.

References:

[1] Friedrich, J. F. et al. Surface & Coatings Technology 2005, 200, 565-568.

Thin Films
Room 317 - Session TF2-TuA
VSHOP Applications I, Membranes and Fluidics

Moderators: Prof. David S. Bergsman, University of Washington, **Prof. Siamak Nejati**, University of Nebraska-Lincoln

4:00pm **TF2-TuA-8 Selective Transport Through Organic Interfaces via Atomic and Molecular Layer Deposition: Durable Materials and Ion-Selective Membranes**, ***Tamar Segal-Peretz,*** Department of Chemical Engineering, Technion, Israel **INVITED**

The ability to control molecular transport through organic interfaces is crucial to a wide array of applications, including polymer and composite materials durability in harsh environmental conditions and membrane-based separations. In this talk, I will discuss how vapor-phase processing, specifically atomic layer deposition (ALD), vapor phase infiltration (VPI), andmolecular layer deposition (MLD) can be used to engineer organic interfaces with nanoscale precision for controlled molecular transport across them.

First, we utilized vapor-phase growth of inorganic materials on polymers and carbon fibers to enhance their durability under UV radiation and elevated temperatures. We showed that sequential VPI and ALD enable robust ZnO–polymer hybrid structures on poly(lactic acid) (PLA), where VPI creates subsurface and surface nucleation sites that promote conformal ZnO growth during ALD. While VPI or ALD alone provides limited protection, their combination yields polycrystalline ZnO coatings that reduce polymer photodegradation by more than two orders of magnitude, while preserving transparency in the visible range. In addition, we employed Al_2O_3 ALD on carbon fibers to reduce oxygen transport into the fibers and oxidative degradation at elevated temperatures. The Al_2O_3-coated fibers showed superior thermal durability and mechanical properties under these conditions.

Second, we used MLD to fabricate ion-selective polyamide membranes. MLD provides a unique route to synthesize ultrathin polyamide films with molecular-level control over thickness and chemistry. Using MLD, we grew ultrathin, ultrasmooth, and highly cross-linked aromatic polyamide selective layers directly on porous supports, achieving tunable, Angstrom-level controlled thickness in the 2-30 nm range. The MLD-based exhibited high water-ion and ion-ion selectivities. Beyond enhanced performance, MLD provides a powerful experimental platform for probing structure–composition–transport relationships with unprecedented precision. This approach opens new pathways toward rational design of polymer layers, building one molecular layer at a time.

4:30pm **TF2-TuA-10 Investigating the Impact of Membrane Hydrophilicity on Long- and Short-Chain PFAS Remediation via Molecular Layer Deposition**, ***Joelle Scott***, *Jocelyne Booth, Kacey Taylor, Mathangi Venkatesh, Jay Werner, David S. Bergsman,* University of Washington

Per- and polyfluoroalkyl substances (PFAS) are a class of toxic contaminants in water that have become a topic of increasing concern. While long-chain PFAS have seen decreased use due to environmental regulation, short-chain PFAS continue to proliferate. Unfortunately, these smaller molecules are more environmentally mobile, harder to remove from water, and just as toxic, undermining environmental protection efforts. Membrane separations have been explored as a low cost technology to remove PFAS from water. However, membrane permeability usually must be sacrificed to be able to achieve high removal rates of these short-chain PFAS, like with desalination membranes. To combat this, using more hydrophilic membranes may increase the rejection of both long- and short-chain PFAS by reducing hydrophobic interactions between the membrane and PFAS compounds, resulting in an opportunity to improve rejection without compromising permeability. Current interfacial polymerization methods of membrane synthesis rely on identifying monomers that can be dissolved in immiscible solvents, greatly limiting the possible membrane chemistries that can be explored. Molecular layer deposition (MLD) is an alternative method for synthesizing thin film composite membranes that uses vapor-phase reactions, allowing for a wider range of selective layer chemistries to be explored. In this work, we use MLD to synthesize thin film composite membranes of different hydrophilicities, with the aim of investigating the impact of hydrophilicity on PFAS selectivity. To demonstrate the effectiveness of this technique for controlling membrane properties, polyurea and polyurethane films were deposited as membrane selective layers, and their film composition was confirmed using FTIR and XPS. These membranes were then examined for their pure water permeability and PFAS rejection, correlating these properties to their hydrophilicity to determine the impact of monomer chemistry. As part of this work, a polyurethane MLD process was developed and fully optimized for the first time. This work highlights the challenges of depositing thin films without interfacial polymerization, but the rewards of using techniques with independent compositional control for exploring polymer chemistry in membrane separations.

4:45pm **TF2-TuA-11 Vapor Phase Infiltration of Metal Oxides into Polymeric Water Treatment Membranes**, *Jiaman Wang, Chenhao Yao,* ***Bezawit Getachew***, Rice University

Vapor phase infiltration (VPI) of metal oxides into polymeric membranes may offer a novel way to combine the benefits of polymeric and ceramic membranes and enable improved capabilities in water treatment membranes. In this paper, we investigate the infiltration of alumina into two types of membranes, namely polyamide nanofiltration (NF) membranes and commercial anion exchange membranes (AEMs). The infiltration is characterized by using X-ray photoelectron spectroscopy (XPS) to confirm the presence of metal oxide, quantify the amount of incorporation at the surface and as a function of depth, and probe the type of bonding taking place. Complementary SEM-EDX (Scanning Electron Microscopy with Energy Dispersive X-ray Spectroscopy) and time of flight secondary ion mass spectrometry (ToF-SIMS) experiments show the distribution of the inorganic phase within the membranes. We find an increase in NaCl rejection from 90 to >95% for NF90 and MgSO4 rejection from 80 to 90% for NF270 membranes with minimal impact on water flux. For the AEMs, we find that the infiltrated membranes show improved resistance to degradation by chlorine without any changes in membrane resistance and permselectivity after infiltration. These results show that infiltration of metal oxides into polymeric membranes holds promise for improving the selectivity and stability of polymeric membranes without compromising other important performance metrics.

5:00pm **TF2-TuA-12 Molecular Layer Deposition of Salt Sieving Polyamide Membranes**, ***Brian Welch***, University of Missouri*; Ruoke Cai, Tamar Segal-Peretz,* Technion Israel Institute of Technology, Israel **INVITED**

Membrane separations offer a vital pathway for recovering critical minerals such as lithium from magnesium-rich brines. However, conventional polymerization methods produce selective layers with poorly controlled molecular structure, resulting in low selectivity between Li^+ and Mg^{2+}. To overcome the limitations of solution-based polymerization, we used molecular layer deposition (MLD) to fabricate polyamide selective layers for

nanofiltration (NF) and reverse osmosis (RO) membranes, using trimesoyl chloride/piperazine (NF) and trimesoyl chloride/m-phenylenediamine (RO) precursors. MLD-grown polyamide films exhibited structural advantages, including high crosslinking, high mass density, low surface roughness, morphological homogeneity, and precise thickness control. Inverse gas chromatography measurement of surface energy revealed that amine-terminated cycles were free of surface defects. MLD NF membranes deposited at 1.3 Å/cy achieved Li^+/Mg^{2+} selectivity as high as 35, compared to 3 for commercial membranes, while maintaining comparable Li^+ flux. While the Li^+/Mg^{2+} selectivity of conventional NF membranes relied on Donnan exclusion arising from strong surface charges, MLD NF membranes achieved high selectivity with negligible surface charge through molecular sieving via 5 ± 1 Å ultramicropores. While conventional, solvent-based synthesis results in selective RO layers with overall thickness > 100 nm, MLD RO films grew at a rate of 2.4 Å/cy, enabling fabrication of functioning membrane films as thin as 2 nm. By probing the extreme low end of thickness, we improved water flux, but ultimately reached a performance limit, demonstrating that selective films with thickness below their Bjerrum length exhibited reduced salt selectivity due to decreased dielectric self-energy. These results establish a high-precision platform for probing and optimizing molecular transport in thin-film composite membranes and advancing membrane materials.

5:30pm **TF2-TuA-14 Tertiary and Aromatic Polyurea Films Deposited Using Molecular Layer Deposition as a Method of Producing Cationic Thin Film Coatings for Use in Microfluidic Design**, ***Jay Werner***, *David S. Bergsman,* University of Washington

The application of cationic thin film coatings has gained interest as a method of producing antibacterial surfaces which can passively resist bacterial contamination and reduce the spread of infectious microbes. One common method of producing these cationic surfaces is through the exposure of surface amine groups to methyl iodide to produce quaternary ammonium compounds (QACs). These films are typically deposited from the liquid phase using spin coating, spray coating, or dip coating, but these coating methods can be difficult or impossible to implement effectively for high aspect ratio or enclosed microfluidic devices. Molecular layer deposition (MLD) is a vapor phase process involving the exposure of a surface to reactive precursors in a cyclic manner, forming a polymer film layer by layer in a highly precise and conformal way. To vaporize precursors, they must be neutrally charged, but the deposition of a polyurea film with tertiary or aromatic amine sites could be used as a substrate for post-synthetic surface quaternization with liquid or vapor-phase treatment with methyl iodide.

In this work, we investigate the formation of polyurea MLD chemistries based on low melting point 2,4-toluene diisocyanate (TDIC) combined with substituted diamines including bis(2-aminopropyl)(methyl)amine (BAPMA) and 2,6-diaminopyridine (DAP). These precursors enable incorporation of tertiary and aromatic nitrogen functionalities into polyurea thin films, providing reactive sites for subsequent in situ or ex situ quaternization. The resulting substituted polyurea films are investigated as candidate substrates for vapor-phase fabrication of cationic antimicrobial coatings compatible with microfluidic device architectures, characterizing their film thickness, composition, and surface charge before and after exposure to methyl iodide. These results demonstrate a new avenue towards the creation of films with MLD and a possible new approach toward the functionalization of surfaces with cationic coatings.

The Future of Temperature Sensing
Room 320 - Session TS-TuA

The Future of Temperature Sensing I

Moderators: Dr. Nikolai Klimov, National Institute of Standards and Technology, **Dr. Sesha Challa**, NIST-Gaithersburg

4:00pm **TS-TuA-8 Keynote Talk: The Transformation of Temperature Traceability**, ***Graham Machin FREng FRS***, National Physical Laboratory, U.K. **INVITED**

In May 2019 the kelvin was redefined in terms of a fixed value for the Boltzmann constant, *k*. Since then global temperature traceability has been regulated through the Consultative Committee of Thermometry (CCT) *mise-en-pratique* for the definition of the kelvin (*MeP*-K-19).

The *MeP*-K-19 introduced a gradualist but transformational approach to temperature traceability. Whilst allowing for continuity in temperature traceability through the long defined temperature scales of ITS-90 and PLTS-2000, it opened, for the first time, the possibility for temperature traceability to be derived directly from the kelvin definition through use of a *MeP*-K-19 approved primary thermometry approach, such as acoustic gas thermometry or dielectric constant gas thermometry. Some of these approaches are currently close to maturity and likely to be implemented and trial comparisons in train before the end of the decade.

However, that form of traceability is essentially still traditional in that reference thermometers would still be calibrated at National Metrology Institutes (NMIs) and sent to calibration laboratories to act as reference standards for the calibration of user thermometers. The only difference, from a user perspective, is that thermodynamic temperature, *T*, rather than a defined scale (T_{90} or T_{2000}) would be disseminated to them. More radical traceability approaches, envisaged in the CCT Strategy 2030+, is the development of temperature sensors that provide traceability at the point of measurement. These could be conventional based self-validating thermometers, or reliable practical primary thermometers, that require no calibration, based on fundamental physical principles that would provide trustworthy thermodynamic temperature values for the lifetime of the application.

In this talk I will outline the kelvin redefinition, introduce the concept of traceability, describe the *MeP*-K-19 and its function and then go on to speak about emerging approaches to temperature traceability. This will be illustrated with examples ranging from traditional approaches to temperature traceability that disseminate *T*, to more radical approaches under development such as self-validating thermometers and practical primary thermometry such as Doppler broadening or ring-resonator thermometry.

4:45pm **TS-TuA-11 Dual-Mode Fiber-Optic Refractive-Index Gas Thermometry for Primary Calibration and Continuous Temperature Tracking to 1000 K**, *Musaddeque Syed,* ***Ming Han***, Michigan State University

Accurate, drift-resistant temperature measurement is essential for harsh industrial processes, where conventional secondary sensors often degrade under sustained thermal and mechanical stress or experience radiation-induced drift in nuclear reactor environments. Refractive-index gas thermometry (RIGT) provides a driftless primary route to thermodynamic temperature measurement, but practical deployment has been limited by pressure-cycling requirements that reduce measurement speed and complicate field operation. Here, we advance an argon-filled, fiber-optic Fabry-Perot (FP) RIGT sensor into a dual-mode temperature metrology platform that combines absolute primary calibration with continuous temperature tracking up to 1000 K.

The thermometer consists of an external FP cavity formed at the end of a single-mode optical fiber and filled with argon gas. In primary mode, absolute thermodynamic temperature is determined from spectral fringe shifts measured between two pressure states and interpreted using a virial-coefficient refractivity model, eliminating dependence on empirical calibration. In secondary mode, the same fiber-optic FP sensor operates at a fixed pressure to continuously track temperature-induced optical path-length changes with faster temporal response. This mode provides practical monitoring capability between primary calibration points while retaining traceability to the underlying RIGT measurement framework.

We develop working equations for both primary-mode and secondary-mode operation, establishing a unified analytical framework for absolute temperature determination and continuous temperature tracking using the same fiber-optic FP sensor. The dual-mode operation is experimentally demonstrated from room temperature to 1000 K. The resulting architecture links the driftless accuracy of a primary gas thermometer with the compactness, remote interrogation capability, and deployment advantages of a fiber-optic FP sensor. This work establishes a practical pathway toward high-accuracy temperature metrology for extreme industrial, energy, nuclear, and process-control environments.

5:00pm **TS-TuA-12 A Projected Refractive Index Gas Thermometer Revisited**, ***Patrick Egan***, National Institute of Standards and Technology (NIST)

In 1974, Colclough of the National Physical Laboratory UK lamented the difficulties associated with the primary thermometry methods: constant volume gas thermometry, acoustic gas thermometry, and Johnson noise thermometry. As an alternative to those established methods, Colclough projected a refractive index gas thermometer as a viable alternative for primary thermometry.

There were two oversights in Colclough's projections. The first is merely a minor point that the proposed refractometer system (gas cell in a Michelson interferometer) never worked! The second issue is that Colclough did not foresee the 2025 breakthrough "dispersion gas barometry" which derives thermodynamic temperature using simultaneous measurements of refractive index at widely separated wavelengths. Fifty year's after Colclough's original projection, I would now argue that refractive index gas thermometry has become superior to every other primary thermometry methodology.

My presentation will explain some key advantages of dispersion gas barometry. I will present a roadmap for primary thermometry covering the range 4 K to 1234 K using only two refractometers.

- A. R. Colclough, "A Projected Refractive Index Thermometer for the Range 2--20 K," Metrologia 10, 73 (1974). https://doi.org/10.1088/0026-1394/10/2/006
- Y. Yang, J. A. Stone, and P. F. Egan, "Demonstration of dispersion gas barometry," Physical Review Applied 23, 064041 (2025). https://doi.org/10.1103/z9zz-lqzh

5:15pm **TS-TuA-13 Wide-Temperature-Range Luminescence Thermometry***, **Yuanbing Mao**,* Illinois Institute of Technology

Luminescence-based temperature sensing holds great promise thanks to their attractive properties including rapid response, high spatial resolution, and remote non-invasive detection, ultimately their applicability in chemically and electromagnetically harsh environments. Relevant to their practical use, a wide temperature sensing range is urgently required for thermometric phosphors along with high relative sensitivity. Herein, we have designed several thermometric phosphors for wide-temperature-range sensing in recent years. In this talk, I will focus on discussing relevant strategies to broaden the working range of thermometric phosphors with enhanced temperature sensitivity, such as intervalence charge transfer and thermally stable hosts, particularly negative thermal expansion compounds. Our work provides inspiration for exploring desirable wide-temperature-range thermometric phosphors insensitive to surface emissivity and reflected radiation with broad application potential.

5:30pm **TS-TuA-14 Group V Metalates as High-Temperature Thermosensitive Phosphors***, **Federico Rabuffetti**,* Wayne State University

Refractory niobates and tantalates are ideal hosts for high-temperature thermosensitive phosphors activated with rare-earths.A distinct feature of these materials is their chemical tunability, which makes them ideal platforms to understand the interplay between crystal structure, electronic structure, and luminescence thermal quenching. This understanding provides the basis to exercise synthetic control over temperature-dependent luminescence and thermometric response.

In this talk I will use group V metalates to illustrate how we are approaching the challenge of establishing a set of crystal-chemical principles that enable the design of high-temperature thermosensitive phosphors. Synthesis, high-end structural analysis, and luminescence studies of dysprosium-doped $Ba_3MgTa_2O_9$ and Y_3NbO_7 will be described to demonstrate how chemical substitutions may be used to rationally tune structural and electronic features governing thermal quenching. From a luminescence thermometry standpoint, I will show that both phosphors are capable of temperature sensing up to 1200 °C, thus expanding the compositional library of high-temperature thermosensitive phosphors [1,2].

[1] M.R. Imer, A. Afugu; Z.-F. Liu; and F.A. Rabuffetti. Luminescence of Triple Perovskite $Ba_3MgTa_2O_9:Dy^{3+}$ Up to 1100 °C. *The Journal of Physical Chemistry C* **2024**, 128, 16628–16639.

[2] M.R. Imer and F.A. Rabuffetti. Luminescence of Y_3NbO_7:Dy Up to 1000 °C. *Journal of Luminescence* **2025**, 278, 121017.

2D Materials

Room 304 - Session 2D-WeM

2D Materials: Electronic, Magnetic, Mechanical, and Optical Properties

Moderators: Prof. Victor Brar, University of Wisconsin - Madison, **Souvik Sasmal**, Argonne National Laboratory

8:00am **2D-WeM-1 Functionalizing 2D Materials with Defects and Dopants Using Ultra-Low Energy Ions**, ***Harriet Åhlgren,*** Uppsala University, Sweden

The inert surface plane of 2D materials can be functionalised by defects and the incorporation of foreign atomic species for applications in catalsysis, energy conversion and optoelectronics. Various methods are available for this, but major challenges still lay in the control of the defect types and their concentrations. Irradiation with energetic ions at ultra-low energies (< 100 eV) offers a powerful tool to create modifications with selected type and concentration in 2D materials by adjusting the kinetic energy of the ion and the exact number of the ions. In this talk, I will discuss our recent efforts in applying this methodology to functionalise and manipulate 2D materials. Specifically, I will review our recent results on introducing substitutional metal atoms in graphene [1,2], and how these functional sites are then used as anchoring sites to build single atom thick planar metal structures (metallenes) on the graphene surface [3]. Structural analysis via high-resolution transmission electron microscopy reveals the defect structures and metallenes at single atom scale, while atomistic simulations provide complementary information about at the dynamic processes of the synthesis at picosecons timescales.

[1] Trentino,.., Åhlgren et al. Micron 184, 103667, 2024.
[2] Trentino,.., Åhlgren, 2D Materials 9, 025011, 2022.
[3] Joudi, .., Åhlgren, ACS Nano 19, 22032-22043, 2025.

8:15am **2D-WeM-2 Clean Integration of h-BN Encapsulated Graphene Heterostructures with Ferroelectric $Al_{1-x}B_xN$ Thin Films for Robust Carrier Concentration Modulation**, ***Joseph Hladik,*** Penn State University; *Aswini Ramankutty,* University of Pittsburgh; *K. M. Daiyan,* Penn State University; *Jeremy Levy, Patrick Irvin,* University of Pittsburgh; *Beth Dickey,* Carnegie Mellon University; *Morteza Kayyalha, Jon-Paul Maria,* Penn State University

Since the discovery of graphene, there have been significant efforts to manipulate its band structure to further probe its interesting properties. However known band structure engineering methods, such as nanostructuring, twistronics, and chemical doping, can present practical challenges and may degrade the delicate structure of graphene that brings about these interesting properties in the first place. A new platform for precise, nondestructive tuning of energy landscapes in graphene has been developed, which involves the interaction of graphene with the electrostatic field effect generated by a thin film of ferroelectric $Al_{1-x}B_xN$. Using resist-free ultra-low-voltage electron-beam lithography (ULV-EBL), ferroelectric domains can be patterned and reprogrammed through an existing graphene-to-AlBN interface at resolutions below 20 nm, where the graphene acts as a capacitor top electrode during writing. These ferroelectric domains in AlBN are highly robust, showing polarization of up to 130 $\mu C/cm^2$ and capable in principle of inducing theoretical carrier concentrations of up to 10^{15} cm^{-3} in an adjacent graphene layer. However, this limit of carrier modulation assumes the full polarization field has been screened by the graphene. To achieve this theoretical limit, interfacial contamination during device preparation must be eliminated so as to block alternative compensation paths. We have demonstrated the preparation of defect-free single layer graphene encapsulated with multilayer h-BN via a dry transfer method under argon atmosphere to prevent moisture accumulation between layers. This dry transfer method involves a PC film-assisted PDMS stamp for easy pickup and stacking of exfoliated flakes, as well as precise placement of full 2D heterostructures within defined device AlBN windows. Gold metal is used to make contact to encapsulated graphene via a 1D edge contacting method. In this presentation, we detail the specific process flow for the clean transfer of standalone 2D single layer graphene as well as 2D h-BN encapsulated graphene heterostructures onto $Al_{1-x}B_xN$ surfaces. Transport property measurements will be shown that measure the graphene carrier density and explore the modulation limits possible using the ferroelectric polarization.

8:30am **2D-WeM-3 Hidden in Plain Sight: Aromaticity of Hexagonal Boron Nitride**, *Suryakanti Debata,* Laboratory for Physical Sciences; *Sai Krishna Narayanan,* University of Maryland College Park; ***Pratibha Dev,*** Laboratory for Physical Sciences **INVITED**

Hexagonal boron nitride (hBN), which is isoelectronic to graphene, is of interest for a wide range of applications in electronics, photonics, catalysis, and quantum information science. Despite this broad interest, it is not known if hBN is aromatic. Aromaticity (or lack thereof) of a planar structure is related to its structural and chemical stability, and hence, its determination is of fundamental importance to different applications. With the help of energetic and magnetic criteria, we determine the aromaticity of hBN flakes of different sizes. We show that although hBN is aromatic, it is weakly so as compared to graphene. Ultimately, the differences in the aromaticity of hBN and graphene can be linked to the differences in their symmetry-allowed transitions between the occupied and unoccupied molecular orbitals.

9:00am **2D-WeM-5 Damage-Free Fabrication of Single Photon Emitters in Hexagonal Boron Nitride by Remote Plasma Generation of Vacancies**, *Souvik Bhattacharya, Swetapadma Sahoo,* University of Illinois Urbana-Champaign; *Simeon Bogdanov,* University of Illinois Urbana Champaign; ***R. Mohan Sankaran,*** University of Illinois Urbana-Champaign

Hexagonal boron nitride (hBN) has emerged as a promising material for quantum photonics and sensing because of its unique ability to host single room-temperature optically active color centers that exhibit bright and stable emission. However, scalable and deterministic fabrication of the emitters remains challenging. Color centers often appear near an edge or fold in the material, or require methods that produce undesired damage. Emitters are produced from combinations of impurities and vacancies, which are difficult to control at the atomic level. In particular, the controlled production of vacancies has been so far elusive.

In this study, we present a remote plasma whereby the energetic species, particularly ions, are separated spatially from hBN, to controllably generate vacancies.[1] Properties of the remote plasma are characterized by Langmuir probe measurements and binary collision approximation simulations. Combined with atomic force microscopy (AFM) imaging of the hBN surface helps provide insight into structural changes resulting from ion bombardment. We then show by photoluminescence mapping and time-correlated photon counting that process conditions exist where damage is minimized but emitters are created without preference for structural imperfections (i.e., edges or folds). The results establish remote plasma processing for the fabrication of single photon emitters in ultrathin hBN, and show the importance of vacancy generation as another knob in addition to impurities for the tuning of emitter properties.

1. Bhattacharya et al., Appl. Phys. Lett. 128, 214103 (2026).

9:15am **2D-WeM-6 Probing Static and Dynamical Phenomena in Magnetic Systems Using Spin Defects in Hexagonal Boron Nitride**, ***Kartik Shah,*** *Pratyush Saud,* Carnegie Mellon University; *Anshuman Sahoo, Ravi Kumar Bandapelli, Raghvendra Posti, I-Hsuan Kao,* Carnegie Mellon University, USA; *James Edgar,* Kansas State University; *Jyoti Katoch, Simranjeet Singh,* Carnegie Mellon University, USA

Atomic vacancies in van der Waal materials, like hexagonal Boron Nitride (hBN), have emerged as a versatile quantum sensing platform. The exceptional ease of integration of hBN based quantum sensors with various 2D systems has proven to be of substantial importance as a quantum probe. In this work, we will present the characterization techniques for the establishing properties of optically active spin defects in hBN. We employ Photoluminescence (PL) spectroscopy and PL mapping to probe the defect ensemble and lateral uniformity of the defect centres in hBN. As a primary application of these defects as quantum sensors, we explore its utility to study magnetism in a van der Waals (vdW) ferromagnet, particularly $Fe_xGa_yTe_2$, at room temperature. By integrating ion flux irradiated hBN flakes (containing spin defects) with vdW magnetic layer, via a dry transfer method, we probe spatially resolved spin phenomena in the ferromagnet layer at a microscopic level. Our work will establish the utility of hBN based sensors to probe spin related interactions/phenomena in vdW-based systems with high spatial resolution, thus providing a robust framework for probing emergent magnetism in low-dimensional systems.

9:30am **2D-WeM-7 Characterization of Optically Active Spin Defects in hBN as Quantum Sensors**, ***Pratyush Saud***, *Anshuman Sahoo, Kartik Shah,* Carnegie Mellon University, USA*; I-Hsuan Kao,* Taiwan Semiconductor Manufacturing Company*; Raghvendra Posti, Ravi Kumar Bandapelli,* Carnegie Mellon University, USA*; James H. Edgar,* Kansas State University*; Jyoti Katoch, Simranjeet Singh,* Carnegie Mellon University, USA

Abstract:

Quantum sensing employing optically active spin defects in hexagonal boron nitride (hBN), specifically the negatively charged boron vacancy (V^-_B), has shown a capacity to investigate local spin dynamics[1]. Building upon the initial principles established by V^-_B-based sensing platforms, our work aims at expanding capabilities of 2D-based material characterization by moving toward more stable and spin-active carbon-related defects in hBN, as well as defects generated through neutron irradiation. Carbon-related defects possess optical and spin characteristics that make them suitable for precise spin manipulation and improved quantum sensing[2]. In this study, we present comprehensive time-resolved measurements of these defects to evaluate their potential as sensors for probing static and dynamical phenomena in magnetic systems. Through the driving of Rabi oscillations and the determination of longitudinal spin-lattice relaxation (T_1) times, the study characterizes the coherence limits and manipulation fidelity of these centers. These time-resolved protocols demonstrate the benefits of carbon-related centers compared to standard V^-_B ensembles for investigating weak, spatially localized magnetic fields. This optimized quantum sensing architecture is intended to address the metrological limitations of 2D-based systems' characterization, providing a sensitive platform for the discovery of new physical phenomena and the direct observation of spin interactions in emergent 2D magnetic materials.

References:

[1] Shekhar Das, Alex L. Melendez, I-Hsuan Kao, Janeth A. Garcia-Monge, Daniel Russell, Jiahan Li, Kenji Watanabe, Takashi Taniguchi, James H. Edgar, Jyoti Katoch, Fengyuan Yang, P. Chris Hammel, and Simranjeet Singh. Quantum sensing of spin dynamics using boron-vacancy centers in hexagonal boron nitride. Phys. Rev. Lett., 133:166704, Oct 2024

[2] Xingyu Gao, Sumukh Vaidya, Kejun Li, Zhun Ge, Saakshi Dikshit, Shimin Zhang, Peng Ju, Kunhong Shen, Yuanbin Jin, Yuan Ping, and Tongcang Li. Single nuclear spin detection and control in a van der waals material. Nature, 643:943–949, 2025.

9:45am **2D-WeM-8 Towards Probing spin dynamics in mesoscopic sized 2D magnets**, ***Anshuman Sahoo***, *Pratyush Saud, I-Hsuan Kao, Raghvendra Posti,* Carnegie Mellon University*; Kartik Shah,* carnegie Mellon University*; Ravi Kumar Bandapelli,* Carnegie Mellon University*; Bing Lv,* University of Texas at Dallas*; Jyoti Katoch,* Carnegie Mellon University*; Simranjeet Singh,* carnegie Mellon University

Absttrat:

van der Waals (vdW) based antiferromagnets (AFMs) are an emerging class of materials, which can enable high density and ultrafast magnetic memory technologies. The spin dynamics in conventional AFMs is not well studied because magnetic resonance frequency often lies in the terahertz regime, which is not easy to access in research labs. However, vdW based materials that exhibit weak interlayer coupling, resonance frequency is in the gigahertz regime, and yet existing studies (using conventional techniques) are mainly limited to bulk crystals [1][2]. The understanding of spin dynamics in AFMs in the 2D atomic limit is needed for envisoned devices but it remains critically missing. A long-standing challenge has been the requirement of ultra-high-sensitive technique to probe spin dynamics in exfoliated flakes of 2D materials. Here, we present our work on developing a new technique for the broadband detection of spin dynamics in mesoscopic sized samples of 2D materials at cryogenic temperatures. We employ microwave interferometry to enhance the signal to noise ratio (SNR) [3], thus enabling the detection of spin dynamics in mesoscopic sized 2D materials. We will present the results of antiferromagnetic resonance experiments performed on CrSBr, which is layered A-type AFM. Our interferometer provides a versatile platform for studying the magnetic properties, i.e. magnetic damping, interlayer coupling, and anisotropy effects in low-dimensional systems.

References:

1] D. MacNeill, J. T. Hou, D. R. Klein, P. Zhang, P. Jarillo-Herrero, and L. Liu. Gigahertz frequency antiferromagnetic resonance and strong magnon-magnon coupling in the layered crystal crcl3. Physical Review Letters, 123(4):047204, 2019.

[2] T. M. J. Cham, S. Karimeddiny, A. H. Dismukes, X. Roy, D. C. Ralph, and Y. K. Luo.Micrometer-scale magnetic resonance imaging of two-dimensional ferromagnets. NanoLetters, 22(16):6716–6721, 2022.

[3] S. Tamaru, K. Yakushiji, A. Fukushima, S. Yuasa, and H. Kubota. Highly sensitive ferromagnetic resonance detection using a microwave interferometer. IEEE Magnetics Letters, 5:3700304, 2014.

11:00am **2D-WeM-13 A New Topological Monolayer**, ***Qiong Ma***, Boston College **INVITED**

I will present experimental studies of the topological and correlated electronic properties of monolayer TaIrTe4. I first discuss the realization of a *dual quantum spin Hall (QSH) insulator* arising from the interplay between single-particle band topology and density-tuned electronic correlations. At charge neutrality, monolayer TaIrTe4 exhibits QSH behavior, characterized by enhanced nonlocal transport and quantized helical edge conduction. Upon electron doping, the system briefly becomes metallic before entering a correlated insulating state, likely driven by an electronic instability near conduction-band van Hove singularities, such as a charge density wave. Remarkably, within this correlated gap, the QSH state re-emerges. I will then report the discovery of a *nonvolatile superlattice memory effect* in the same material. In a pristine monolayer, we observe the spontaneous formation of a long-period superlattice that can be reversibly programmed ON and OFF via electrostatic tuning of low-energy electronic states. This switching toggles between two lattice configurations with unit-cell areas differing by nearly two orders of magnitude. Our results reveal two distinct but coupled instabilities—one electronic and one structural—enabling electrostatic control of lattice configurations with nonvolatile memory. These findings are established through a combination of nonlinear Hall measurements that probe quantum geometry and Raman spectroscopy that tracks lattice reconstruction.

11:30am **2D-WeM-15 Spatially-resolved Voltage-reversal due to Bernoulli Potentials in Dissipative Bi2Sr2CaCu2O8+x**, ***Sharadh Jois***, *Gregory M. Stephen, Samuel W. LaGasse,* Laboratory for Physical Sciences*; Genda Gu,* Brookhaven National Laboratory*; Aubrey T. Hanbicki, Adam L. Friedman,* Laboratory for Physical Sciences

We measure magneto-transport and critical currents in $Bi_2Sr_2CaCu_2O_{8+x}$ Hall bar devices. Above critical current in an applied magnetic field, we observe longitudinal differential voltage along one edge comparable in magnitude but opposite in sign to the other edge. This phenomenon is unaffected by reversal of the applied field, and seems unique to devices with invasive voltage contacts. We attribute the source of this behavior to particle-hole symmetry breaking in moving vortices and the formation of opposite Bernoulli potentials due to opposing vortex velocities at the edges where the invasive contacts create hotspots for rapid vortex nucleation and flux flow. These results are fundamental to the composition and flow of dissipative currents in layered superconductors.

https://arxiv.org/abs/2604.19467

11:45am **2D-WeM-16 Signature of Ferromagnetic and Ferroelectric Coupling in WTe_2/$Cr_2Ge_2Te_6$ Heterostructures**, ***Zhenhong Cui***, *Ravi Kumar, I-Hsuan Kao, Raghvendra Posti, Jyoti Katoch, Simranjeet Singh,* Carnegie Mellon University

Electric-field control of magnetism is a central goal in multiferroic and spintronic devices, where ferroelectric polarization can be used to tune the magnetic states without a global magnetic field or large writing current. Van der Waals heterostructures provide a flexible platform for exploring this coupling by stacking a ferroelectric layer with a ferromagnetic layer. In this work, we study a dual-gated bilayer heterostructure, combining gate-switchable ferroelectric weyl semimetal WTe_2 and the ferromagnetic semiconductor $Cr_2Ge_2Te_6$ (CGT). The bilayer WTe_2 exhibits ferroelectric hysteresis in longitudinal resistance under electric field switching. Since WTe_2 can also generate a current-induced spin polarization with an out-of-plane component due to the low-symmetry crystal structure, this allows us to used unconventional unidirection magnetoresistance, which is sensitive to both spin-polarization and magnetization, as an electrical readout for the out-of-plane magnetization of CGT. Given the advantage of dual-gated geometry, the carrier density and displacement field can be independently tuned in the heterostructure, and we show that the UMR amplitude is strongly modulated by electrostatic gating. In addition, the displacement-field-dependent UMR response follows the ferroelectric hysteresis in bilayer WTe_2, suggesting that ferroelectric switching can modulate the spin-dependent magnetotransport response of the WTe_2/CGT heterostructure.

These results suggest bilayer WTe_2/CGT as a possible platform for studying ferroelectric and ferromagnetic coupling and gate-tunable spin polarization in van der Waals devices.

12:00pm **2D-WeM-17 Electrical Detection of NéEl Vector Reversal in a Van Der Waals Antiferromagnet**, ***Raghvendra Posti***, *Ravi Kumar Bandepalli,* Carnegie Mellon University*; Wenhao Liu,* The University of Texas at Dallas*; Anshuman Sahoo, Pratyush Saud,* Carnegie Mellon University*; Zixin Zhai,* The University of Texas at Dallas*; Zhenhong Cui, I-Hsuan Kao, Aalok Tiwari,* Carnegie Mellon University*; Thomas Poirier, James H. Edgar,* Kansas State University*; Kenji Watanabe, Takashi Taniguchi,* National Institute for Materials Science, Japan*; Bing Lv,* The University of Texas at Dallas*; Jyoti Katoch, Simranjeet Singh,* Carnegie Mellon University

Antiferromagnets (AFMs) are a promising platform for next-generation spintronic and magnonic technologies owing to their intrinsic ultrafast spin dynamics, absence of stray magnetic fields, and robustness against external perturbations. In particular, electrical control and detection of the Néel vector, the fundamental order parameter of AFMs, is central to realizing ultrafast magnetic memory devices. Recent discoveries of two-dimensional van der Waals AFMs have provided a versatile material platform for exploring antiferromagnetic spin transport and dynamics, where reduced dimensionality and weak interlayer exchange coupling enable access to different magnetic phases at relatively low magnetic fields. Despite these advances, electrical detection of complete 180° reversal of the Néel vector remains a major challenge due to the absence of net magnetization in antiferromagnets. Here, we focus on the layered A-type antiferromagnet CrSBr, which exhibits highly spin-dependent transport arising from its spin-polarized electronic structure. Utilizing this spin-dependent transport, we probe the Néel-vector orientation in CrSBr through tunnel magnetoresistance between CrSBr and a ferromagnetic spin-polarized electrode. To realize this, we fabricate Co/hBN/CrSBr tunnel junctions and perform magnetotransport measurements. We demonstrate that spin-dependent tunnelling between Co and CrSBr enables electrical detection of the Néel vector and its 180° reversal. Furthermore, this detection scheme is robust for both even- and odd-layer CrSBr devices and remains observable up to Néel transition temperature of CrSBr.

Atomic Scale Processing Mini-Symposium
Room 316 - Session AP+EL+PS+TF-WeM

Thermal and Plasma Enhanced Atomic Layer Etching

Moderators: Dr. Eric A. Joseph, IBM Research Division, T.J. Watson Research Center, **Prof. Dr. Erwin Kessels**, Eindhoven University of Technology, the Netherlands

8:00am **AP+EL+PS+TF-WeM-1 Cyclic dielectric etching challenges for next-generation FDSOI logic and quantum devices**, ***François Boulard***, CEA-LETI, France*; Ramy Ayoub,* CEA-LETI, France, Lebanon*; Emmanuel Petitprez, Stéphane Pocas, Nicolas Gauthier, Benoit Martin, Pierre Brianceau, Antoine Ronco,* CEA-LETI, France*; Bernard Pelissier,* LTM-CNRS, France*; Nicolas Posseme,* CEA-LETI, France **INVITED**

As logic devices dimensions scale down[(1)] and quantum gates advance in scalability and environment resilience[(2)], the demand for gentle, selective, and highly controlled fabrication processes has become critical. Atomic-scale processing—particularly cyclic approaches like Atomic Layer Etching (ALE) and quasi-ALE—has emerged as a potential solution. By leveraging fluorocarbon-based chemistries in sequential deposition/removal cycles, these methods have already demonstrated superior performances in terms of SiO_2 to Si_3N_4 selectivity, such as in Self-Aligned Contact (SAC) etching[(3)]. While the fundamental mechanisms of these cyclic processes are increasingly well understood[(4)], their industrial applicability—especially for advanced integration schemes—still faces challenges in versatility, robustness, and throughput. In this presentation, we will highlight recent advances in adapting cyclic etching strategies to selectively etch dielectric materials (SiO_2, SiON, Si_3N_4) for two cutting-edge applications: Contact multipatterning in next-generation FDSOI CMOS logic devices and intertwined gate patterning for cryogenic FDSOI quantum chips. This study explore the critical role of process parameters, including fluorocarbon precursor selection, multi-step cyclic strategies, substrate temperature and plasma power modulation, and their collective influence on etch per cycle stability, selectivity, uniformity, throughput, and pattern transfer fidelity.

By bridging fundamental insights with integration-driven optimization, this work clears the path to highly scalable, atomic-precision etching—a key enabler for both classical and quantum semiconductor technologies.

The research work presented in this paper was carried out in the framework of the FAMES Pilot Line of the Chips JU, funded by Horizon Europe grant 101182279 and the ANR NextGen project ANR-22-NEXTG001 of the France 2030 initiative. Part of this work, carried out on the Platform for Nanocharacterisation (PFNC), was supported by the “Recherche Technologique de Base” and "France 2030 - ANR-22-PEEL-0014" programs of the French National Research Agency (ANR).

(1)C. Fenouillet-Beranger, et.al., Solid-State Electronics, 2026, 231, 109264, https://doi.org/10.1016/j.sse.2025.109264

(2)B. Bertrand, et.al., International Electron Devices Meeting, IEDM 2023, DOI: 10.1109/IEDM45741.2023.10413763

(3)M. Honda, et.al, 2017, J. Phys. D: Appl. Phys. 50 234002 [tel:50 234002], https://doi.org/10.1088/1361-6463/aa6f27

(4)R.J. Gasvoda, J. Vac. Sci. Technol. A 38, 050803 (2020); https://doi.org/10.1116/6.0000395

8:30am **AP+EL+PS+TF-WeM-3 Atomic Layer Etching of TiN using O_2/Ar Plasma and SF_6/H_2/Ar Plasma Half-Cycles**, ***Kazuya Tajima,*** Hitachi High-Tech Corporation, Japan*; Andrew P. Kaye,* Colorado School of Mines*; Kazumasa Okuma, Hiroaki Ishimura,* Hitachi High-Tech Corporation, Japan*; Sumit Agarwal,* Colorado School of Mines

Titanium nitride (TiN) has become a widely adopted material for both logic and memory devices due to its appropriate work function with high-k gate stacks and excellent barrier properties against fluorine and oxygen diffusion. Atomic layer etching (ALE) of TiN was performed by a combination of surface modification by oxidation during the O_2/Ar plasma half-cycle and release of volatile etch products in the SF_6/H_2/Ar plasma half-cycle. [1,2] For the ALE experiments, we used low-resistivity TiN deposited by atomic layer deposition. In the O_2/Ar plasma half-cycle, TiN was oxidized to TiO_x with O radicals. For the SF_6/H_2/Ar plasma cycle, the SF_6-to-H_2 flow ratio was tuned to minimize continuous etching of TiN. Quadrupole mass spectrometry (QMS) was used to identify conditions that maximize the production of HF in the SF_6/H_2/Ar plasma, which acts as the etchant for surface modified TiO_x layer, and does not spontaneously etch TiN. Using QMS, we also identified the primary reaction products produced in each half-cycle. Our data show that NO was the primary nitrogen-containing product in the Ar/O_2 plasma half-cycle. TiF_2^+ and TiF^+ ions were detected by the QMS in the SF_6/H_2/Ar plasma half-cycle, which most likely originate due to cracking of TiF_4 parent molecules in the ionizer. The likely O-containing product during the SF_6/H_2/Ar plasma half-cycle is H_2O, which could not be detected due to the background signal in the QMS. In addition, we also detected SO^+ and SO_2^+ ions during both half-cycles due to the presence of S on the substrate and/or the chamber walls.

The etching process was performed at 200 °C. While the oxidation of TiN was quasi-self-limiting during the O_2/Ar plasma half-cycle, subsequent etching in the SF_6/H_2/Ar plasma half-cycle was not self-limiting. The synergy parameter, *S*, [3] is an indicator of the ideality of the ALE process. We show that the ALE end point could be determined by the time decay of the reaction products measured by the QMS, and the synergy parameter could be optimized by limiting the duration of the SF_6/H_2/Ar plasma half-cycle. We were able to obtain a synergy parameter of ~82% under optimized conditions.

[1]Lee et al., Chem. Mater. 29, 8202 (2017);

[2]Hossain et al., J. Vac. Sci. Technol. A 41, 062601 (2023);

[3] Kanarik et al.,J. Vac. Sci. Technol. A 35, 05C302 (2017);

8:45am **AP+EL+PS+TF-WeM-4 Atomic Layer Etch Process for InGaAs Using (CH4+H2)/Ar+ Plasma**, ***Burak Okur***, *Ryan Walsh, J. Russell Renzas,* University of Nevada, Reno

Precise, damage-free etching of InGaAs with Angstrom-scale control is a critical requirement for next-generation III-V semiconductor device fabrication, including gate recess etching in InGaAs HEMTs, which require very precise etching of ~20 nm of InGaAs. Conventional plasma etching is insufficiently precise for this application and introduces subsurface damage and surface roughness, motivating the development of atomic layer etching (ALE) processes that achieve controlled material removal through sequential, self-limiting surface reactions.

In this work, we investigate a plasma-based ALE process for InGaAs using $(CH_4+H_2)/Ar^+$ chemistry, consisting of alternating surface modification and removal half-cycles. The expected volatile products are $In(CH_3)_3$, $Ga(CH_3)_3$, and AsH_3. The effects of chamber conditioning, process pressure, and Ar flow rate are systematically investigated to achieve self-limiting ALE behavior. Real-time optical emission spectroscopy (OES) measurements are

used to monitor plasma species and investigate the role of residual CH-related species in the transition between self-limiting ALE and RIE-like behavior. For a process at 10 mTorr with 200 W ICP power, 5 sccm Ar, a 1 sec dose of 5 sccm CH_4 and 20 sccm H_2, and 5 sec etch time, an ALE window is present from 10-15 W RF bias, with EPC of 0.25 nm/cycle. The etched surfaces are characterized using scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), atomic force microscopy (AFM), and profilometry to evaluate etch per cycle (EPC), surface morphology, roughness evolution, and compositional uniformity of the InGaAs surface. Synergy is also measured.

9:00am **AP+EL+PS+TF-WeM-5 O2/CF4/Ar+ 3-Step Plasma Atomic Layer Etch Process for Aluminum***, **Ryan Walsh**, Burak Okur, J. Russell Renzas,* University of Nevada, Reno

Aluminum is a light, conductive metal used in an incredible assortment of device fabrication processes, including in superconducting devices, where performance is highly sensitive to material impurities, interface damage, and critical dimensions. Most aluminum reactive ion etch processes use Cl_2 or BCl_3, which have the dual disadvantages of toxicity and post-etch corrosion. Fluorine is not typically used as an etchant for Al films because of the high melting point of AlF_3. It is known, however, that fluorinated AlO_x has a lower sputter threshold than untreated AlOx[1]. We present a novel 3-step plasma Atomic Layer Etch (ALE) process for Al using O_2, CF_4, and Ar^+. This room-temperature cyclical process starts by oxidizing Al in O_2 in Step A. Step B consists of a tetrafluoromethane dose to create an aluminum oxyfluoride modified layer. In Step C, this modified layer is removed via argon ion bombardment, using the oxide as an etch stop for the removal of the more easily sputtered oxyfluoride layer.

EPC of 0.08 nm/cycle and synergy of >99% were achieved with 100 W ICP power and 7 W table bias during step C. Etch control is governed by the thickness of the grown oxide and the depth of fluorine diffusion. We also present AFM, SEM, and XPS to show the effect of this process on the Al surface. This process could provide an avenue toward improved performance in aluminum-based superconducting devices.

[1] Chittock, N. J. (2024). Plasma processes for atomic layer etching. [Phd Thesis 1 (Research TU/e / Graduation TU/e), Applied Physics and Science Education]. Eindhoven University of Technology.

9:15am **AP+EL+PS+TF-WeM-6 Directional Atomic Layer Etching of Lithium Niobate for Nonlinear Integrated Nanophotonics***, **Ivy Chen,*** California Institute of Technology*; Frank Greer,* Jet Propulsion Laboratory (NASA/JPL)*; Austin Minnich,* California Institute of Technology

Atomic layer etching (ALE) is of intense interest in microelectronics, photonics, and other fields owing to increasing demands for nanofabrication with nanometer-scale precision, aspect-ratio independent etching, and sub-nanometer surface roughness. Nonlinear integrated nanophotonic devices typically employ complex oxides like lithium niobate for which dry etching processes perform poorly. Fundamental improvements in nanofabrication processes are vital to realize the full potential of nonlinear integrated nanophotonics for on-chip quantum information processing and beyond. Here, we report a directional ALE process for LN consisting of sequential exposures of HBr/BCl_3/Ar plasma for surface modification and Ar plasma for removal. We observe an etch rate of 1.04 ± 0.01 nm/cycle with a synergy of 84.6% at a temperature of 0°C. At higher process temperatures, the HBr chemistry is found to decrease redeposition compared to F- and Cl-based plasmas, which we attribute to the higher vapor pressures of Br-based products. A grating pattern etched entirely by the process (total etch depth of 220 nm) exhibits no aspect-ratio dependent etching (ARDE) down to the smallest tested gap of 150 nm, in contrast to ion milling in which ARDE manifests even at 300 nm gaps for the same etch depth. Additionally, we present results on applying our ALE processes to TFLN devices to obtain higher aspect ratios, smoother sidewalls, and precise etch depths, yielding enhanced performance metrics for coupler gratings, ring resonators, and spontaneous parametric downconverters for on-chip quantum information processing.

9:30am **AP+EL+PS+TF-WeM-7 Native Oxide Removal and Passivation of Niobium for Superconducting Devices***, **Jessica Jones,*** Argonne National Laboratory*; Jeffrey Elam,* Argonne National Laboratory, USA

Superconducting materials are foundational to many quantum technologies, yet surface and interfacial disorder remain important barriers to device performance and scalability. In particular, native oxide formation on superconducting metals is believed to contribute to loss and decoherence, creating a need for processing methods that provide precise surface control while maintaining the integrity of the underlying material. Niobium is an attractive superconducting material because of its relatively high critical temperature and broad relevance to quantum circuit platforms. However, complex native oxide formation and near-surface chemical disorder complicate its integration into devices such as Josephson junctions and other superconducting circuit elements. Here, we investigate an atomic-scale surface treatment and passivation approach for niobium thin films aimed at improving control over the metal/oxide interface. Our results show that thermal atomic layer etching can effectively remove native surface oxides from niobium while preserving the underlying metallic surface. Subsequent atomic layer deposition prevents reformation of the native oxide layer on the surface. Together, these findings establish a promising pathway for interface control in superconducting niobium and support the development of improved fabrication strategies for quantum circuit technologies.

9:45am **AP+EL+PS+TF-WeM-8 Thermal Atomic Layer Etching of the Semiconductor Oxide Channel Materials by Sequential Surface Modification and Volatile Release Reactions***, **Muhammad Hamza Ansar**, Steven George,* University of Colorado Boulder

Indium gallium oxide (IGO) and Indium gallium zinc oxide (IGZO) can be used as channel materials in metal oxide semiconductor thin-film transistors (TFTs). These TFTs have high carrier mobility, low leakage current and a wider bandgap compared with silicon. Etching the channel material to a precise and controlled thickness is important for device performance. Thermal atomic layer etching (ALE) of these metal oxide semiconductors is possible using surface modification and volatile release reactions.

In this study, the thermal ALE was performed with sequential exposures of boron trichloride (BCl3) and hydrogen fluoride (HF). In situ spectroscopic ellipsometry (SE) measurements on flat films determined etch rates for IGO of 2.1 Å/cycle at 225°C and 3.0 Å/cycle at 255°C. The etch rate for IGZO was 2.5 Å/cycle at 205°C and 5.6 Å/cycle at 255°C. The etch rates were observed to be nearly self-limiting versus the BCl3 and HF exposures.

Quadrupole mass spectrometry (QMS) investigations identified the volatile products during the BCl3 and HF exposures on In2O3, Ga2O3 and ZnO powders. The initial BCl3 exposure reacted with the In2O3, Ga2O3 and ZnO powders and produced InCl3, GaCl3 and ZnCl2, respectively. These products are consistent with conversion to B2O3. The next HF exposure then produced BF3 and H2O from the spontaneous etching of B2O3. The HF then proceeded to yield additional H2O from the fluorination of the metal oxide. The subsequent BCl3 exposure first yielded BF3 from ligand-exchange with the metal fluoride. The BCl3 exposure then proceeded to produce metal chloride by conversion of the underlying metal oxide. The QMS results for Ga2O3 powder are displayed in **Figure 1**.

Additional studies on flat films explored the effect of IGO composition on the etch rate. **Figure 2** shows that the IGO etch rates were 2.8, 3.6, and 4.2 Å/cycle at In:Ga ratios of 1:1, 2:1 and 4:1, respectively at 230 °C. The etch rate then decreased to 0.8 Å/cycle at an In:Ga ratio of 8:1. The thermal ALE was also observed to smooth the initial roughness of the IGZO surface.

11:00am **AP+EL+PS+TF-WeM-13 Isotropic Atomic Layer Etching via Thermal-Cyclic Processing: Broad Material Capabilities with a Focus on Work–Function Metal Films***, **Kazunori Shinoda,*** Hitachi High-Tech Corporation, Japan*; Thi-Thuy-Nga Nguyen, Shunya Hirai,* Nagoya University, Japan*; Nobuya Miyoshi,* Hitachi, Ltd., Japan*; Masaru Izawa,* Hitachi High-Tech Corporation, Japan*; Kenji Ishikawa, Masaru Hori,* Nagoya University, Japan **INVITED**

An isotropic atomic layer etching (ALE) process based on thermal–cyclic processing (thermal-cyclic ALE), consisting of repeated plasma exposure and infrared lamp heating, has been developed for advanced semiconductor manufacturing applications. This approach enables highly controllable and selective isotropic material removal through self–limiting surface reactions driven by cyclic thermal activation. A key advantage of this approach is the independent optimization of the adsorption and desorption temperatures, which enables enhanced material selectivity, improved surface smoothness, and sufficient etch per cycle (EPC). To realize this process at a manufacturing scale, a dedicated 300–mm wafer tool, referred to as a Dry Chemical Removal (DCR), has been developed and commercialized. Using this DCR tool, isotropic ALE processes have been developed for a wide range of materials used in semiconductor device fabrication, including oxides, nitrides, carbides, metals, and compound films. Furthermore, surface reaction mechanisms during the ALE steps have been systematically investigated using in–situ X–ray photoelectron spectroscopy (XPS), providing direct insight into adsorption and desorption steps governing the self–limiting etching behavior. These analyses reveal material–dependent reaction pathways and clarify the roles of plasma–

induced surface modification and thermally activated removal of the modified surfaces. This invited presentation provides a comprehensive overview of the thermal–cyclic ALE technology, covering its historical development, process fundamentals, tool design, and mechanistic understanding across multiple material systems.In particular, recent progress in the isotropic ALE of work–function metal films, such as TiC and TiN, will be highlighted, with an emphasis on surface reaction mechanisms investigated by in–situ XPS. These materials are of increasing importance for advanced semiconductor devices, where precise thickness and surface control are critical. Process characteristics and surface chemistry insights obtained by in–situ XPS will be discussed.

11:30am **AP+EL+PS+TF-WeM-15 Selective Thermal Chemical Vapor Etching (CVE) and Atomic Layer Etching (ALE) of Ge Versus Si**, ***Micah Duffield,*** *Marcel Junige, Steven George,* University of Colorado at Boulder

The fabrication of gate-all-around nanosheet transistors employs multi-layer stacks of crystalline SiGe and Si. Completely removing sacrificial SiGe and precisely recessing SiGe may be accomplished by chemical vapor etching (CVE) and atomic layer etching (ALE), respectively. Facile Si CVE has been shown previously using anhydrous HF vapor above 150°C. This Si CVE is ceased by co-dosing H_2O+HF. The present work explored selective CVE and ALE pathways for Ge compared with Si using HF only or with oxidants.

Quadrupole mass spectrometry (QMS) measurements identified the volatile etch products during different reactant gas exposures at ramped or isothermal temperatures. Exposing Ge nanopowder to HF during an up-ramp from 25 to 400°C discovered that facile Ge CVE produced volatile GeF_4 at 50-75°C and then turned off due to non-volatile GeF_2 polymer formation. The GeF_2 polymer could then be volatilized at >300°C. Additional experiments at varied ramp rates, a reversed down-ramp, and isothermal HF exposures corroborated this non-volatile GeF_2 polymer formation.

Exposing a mixture of Ge & Si nanopowders to HF during a temperature ramp showed that the GeF_4 etch product in turn etched Si, producing volatile SiF_4 at 75-110°C (**Figure 1a**). Co-dosing H_2O+HF still etched Ge (or GeO_2) and produced volatile GeF_4. However, co-dosing H_2O+HF eliminated the parasitic Si etch pathway via GeF_4 (**Figure 1b**). Introduced H_2O oxidized Si and formed an ultra-thin chemical oxide. This SiO_2 was not etched by GeF_4.

Repeatedly exposing GeO_2 nanopowder to HF at 100°C revealed that GeO_2 etched spontaneously without the self-termination observed for Ge. This finding inspired a unique Ge ALE mechanism: A first oxidant exposure may oxidize Ge to form an ultra-thin GeO_2 surface layer. A subsequent HF exposure may volatilize this GeO_2 surface layer but self-terminate on the underlying Ge due to GeF_2 polymer buildup. The following oxidant exposure may remove the GeF_2 polymer and again oxidize Ge.

Exposing Ge nanopowder to a sequence of oxidant and HF exposures at 100 and 150°C, respectively, revealed that volatile GeF_4 was released after each oxidant exposure in a self-terminating fashion. To refresh the Ge surface after HF exposures, H_2O was ineffective, whereas O_2 was effective, and O_3 was even more effective than O_2 (**Figure 2**). To verify these QMS findings, *in situ* spectroscopic ellipsometry (iSE) studies were employed on Ge thin film samples. Ge ALE using an alternating O_2/HF sequence at 150°C exhibited an etch per cycle of 1.38 Å, near-ideal ALE synergy of 97%, and selectivity versus Si (**Figure 3**).

11:45am **AP+EL+PS+TF-WeM-16 Controlled SiO_2 Etch Rates Using a HF/H_2O Liquid-Layer in a Vacuum Environment: Dependence on H_2O and HF Pressures**, ***Samantha Rau,*** University of Colorado at Boulder*; Antonio Rotondaro, Hanna Paddubrouskaya, Kate Abel,* Tokyo Electron America, Inc.*; Steven George,* University of Colorado at Boulder

Our earlier research demonstrated SiO_2 etching by HF using a H_2O liquid-layer in a vacuum environment. The current work characterized the dependence of SiO_2 etch rate on the H_2O and HF pressures. We have observed a dramatic increase in SiO_2 etch rates at higher H_2O and HF pressures. This behavior suggests that the thickness of the HF/H_2O liquid-layer may be increasing rapidly at higher pressures.

SiO_2 etch rates may be sensitive to the HF/H_2O liquid-layer thickness when the thickness is close to the size the hydrated F^-, HF_2^- and SiF_6^{2-} ions that are involved during SiO_2 etching. For example, the size of the hydrated F^- ion is 7 Å. Lower SiO_2 etch rates may result from incomplete hydration of these ions. SiO_2 etch rates may approach the SiO_2 etch rates observed in solution for thicker liquid-layers.

Investigations were performed to determine the thresholds for HF/H_2O condensation versus H_2O and HF pressure. Spectroscopic ellipsometry was employed to measure the liquid-layer thickness, the mean squared error (MSE) in the thickness model, and the transmitted light intensity. Condensation was assumed to occur when the increase in liquid-layer thickness, the increase in MSE, and the decrease in light intensity all occurred rapidly at higher H_2O and HF pressures. Figure 1 shows that rapid changes in the liquid-layer thickness, MSE and transmitted light intensity are observed at a total pressure of 22.9 Torr (18 Torr H_2O and 4.9 Torr HF) at 30.4°C.

Experiments were conducted at initial H_2O pressures from 0-35 Torr and increasing HF pressures from 0-40 Torr to determine the threshold H_2O and HF pressures for condensation at 30.4°C. The resulting condensation points were then compared with the measured SiO_2 etch rates at various H_2O and HF pressures in Figure 2. Below the condensation curve in the ultrathin liquid layers, there were lower SiO_2 etch rates ranging from ~1-100 Å per 5 s HF exposure. These lower SiO_2 etch rates may result from incomplete hydration of the F^-, HF_2^- and SiF_6^{2-} ions. Above the condensation line, the measured SiO_2 etch rates of ~100-1000 Å per 5 s HF exposure were comparable with SiO_2 etch rates in bulk HF solutions with HF wt% values of 25-40%.

12:00pm **AP+EL+PS+TF-WeM-17 Thermal Selective Etching of $Si_{1-x}Ge_x$ in XeF_2**, ***Daniel Cho,*** *Yi Chen,* UCLA*; John Hoang, Nick Altieri, Ji Zhu, Samantha Tan,* Lam Research Corporation*; Jane P. Chang,* UCLA

In GAAFET fabrication, $Si_{1-x}Ge_x$ is etched selectively from Si. Wet, plasma, and thermal chemistries have been investigated to etch $Si_{1-x}Ge_x$ with a range of selectivity [1]. Thermal fluorine-based etch processes, including F_2 and XeF_2, show high selectivity with etch rates exhibiting a volcano-shaped dependence on x [2, 3].

In this study, we report $Si_{1-x}Ge_x$ (x = 0 to 1) etch by a XeF_2 beam. XeF_2 was sublimed into an expansion chamber to a target pressure, then pulsed into the reaction chamber. In each pulse, ΔP_{XeF2} was proportional to the XeF_2 dose. *Ex situ* x-ray photoelectron spectroscopy (XPS) identified the chemical bonding states on the $Si_{1-x}Ge_x$ surface from XeF_2, while scanning electron microscopy (SEM) measured the etch depth for etch rate (ER) calculations.

XeF_2 exposure on as-received $Si_{1-x}Ge_x$ samples showed no etch, confirmed by XPS and SEM. This was attributed to a native oxide which prevented XeF_2 from interacting with the underlying $Si_{1-x}Ge_x$. Prior to XeF_2 exposure, *in situ* Ar ion sputtering was used to remove the native oxide for all sequential etch conditions.

XPS results of XeF_2-processed $Si_{0.75}Ge_{0.25}$, Si, and Ge identified Ge-F, Si-F, and C-F bonding in the F 1s region at binding energies of 685.0 eV, 687.1 eV, and 689.6 eV, respectively, consistent with literature values [4-6]. Ge-F, Si-F, and C-F made up 20.8%, 37.4%, and 41.8% of the total fluorine content on the XeF_2-processed $Si_{0.75}Ge_{0.25}$. Quantitative analysis of fluorination by *ex situ* XPS was limited by air exposure between etch and measurement.

Synergistic etching, with Ar ions and XeF_2 simultaneously exposed, showed a Si ER of 6 nm/pulse at an ion beam voltage of 200 V and ΔP_{XeF2} =0.5 Torr, showing a higher ER than the sequential Si ER of 0.4 nm/pulse at the same ion beam voltage and ΔP_{XeF2}.

The peak sequential $Si_{1-x}Ge_x$ ERs for the following Ar ion beam voltage and ΔP_{XeF2} conditions, 100 V and 0.5 Torr, 200 V and 0.5 Torr, and 100 V and 0.2 Torr, were 7.8 nm/pulse, 9.9 nm/pulse, and 4.1 nm/pulse, respectively. For all conditions, ER increased from x = 0 to 0.1, followed by a decrease or plateau past x = 0.15. Higher pretreatment ion beam voltage and higher ΔP_{XeF2} both led to an etch rate increase for x = 0 to 0.25. The peak $Si_{1-x}Ge_x$/Si etch selectivity ranged from 20 to 30 under all conditions.

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References

[1]T. Salvetat, et al., ECS Transactions **16**, 439 (2008).[2]G. Xuan, et al., J. Vac. Sci. Technol. A **26**, 385 (2008).[3]Y. Chen, et al., J. Vac. Sci. Technol. A **43**, 042604 (2025).[4]T. J. Chuang, J. Appl. Phys. **51**, 2614 (1980).[5]S. W. Robey, et al., J. Vac. Sci. Technol. B: Microelectron. Process. Phenom. **6**, 1650 (1988).[6]M. C. Peignon, et al., J. Vac. Sci. Technol. A **14**, 156 (1996)

Applied Surface Science
Room 319 - Session AS-WeM

Advances in Sputtering

Moderators: Dr. Alexander Shard, National Physical Laboratory, **Dr. Lyndi Strange**, Pacific Northwest National Laboratory

8:00am **AS-WeM-1 Non-destructive XPS Depth Profiling Using a Three-Anode HAXPES Source with Simultaneous (Angle-Resolved) Data Collection over a Range of Angles**, ***Max Clark,*** Brigham Young University*; Paul Dietrich,* SPECS Surface Nano Analysis GmbH, Germany*; Joshua Pinder,* specs Surface Nano Analysis GmbH*; Andreas Thissen,* SPECS Surface Nano Analysis GmbH, Germany*; Matthew Linford,* Brigham Young University

In traditional X-ray photoelectron spectroscopy (XPS), depth profiling is achieved by alternating analysis scans with sputtering of the outermost layer, although at the cost of a damaged sample and increased analysis time. Angle-resolved XPS (ARXPS) can produce information at shallower depths nondestructively, but it is still constrained by the information depth (mean free path) of the photoelectrons. Using HAXPES sources and simultaneously collecting data from a range of angles (10 - 70 degrees with respect to the surface normal) increases information content, depth, speed and allows the user to see deeper into a sample. In particular, by collecting angle-resolved measurements with three X-ray sources (Al Kα, Ag Lα, and Cr Kα) focused at the same spot, non-destructive depth profiling from ca. 0 - 30 nm can be achieved with good resolution and reasonable speed. This technique has been demonstrated on samples with variable compositions and film-thicknesses.

8:15am **AS-WeM-2 XPS Depth Profiling of Multilayer Stacks using Femtosecond Laser Ablation (fs-LA)**, ***Charlie Chandler,*** University of Surrey, UK*; Dhilan Devadasan, Paul Mack, Robin Simpson, Tim Nunney,* Thermo Fisher Scientific, UK*; Mark Baker,* University of Surrey, UK

Multilayer stacks of different materials are commonly employed across a wide range of technical fields. XPS depth profiling of multilayers has been investigated previously using traditional ion beam sputtering techniques, with rotation of the sample during etching increasing the depth resolution. With the recent introduction of femtosecond laser ablation (fs-LA) as a novel depth profiling method, it is important to optimise the analytical approach to enhance depth resolution. A femtosecond laser with a 1030 nm peak wavelength, pulse length of 160 fs and top-hat optical beam shaper has been employed to perform the XPS depth profiles. Results will be shown for different classes of material using analytical set-ups with and without laser polarisation rotation and sample rotation. Discussion of the results will consider the origins of crater roughening in fs-LA depth profiling, influence of top-hat uniformity, material related effects and describe the best analytical approach for optimisation of depth resolution.

8:30am **AS-WeM-3 Calibration of Removal Rates for fs-Laser Ablation XPS Depth Profiling**, ***Tim Nunney,*** Thermo Fisher Scientific, UK*; Charlie Chandler,* University of Surrey, UK*; Robin Simpson, Paul Mack,* Thermo Fisher Scientific, UK

Femtosecond laser ablation offers new opportunities for XPS depth profiling. It has been shown that by using an ultra-fast laser for removing material from the surface, chemical damage and other effects that can distort the measured composition in an ion beam profile can be avoided [1]. For example, a tantalum nitride layer that has been deposited on silicon, with a stoichiometry of Ta_2N_3 measured by Rutherford backscattering spectroscopy, retains that composition through a fs-laser depth profile, but shows depletion of nitrogen during a monatomic ion beam profile [2]. With the introduction of this method, there is a necessity to understand the relationship between the laser energy and the ablation rate, to be able to control the removal process to match experimental requirements of the sample. This presentation will describe a simple method to determine the ablation threshold of a material, and how to use the threshold to determine the laser energy required to remove the desired amount of material per laser shot.

1. M.A. Baker et al, Applied Surface Science 654 (2024) 159405
2. C.W. Chandler et al, Applied Surface Science Advances, 34 (2026) 101008

8:45am **AS-WeM-4 IR Femtosecond-Laser Ablation of IR-Transparent Coatings - Consequences for XPS Depth Profiling**, ***Miroslav Michlicek,*** Thermo Fisher Scientific, Czechia*; Paul Mack,* Thermo Fisher Scientific, UK*; Veronika Hammerova,* Thermo Fisher Scientific, Czechia

Femtosecond-laser depth profiling is emerging as a practical complement to ion sputtering for XPS analysis of materials that are either difficult to profile by conventional monoatomic or cluster ion beams, or to simply speed up the depth profiling process. In our current implementation - Hypulse, ultrashort IR (1030 nm) pulses remove material rapidly while minimizing the extended collision cascades, preferential sputtering, and chemical reduction often associated with ion sputtering. The ablation rate, crater growth and material removal uniformity are largely defined by the energy distribution of the shaped laser beam relative to the material ablation threshold. For quantitative XPS depth profiling, this creates a fundamental tradeoff between removal rate and crater uniformity.Notably for IR transparent materials, the ablation threshold can be relatively large and easily above the ablation threshold of the substrate. In sample configurations where the overlaying thin film transmits the beam while the substrate is ablated, generally the interface tends to fail, leading to thin film tearing or lateral crater growth from point defects. Here, we investigate this behavior on a simple model of SiN on Si. The results show the described non-uniformity near the ablation threshold, however, due to the non-linear nature of the ablation process, we can largely mitigate it by a significant increase in the pulse energy.

9:00am **AS-WeM-5 AFM Analysis of Surface Morphology and Grain Growth in Ag Thin Films Prepared by RF Magnetron Sputtering**, ***Kenneth Lathrum,*** *Samuel Goutierrez, Jhonatan Gil Romero, Seonhee Jang,* University of Louisiana

Silver (Ag) thin films have unique electrical and optical properties that make them more desirable than other metals in applications such as solar cells, semiconductor chips, and optical coatings. The properties of these films depend significantly on surface morphology, uniformity, and thickness. Atomic Force Microscopy (AFM) is frequently used to analyze these characteristics at a sub-nanometer level. AFM measurements can be performed in either contact mode or tapping mode, distinguished by the positioning and movement of the cantilever beam. In contact mode, the cantilever tip maintains physical contact with the film's surface. In tapping mode, the tip is held a few nanometers above the film's surface and oscillates near its resonant frequency.

In this study, Ag thin films were prepared on n-type Silicon (Si) wafers (with a resistivity of 1-10 Ω cm) using radio frequency (RF) magnetron sputtering. The sputtering deposition process varied the plasma power and reactor pressure. Following deposition, the films were subjected to various thermal and laser annealing conditions. AFM measurements were conducted in tapping mode to prevent damaging the film surface. Gwyddion software was used to process the AFM measurement data, specifically utilizing equivalent disc radius analysis to characterize the grain distribution. This analysis is particularly useful for comparing grain distribution across different samples, such as those subjected to varying deposition parameters or annealing conditions. The equivalent disc radius is calculated using Gwydion's watershed method through the following steps: (1) determination of the grain area, (2) transformation of the grain area into an equivalent circle, and (3) calculation of the equivalent circle radius.

It was determined that the surface morphology, thickness, and electrical properties of the Ag thin films were significantly impacted by the deposition plasma power, reactor pressure, and annealing conditions. As deposition power increased, grain size, crystallite size, surface roughness, and film thickness increased, while sheet resistance decreased. In comparison, as deposition pressure increased, surface roughness and sheet resistance increased, while grain size, crystallite size, and film thickness decreased. Following thermal and laser annealing, grain size and crystallite size increased, while surface roughness, film thickness, and sheet resistance decreased. These results demonstrate that RF magnetron sputtering deposition parameters can be optimized and combined with post-deposition annealing to precisely tune the electrical and optical properties of Ag thin films.

9:15am **AS-WeM-6 Non-Destructive Depth Profiling with a Multi-Colored Monochromated X-Ray Source**, ***Paul Dietrich,*** *Emilie Gérouville, Andreas Thissen,* SPECS Surface Nano Analysis GmbH, Germany

X-ray photoelectron spectroscopy (XPS) is a powerful technique to gather information on elemental composition and chemical states of sample surfaces. Modern thin film architectures, multilayer devices, and buried interfaces have become increasingly relevant for various fields such as semiconductor technology and energy materials. Therefore, the need to characterize chemical states deeper than the topmost surface layers grows significantly.

Ion sputtering depth profiling is a well-established approach to access deeper layers but is inherently destructive and alters chemical states and morphology of the surfaces under investigation. Non-destructive

alternative is to extend into hard X-ray photoelectron spectroscopy (HAXPES). Higher photon energies increase the kinetic energy of emitted photoelectrons, which extends their inelastic mean free path and enables access to deeper layers without modifying the sample.

Traditionally, accessing multiple excitation energies and/or hard X-rays requires either synchrotron beamtime or the use of several separate X-ray sources. Unfortunately, these impose accessibility, cost, and experimental complexity constraints. We present an extended compact, small spot monochromated X-ray source that integrates up to four anode materials and their corresponding individually optimized crystal optics within a single Rowland circle-based housing. This all-in-one design enables fully automated, software-controlled in-situ switching between multiple excitation energies spanning from soft to the hard X-ray regime.

By combining measurements at different photon energies with parallel detection angle-resolved XPS (PARXPS), comprehensive depth-resolved chemical information can be obtained non-destructively from a single measurement session. The approach of PARXPS with variable excitation energy provides complementary information depths, allowing for reliable layer thickness determination and chemical state analysis from the surface through to deeper buried layers. We demonstrate the capabilities of this variable energy PARXPS approach with the latest results on different samples including (multi)layer stacks, highlighting how the combination of multiple excitation energies can study depth-dependent chemistry.

9:30am **AS-WeM-7 Evaluating Oxygen Gas Cluster Ion Beams for Inorganic Depth Profiling in Tof–Sims***, **Thierry Conard**,* IMEC, Belgium*; Wilfried Vandervorst, Claudia Fleischmann,* imec and KU Leuven (University of Leuven), Belgium

Large gas cluster ion beams have enabled major advances in ToF–SIMS depth profiling by strongly reducing sputter–induced damage and preserving molecular information in organic materials. However, their application to heterogeneous systems containing inorganic components remains problematic. Previous work using Ar gas cluster ion beams has shown that, despite the low energy per atom, depth profiling of inorganic layers is often limited by strong profile broadening arising from roughness development, ion–beam–induced mixing, and unexpectedly large information depths. Whether chemically reactive gas cluster ion beams can modify these limitations remains an open question.

In this work, we investigate the hypothesis that oxygen gas cluster ion beams alter the sputtering dynamics of inorganic materials sufficiently to change erosion behavior, mixing, and apparent depth resolution compared to inert Ar clusters. A model system consisting of aluminum delta layer(s) embedded in a silicon matrix is employed, providing a sensitive probe of sputter–induced mixing and interface distortion. Depth profiles acquired using oxygen cluster sputtering are systematically compared to reference data obtained with Ar clusters under comparable total cluster energies.

The study examines how the introduction of chemical reactivity through oxygen cluster bombardment influences profile shape, signal stability, and the apparent information depth of the delta layers. Particular attention is paid to separating the contributions of roughness development, ion–beam–induced mixing, and chemical modification to the observed depth profiles. The effects of key experimental parameters, including total cluster energy and sample rotation, are evaluated to assess whether trends previously observed for Ar clusters remain valid for oxygen clusters.

By benchmarking oxygen cluster sputtering against an established Ar–cluster reference system, this work aims to establish whether reactive gas cluster beams provide tangible advantages for inorganic depth profiling or introduce new sources of artefacts. The results are intended to define practical operating regimes and limitations for the application of oxygen cluster ion beams to heterogeneous and inorganic material systems in ToF–SIMS.

9:45am **AS-WeM-8 Low-k SiOC Etching: Correlating Surface Reaction Mechanisms with SiOC/poly-Si Etching Selectivity***, **Sang-Jin Chung**,* University of Maryland, College Park*; Pingshan Luan, Adam Pranda, Yusuke Yoshida,* Tokyo Electron America, Inc.*; Gottlieb S. Oehrlein,* University of Maryland, College Park

Front-end low-k dielectric materials, such as SiOC, are important in complementary field-effect transistors (CFET) for reducing RC and LC delay, minimizing power consumption, and mitigating crosstalk. During CFET fabrication, maximizing SiOC etch selectivity to the underlying poly-Si is crucial. To this end, a better understanding of SiOC etch mechanism and the transition of etch behavior from SiOC to poly-Si can inform us on the appropriate etch regime to optimize SiOC etch and poly-Si protection.

In this work, we examine SiOC etch both isotropically and anisotropically using an inductively coupled plasma (ICP) chamber. We investigate CF_4/O_2 isotropic etch on the stacked samples by varying the CF_4/ O_2 ratio and study its effect on the composition of modified layer and SiOC-to-poly-Si transition by combining *in-situ* ellipsometry and post-process vacuum-transferred XPS. *Ex-situ* AFM and SEM measurements will be provided to understand the surface roughening process as well.

Our study shows that during the CF_4/O_2 isotropic etch of ~25 nm SiOC/poly-Si stack a etch transition from SiOC etching to poly-Si etching after~13 nm of SiOC is removed and the remaining 12 nm of “SiOC” becomes highly modified . One possible interpretation of this early poly-Si transition is that carbon composition can be removed quickly compared to the overall SiOC etch rate which creates a carbon-deficient porous modified top layer. This modified layer allows for an earlier poly-Si isotropic etch once it is fully porous. During poly-Si etch, the porous layer remains on the poly-Si while a transitioning SiO_xF_y interfacial layer is being formed on the poly-Si. Consistent with expectations, XPS surface analysis shows a steady decrease in C-Si and C-C/H bonding of SiOC with progressive plasma treatment.

With a better understanding of the etch mechanism, additional experimental results with varying precursor type (HFC vs FC), plasma power, bias voltages, and material carbon concentration will be presented to demonstrate optimal etch regimes for SiOC to poly-Si selectivity. In addition to planar etch of these substrates, aspect ratio dependent etch (ARDE) of SiOC will be discussed using trench structures[1].

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11:00am **AS-WeM-13 Multimodal Surface Analysis and Depth Profiling Using Femtosecond Laser Ablation, Ion Sputtering, and Ion Scattering Spectroscopy***, **Paul Mack**,* Thermo Fisher Scientific, UK

Recent advances in surface and interface analysis are enabling new approaches for characterizing complex materials. The Thermo Scientific™ Hypulse™ XPS system combines X-ray Photoelectron Spectroscopy (XPS), Ion Scattering Spectroscopy (ISS), monatomic and gas cluster ion sputtering, and femtosecond laser ablation within a single platform, allowing characterization across length scales ranging from the outermost atomic layer to buried interfaces tens of microns below the surface.

At the very top surface, Ion Scattering Spectroscopy (ISS) will be used to examine the surface coverage of oxidized tungsten-containing layers on Ni-rich NMC battery powders, demonstrating the ability to distinguish between partial and complete surface coverage with true monolayer sensitivity. This presentation will then demonstrate the use of femtosecond laser ablation for extending XPS depth profiling into regimes inaccessible using conventional sputtering approaches. Example applications will include rapid profiling through thick graphitic battery anode structures (~25 µm), enabling characterization of compositional and chemical variations throughout porous electrode materials and buried interphases. In addition, femtosecond laser-based cleaning and shallow profiling of a thin film material will be presented, illustrating preservation of the characteristic XPS chemical structure during surface preparation compared to conventional sputtering methods.

A combined multimodal depth profiling methodology based on sequential MAGCIS ion sputtering and femtosecond laser ablation will also be described. This approach enables depth profiling of chemically sensitive oxide materials such as HfO_2, Ta_2O_5, and TiO_2 with substantially reduced chemical damage compared to conventional ion sputtering alone. The preservation of characteristic metal oxide spectral features and near-correct oxide stoichiometry during profiling will be discussed.

These examples illustrate how complementary surface analysis and depth profiling methods can be applied across very different length scales and materials systems. The combination of ISS, gas cluster sputtering, and femtosecond laser ablation enables comparison of outermost surface composition, near-surface chemistry, and deeper buried structures within the same experimental workflow. Particular emphasis will be placed on the preservation of chemically sensitive species during cleaning and profiling, and on extending XPS analysis to thicker and more structurally complex materials than are typically accessible using conventional sputtering methods.

11:15am **AS-WeM-14 Velocity-Resolved Snms as a Surface-Analytical Probe of Electronically Driven Sputtering Under Swift-Heavy-Ion Irradiation***, **Lars Breuer**, Tobias Heckhoff,* University of Duisburg-Essen, Germany*; Frieder Koch,* GSI Helmholtzzentrum fuer Schwerionenforschung, Germany*; Marika Schleberger, Andreas Wucher,* University of Duisburg-Essen, Germany

Sputtering under keV ion bombardment is commonly described by nuclear collision cascades, while sputtering under swift-heavy-ion (SHI) irradiation is driven by electronic excitation and the subsequent conversion of deposited energy into atomic motion. This different energy-conversion pathway leads to altered sputtering characteristics, such as ionization probabilities and velocity distributions of sputtered material. Accessing such velocity distributions experimentally is challenging because SHI beams at accelerator facilities are often quasi-continuous and therefore not directly compatible with conventional pulsed ToF-SIMS/SNMS schemes.

Here, we use velocity-resolved secondary neutral mass spectrometry (SNMS) to probe neutral-particle emission from surfaces under nuclear- and electronic-stopping conditions on a common experimental basis. The approach combines laser post-ionization with a laser-delay scheme, in which the delay between the ionizing laser pulse and pulsed extraction into a time-of-flight mass spectrometer is varied. In contrast to classical extraction-delay methods, the timing reference is set by the post-ionization laser rather than by a short primary-ion pulse. The method is therefore applicable to quasi-continuous SHI beams, such as those available at GSI, while retaining sensitivity to the velocity distribution of sputtered neutral species.

Velocity distributions were measured for representative target materials, including indium, bismuth, and sodium chloride. Collision-cascade sputtering was investigated using 5 keV Ar^+ bombardment, whereas electronically driven sputtering was probed with 4.8 MeV/u $^{48}Ca^{10+/19+}$ and $^{197}Au^{26+/54+}$ projectiles quasi simultaneously. For all investigated targets, SHI-induced emission shows a pronounced shift toward lower velocities compared with the keV reference case. This finding demonstrates that electronically driven sputtering cannot be treated as a straightforward extension of nuclear collision cascades. At the same time, the distributions are not reproduced by a simple Maxwell-Boltzmann description, indicating that the emission is not governed by a purely thermal evaporation-like process.

These results establish laser-delay-based, velocity-resolved SNMS as a surface-analytical probe of energy conversion and particle emission under electronic-stopping conditions, providing mechanistic insight into SHI-induced sputtering.

11:30am **AS-WeM-15 Experimental Validation of Monte Carlo Transport Simulations for MoS_2 Sputter Deposition***, **Alexander Mings**, Kyle Dorman, Steven Larson, Tomas Babuska, John Curry, David Adams,* Sandia National Laboratories

Sputter-deposited MoS_2 coatings are widely used in aerospace applications because they provide reliable solid lubrication and ultralow friction in vacuum. However, their layered structure often promotes porous film growth, reducing wear life and increasing susceptibility to oxidation. Process optimization to improve film density is typically empirical, costly, and difficult to transfer between deposition systems. Monte Carlo transport simulations have demonstrated success in streamlining this process, but their reliability depends heavily on experimental validation.

In this work, SRIM and SIMTRA are used to model the transport of sputtered atoms and backscattered neutrals during MoS_2 deposition. Key simulation outputs are validated experimentally at the substrate using a pinhole camera to measure the angular distribution of sputtered species, and wavelength-dispersive spectroscopy (WDS) to map spatial variations in sulfur flux. To indirectly assess post-ionized backscattered neutrals, a retarding field energy analyzer (RFEA) is used to measure the ion flux and energy distributions. Film hardness is further used as a proxy for porosity to connect deposition conditions with coating densification. This work assesses the extent to which Monte Carlo simulations can predict the flux conditions that produce dense MoS_2 coatings and provides a framework for more efficient process development and transfer.

Sandia National Laboratories is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

11:45am **AS-WeM-16 TOF-SIMS Depth Profiling of Inorganic–Organic Multilayers Using a Hybrid Sputtering Approach***, **Shin-ichi IIDA**,* ULVAC-PHI, Japan*; Jacob Schmidt,* Physical Electronics*; Gabriele Di Stadio,* ULVAC-PHI, Italy

Time-of-flight secondary ion mass spectrometry (TOF-SIMS) combined with argon gas cluster ion beam (Ar-GCIB) sputtering is widely used for low-damage depth profiling of organic materials. However, the extremely low sputtering yield of Ar-GCIB for inorganic materials remains a major limitation for the analysis of inorganic–organic multilayer systems. To address this challenge, a hybrid sputtering approach combining low-energy Cs^+ ions and Ar-GCIB was applied to TOF-SIMS depth profiling of inorganic–organic multilayer structures. Periodic multilayer samples consisting of Al interlayers embedded within micrometer-thick Irganox 1010 films were prepared as a model system. Depth profiling was performed using combined Cs^+ and Ar-GCIB sputtering. The hybrid sputtering conditions enabled efficient removal of buried Al layers while preserving characteristic molecular ion signals from Irganox 1010 over extended sputter depths. The results demonstrate that hybrid Cs^+/Ar-GCIB sputtering enables reliable TOF-SIMS depth profiling of inorganic–organic multilayer systems while maintaining molecular information throughout the analysis.

12:00pm **AS-WeM-17 Resolving Chemical Speciation in Complex Nickel-Based Electrocatalysts through Detailed XPS Analysis and Corroborations with ToF-SIMS***, **Emilia McCann**,* Colorado School of Mines*; Doha M. Sayed,* Los Alamos National Laboratory*; Virginia Larson, Meital Shviro,* National Laboratory of the Rockies*; Luigi Osmieri, Piotr Zelenay,* Los Alamos National Laboratory*; Svitlana Pylypenko,* Colorado School of Mines

X-ray photoelectron spectroscopy (XPS) is essential for characterizing nickel-based electrocatalysts, however the Ni 2p region is notoriously challenging due to overlapping peaks, complex satellites and spectral similarities between different oxidation states and chemical environments. This complexity intensifies in complex catalysts where nickel coexists with another metal such as iron or molybdenum and/or is present in the form of phosphides or carbides, in addition to oxides and hydroxides. These various chemistries are widely explored for catalyzing reactions in liquid alkaline water electrolyzers (AWE) and anion-exchange membrane water electrolyzers (AEMWEs), yet poorly characterized and reported in the literature. In this work, a series of Ni-containing electrocatalysts, including pristine and tested iron-doped NiOx , NiMo, NiPx, and NiMoPx supported on Ni substrate (either Ni foam or Ni fiber), were examined using XPS to track differences in nickel surface composition. The approach to deconvoluting Ni 2p XPS spectra is built on established fitting parameters for nickel oxides, hydroxides and mixed iron-nickel compounds [1]. Additional fitting parameters were systematically developed to include mixed Ni, Mo, P, O species, including NiOOH-MoO4, NiMoO4, NixPy and NiPO4, using reference samples, while complementary analysis of the Fe 2p, Mo 3d and P 2p spectral regions was conducted to more effectively capture trends in nickel speciation. Each species is characterized by specific binding energies, full width at half-maximum (FWHM) values, satellite positions and asymmetric line shapes necessary to accurately deconvolute XPS spectra. Additionally, this work used ToF-SIMS to analyze selected samples with the goal of identifying certain relevant molecular fragments. The strong correlation between XPS-derived compositions and ToF-SIMS molecular fragments representing certain species, including NiOOH-, MoO4-, PO4-, NiP+ and NiPO4- species, validated the detailed XPS fitting approach presented here. These results provide a set of fitting parameters for complex nickel systems, demonstrating that rigorous multi-technique characterization can resolve ambiguities in transition metal XPS analysis assisting further electrocatalyst optimization for various electrochemical systems. AcknowledgementFinancial support for this work was provided by the U.S. DOE, Critical Materials and Energy Innovation (CMEI)/Alternative Fuels and Feedstocks Office via Electrocatalysis Consortium (ElectroCat)

Electronic Materials and Photonics
Room 318 - Session EM-WeM

Advances in Wide Bandgap, Piezoelectric Materials and Devices

Moderators: Dr. Erin Cleveland, Laboratory of Physical Sciences, **Dr. Seth King**, University of Wisconsin - La Crosse, **Dr. Daniel Pennachio**, Naval Research Laboratory

8:00am **EM-WeM-1 Rigorous Electrostatic Constraints for Interface State Extraction in Wide-Bandgap MOS Devices**, ***Brian Rummel,*** Sandia National Laboratories **INVITED**

Accurate characterization of interface state densities near the band edges is a fundamental requirement for optimizing metal-oxide-semiconductor (MOS) systems. Such deleterious defects are particularly restrictive in wide-bandgap semiconductors (e.g., SiC and GaN), compromising the efficiency and reliability of power transistor devices. A longstanding problem in device characterization is that conventional capacitance-voltage (C-V) methods fail to accurately report interface states in the energy range most relevant for on-state transistor operation. Traditional frameworks are fundamentally limited by inherent electrostatic ambiguities, preventing reliable defect extraction near the band edge. To resolve this challenge, a novel analytical constraint is derived from foundational energy conservation principles to complete the High-Low C-V framework [1]. By enforcing a strict electrostatic boundary, this method eliminates historical measurement uncertainties and enables precise, physically consistent extraction of accumulation interface states. The theoretical validity of this advanced framework is confirmed using analytical modeling, while its practical application is demonstrated through an exemplar case study evaluating the effects of nitric oxide (NO) annealing on silicon carbide MOS structures. Ultimately, this work provides a robust path for evaluating near-band edge defects in next-generation electronic materials.

[1] B. D. Rummel, S. Dhar, R. J. Kaplar; The completed High-Low method for interface state analysis in MOS capacitors. J. Appl. Phys. 14 May 2026; 139 (18): 185708. https://doi.org/10.1063/5.0305772

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8:30am **EM-WeM-3 Doping Dependent Defect Formation in Heavy Ion Irradiated β-Ga2O3**, ***Mark Gordon,*** University of Dayton*; Daram Ramdin,* Air Force Research Laboratory, Materials and Manufacturing Directorate, USA*; Eric O'Quinn,* University of Tennessee Knoxville*; Jian Li, Brenton Noesges, Prescott Evans,* Air Force Research Laboratory, Materials and Manufacturing Directorate, USA*; Maik Lang,* University of Tennessee Knoxville*; Shin Mou, Adam Charnas, Adam Neal,* Air Force Research Laboratory, Materials and Manufacturing Directorate, USA*; Christopher Muratore,* University of Dayton*; Thaddeus Asel,* Air Force Research Laboratory, Materials and Manufacturing Directorate, USA

Gallium Oxide (β-Ga_2O_3) is an ultrawide bandgap semiconductor material with potential in RF, power electronics, & extreme environment applications. Because of its ultrawide bandgap (4.8 eV), β-Ga_2O_3 has a predicted breakdown field of 8 MV/cm, & a demonstrated breakdown field of 5.4 MV/cm in relevant device structures[1] ,[2]. The ultrawide bandgap & large breakdown field of β-Ga_2O_3 make it an excellent candidate for use in high radiation environments such as low earth orbit because β-Ga_2O_3 devices can be operated at higher voltages than conventionally radiation hardened SiC or GaN devices. At this early stage of development for β-Ga_2O_3 radiation hard devices, it is important to understand the ionizing dose effects of heavy ions at the material level in order to differentiate β-Ga_2O_3 material changes from those associated with device structure, such as contacts and interfaces. In this talk, we will discuss the results of recent heavy ion irradiation experiments on molecular beam epitaxy-grown β-Ga_2O_3 thin films irradiated with 946 MeV gold ions. We have observed experimentally a correlation between higher doping concentrations & an increase in carrier concentration after heavy ion irradiation. Two β-Ga_2O_3 film series with doping concentrations of 1×10^{17} & 5×10^{17} cm^{-3} (N1 & N5, respectively) & a thickness of 300 nm were irradiated with 946 MeV Au ions with fluences of $1x10^6$ to $1x10^8$ cm^{-2}. Before & after irradiation the carrier concentration of the samples was measured using Hg probe capacitance voltage. At a fluence of $1x10^6$ cm^{-2} samples in the N1 series showed no difference in carrier concentration after irradiation. Samples in the N5 series showed a ~31% increase in carrier concentration from 6.5 to $8.5x10^{17}$ cm^{-3}. Given the high energy of irradiation, a defect complex is likely formed instead of simple V_{Ga} or V_O & could explain the increase in carrier concentration after irradiation. These defects are consistent with previous proton irradiation studies of β-Ga_2O_3, where low temperature annealing is hypothesized to induce carrier recovery by complex formation[3]. Depth-resolved cathodoluminescence spectroscopy, deep level optical spectroscopy & deep level transient spectroscopy experiments will further identify the defects and defect complexes which are induced after heavy ion irradiation. These results identify important electronic information that is critical for designing β-Ga_2O_3 based electronics for space applications.

[1] C.N. Shah, et al., *Appl. Phys. Lett.* **122**, 182106 (2023).

[2] A.J. Green, et al., *APL Mater.* **10**, 029201 (2022).

[3] M. E. Ingebrigtsen, et al., *APL Mater.* **7**, 022510 (2019).

8:45am **EM-WeM-4 Influence of Substrate Orientation and Surface Treatments on n-Ga2O3/p-GaN Heterointerface Quality**, ***Daniel Pennachio,*** *Frank Kelly, Katie Gann, Emma Rocco, Michael Mastro,* U.S. Naval Research Laboratory

Gallium oxide is a promising ultrawide bandgap semiconductor due to its phenomenal electrical properties such as its high breakdown field and n-type conductivity. Importantly, compatibility with liquid-phase growth techniques allow large-area β-Ga_2O_3 substates to be produced relatively inexpensively and early in the material's development. Despite these benefits, the lack of shallow p-type dopant and the material's low thermal conductivity hinder device performance. Both disadvantages may be resolved by forming heterostructures with compatible p-type semiconductors. This work explores epitaxy of n-type β-Ga_2O_3:Si via metalorganic chemical vapor deposition (MOCVD) on p-type GaN:Mg, with a focus on atomic configuration and associated defects of the heterointerface as a function of Ga_2O_3 growth initiation and substrate polarity.

This work investigates the effect of GaN surface modifications before Ga_2O_3 growth. Surface treatments include *ex situ* O_2 plasma oxidation or an *in situ* MOCVD Ga "flash" clean of the GaN surface [1]. The effects of the polarity of the GaN substrate and the inclusion of a low-temperature Ga_2O_3 nucleation layer are also studied in addition to the surface treatments. The interfacial structure and composition were measured using scanning transmission electron microscopy (STEM) and X-ray energy dispersive spectroscopy (EDS). All grown films exhibited rotational domains with the epitaxial alignment of Ga_2O_3(-201)||GaN(0001). A 6-fold rotational alignment between the substrate and film were confirmed via X-ray diffraction (XRD). Fourier filtering and 4DSTEM were utilized to map grain alignments throughout the cross-sections, showing both vertical and horizontal grain boundaries, as well as various other defects. Predominant crystallographic alignments observed were Ga2O3(-201){0-10}||GaN(0001)[11-20] and Ga2O3(-201){1-32}||GaN(0001)[11-20]. The film grown with *ex situ* oxidation but without a nucleation layer provided the largest lateral grain size as determined via atomic force microscopy (AFM) analysis of surface structure. This growth also exhibited relatively uniform lateral grain size throughout the film thickness in TEM. In contrast, films grown with a nucleation layer resulted in smaller lateral grain sizes near the interface, followed by wider grains near the film surface.For samples treated with *ex situ* oxidation, the interface showed a ~10 nm wide region containing voids, while samples grown without oxidation showed atomically abrupt interfaces.

[1] Katta, Abishek, et al. *Journal of Applied Physics* 135.7 (2024).

9:00am **EM-WeM-5 A Comparison of Cr/Au and Ti/Au Ohmic Contacts on β-Ga_2O_3**, ***Carlo Schettini,*** Carnegie Mellon University*; Kim Kisslinger,* Brookhaven National Laboratory*; Isabella Williams, Xipin Chen, Reid Captain,* Carnegie Mellon University*; Judith Yang,* Brookhaven National Laboratory*; Lisa Porter,* Carnegie Mellon University

Beta gallium oxide (β-Ga_2O_3) is the most promising ultrawide bandgap semiconductor (~4.7 eV) for power electronic applications. Determining what metals can form ohmic contacts to β-Ga_2O_3 is challenging, especially as no low-work-function metals have been predicted and shown to form thermodynamically stable interfaces.[1], [2] Ohmic contacts on β-Ga_2O_3 are typically fabricated as a Ti/Au bilayer. This metallization is not stable due to the growth of an insulating interfacial TiO_x layer when exposed to high temperatures; techniques to lower its contact resistivity and improve its thermal stability include Si^+-ion implantation.[3] Recently, Cr-based ohmic contacts have been reported in β-Ga_2O_3 devices.

In this study, we compare the electrical behavior and interfacial composition profiles of Ti/Au and Cr/Au ohmic contacts to β-Ga_2O_3 as functions of annealing temperature and time. Circular Ti/Au and Cr/Au

contacts were deposited in Sn-doped (N_D = 5 x 10^{18} cm^{-3}) (001) β-Ga_2O_3 substrates and annealed sequentially to temperatures between 300 and 700°C in a rapid thermal annealer for intervals of 1 min under N_2 flow to determine the optimal processing temperature for each material. The electrical properties were determined through current-voltage measurements. For Ti/Au and Cr/Au contacts, the lowest resistance occurred at processing temperatures of 500 – 600°C, and 450 – 500°C, respectively. Both degraded when annealed to 700°C. Transmission electron microscopy (TEM) cross-section images combined with energy dispersive x-ray (EDX) analysis of as-deposited and 450°C-annealed contacts showed differences in the interfacial chemistry after annealing: e.g. Au nanoclusters that were detected at the interface in the annealed Cr/Au contacts but not in the Ti/Au contacts. In this presentation we will compare the electrical measurements and TEM/EDX characterizations of the Ti/Au and Cr/Au contacts at different annealing temperatures. We will also discuss recent results of a long-term annealing study (at 300°C for > 250 h) of ohmic contacts with and without a Ni diffusion barrier.

[1] Y. Yao, R. F. Davis, and L. M. Porter, *Investigation of Different Metals as Ohmic Contacts to β-Ga_2O_3: Comparison and Analysis of Electrical Behavior, Morphology, and Other Physical Properties*, J. Electron. Mater. **46**, 2053 (2017).

[2] C.-W. Lee, A. Zakutayev, and V. Stevanović, *Computational Insights into Phase Equilibria between Wide-Gap Semiconductors and Contact Materials*, ACS Appl. Electron. Mater. **6**, 2383 (2024).

[3] M.-H. Lee and R. L. Peterson, *Accelerated Aging Stability of β-Ga_2O_3–Titanium/Gold Ohmic Interfaces,* ACS Appl. Mater. Interfaces **12**, 46277 (2020).

9:15am **EM-WeM-6 Temperature-Driven Reversible Carrier-Polarity Switching in Bi-Doped SnSe**, ***Mehmet Ozdogan***, *Thomas Iken, Carlos Munoz, Deniz Cakir, Nuri Oncel,* University of North Dakota

Carrier-polarity switching in semiconductors offers a route toward adaptive electronic and thermoelectric functionality beyond conventional static p- or n-type doping. In this work, we investigate temperature-driven reversible n-to-p carrier-type switching in bulk polycrystalline Bi-doped SnSe by combining temperature-dependent transport measurements, structural/chemical characterization, semiempirical transport modeling, and first-principles calculations.

Pristine and Bi-doped SnSe samples, $Sn_{1-x}Bi_xSe$ with x = 0, 0.02, and 0.06, were synthesized and characterized using X-ray diffraction, scanning/transmission electron microscopy, energy-dispersive X-ray spectroscopy, and X-ray photoelectron spectroscopy. Structural analysis confirms that the orthorhombic Pnma SnSe framework is preserved after Bi incorporation, while chemical analysis verifies Bi incorporation and finds no evidence of metallic Bi secondary phases. Temperature-dependent measurements of Seebeck coefficient and electrical conductivity reveal distinct composition-dependent transport behavior. Pristine SnSe remains p-type over the full measured temperature range, whereas Bi substitution drives electron-dominated conduction. The 2% Bi-doped sample exhibits negative Seebeck coefficients at low temperature, followed by a reversible n-to-p polarity reversal near 550 K, while the 6% Bi-doped sample remains robustly n-type up to 880 K.

To clarify the microscopic origin of this switching, the experimental transport data were analyzed using a self-consistent two-carrier model that accounts for competing electron and hole contributions and incorporates the smooth Pnma-to-Cmcm structural evolution. The nonlinear Seebeck response in lightly Bi-doped SnSe is captured by bipolar transport and carrier compensation rather than by a simple single-carrier picture. Density-functional-theory calculations further show that, at low Bi concentration, temperature-driven bandgap narrowing and Fermi-level repositioning promote thermally activated holes that eventually dominate transport. In contrast, higher Bi content pushes the Fermi level deeper into the conduction band, suppressing compensation and stabilizing degenerate n-type behavior.

These results establish Bi-doped SnSe as a model system for tunable carrier compensation and reversible polarity switching, providing design principles for temperature-responsive thermoelectric and multifunctional semiconductor materials [1].

[1]. *Physical Review B* 113, 205202 (**2026**).

9:30am **EM-WeM-7 Hybrid MBE for Freestanding Ultra-wide Bandgap $CaSnO_3$ Thin Films Using a Water-soluble BaO Sacrificial Layer**, ***Sooho Choo***, *Dong Kyu Lee, Rishi Raj, Alyssa Bragg, Seung Gyo Jeong, Ho-Sung Shin, Shivasheesh Varshney, Jitin Sathish Kumar, K. Andre Mkhoyan, Alexander S McLeod,* University of Minnesota*; Anderson Janotti,* University of Delaware*; Bharat Jalan,* University of Minnesota

In power electronic devices, key figures of merit scale nonlinearly with bandgap, driving significant interest in semiconductors beyond wide-bandgap (WBG) semiconductors, such as GaN (3.4 eV) and SiC (3.2 eV). Ultra-wide bandgap (UWBG) semiconductors, with bandgaps exceeding 3.4 eV, offer superior breakdown electric field resistance and represent a promising pathway for next-generation power electronic devices. Among the UWBG candidates, $CaSnO_3$ is particularly attractive due to its bandgap of 4.3 eV, combined with the compositional and structural versatility of the perovskite framework, enabling bandgap engineering through alloying and performance tunability via heterostructure. In parallel, the realization of monolithically integrated electronic and optoelectronic systems demands flexible heterogeneous integration strategies. Conventionally, integrating 3D crystalline semiconductors has relied on heteroepitaxy, which imposes strict growth requirements on lattice matching and chemical compatibility between the film and substrate, limiting material combinations. Recent advances in freestanding thin films, enabled by remote epitaxy or chemical lift-off, overcome these constraints by decoupling the epitaxial film from the substrate, allowing the epitaxial film to be transferred and integrated onto arbitrary material platforms. Here, we demonstrate epitaxial growth of $CaSnO_3$ thin films with a BaO sacrificial layer on LSAT (001) substrate using hybrid MBE and their successful release and transfer onto other material platforms. Morphological and structural properties were systematically investigated as a function of growth stoichiometry using reflection high-energy electron diffraction (RHEED), atomic force microscopy (AFM), and high-resolution X-ray diffraction (HRXRD). These measurements confirm phase-pure epitaxial growth of $CaSnO_3$ and BaO layers. Furthermore, the dielectric and optical properties of freestanding $CaSnO_3$ thin films were investigated, revealing properties comparable to bulk values, as characterized by impedance spectroscopy, scanning near-field optical microscopy (SNOM), and ellipsometry. This work demonstrates that freestanding $CaSnO_3$ films retain bulk-like properties after transfer, opening a pathway for heterogeneous integration in next-generation power electronic and optoelectronic devices.

11:00am **EM-WeM-13 Suppression of Stacking Fault Expansion in SiC Epitaxial Layers via Substrate Implantation**, ***Rachael Myers-Ward***, *Alec Imhof, Nadeemullah Mahadik,* U.S. Naval Research Laboratory*; Benjamin Sekely, Jenifer Hajzus,* US Naval Research Laboratory*; Atul Gupta, Hank Chen, Fulvio Mazzamuto, Christopher Lamontagne,* Axcelis Technologies

Silicon carbide (SiC) devices can fail during operation due to bipolar degradation [1], where carrier injection causes basal plane dislocations (BPDs) to expand into single Shockley stacking faults (SSFs), leading to increased on-state resistance and reverse current leakage [2,3]. Previous studies have demonstrated that proton and helium implantation within the epitaxial layer can effectively suppress stacking fault expansion [4]. However, at very high carrier injection conditions, such as pulsed-power applications, BPDs propagate from the substrate or highly doped layers into the epitaxial drift layer [5]. This study explores an alternative approach for mitigating BPD propagation and SSF expansion by performing implantation into substrates prior to epitaxial growth of the drift layer. This approach offers a pathway toward improved high-power device reliability.

In this work, 200 mm diameter 4H-SiC substrates were subjected to implants with different species (silicon, carbon, and phosphorus) at varying energy (50-200 keV) and doses ($5x10^{14}$ – $2.5x10^{15}$ cm^{-2}). Each wafer had 5 implant regions with one region receiving no implant to allow for a direct comparison of the implantation impact on the BPD faulting and SSF expansion. A 10 µm intentionally doped n-type, ~$2x10^{16}$ cm^{-2}, SiC epitaxial layer was deposited on each of the implanted substrates. During the ramp to growth temperature, the H_2 carrier gas was reduced and the pressure was increased to suppress the etching of the implanted SiC substrate.

Ultraviolet photoluminescence (UVPL) was used to image the wafers before and after prolonged (3hr) UV carrier injection stressing at 9 $kWcm^{-2}$. We observed in several wafers, at such high injection conditions, BPDs from untreated SiC substrates propagate into the epi-layer. However, for the majority of the implant conditions, over a magnitude reduction in SSF densities were seen. The SSF blocking mechanism is likely due to reduction in carrier lifetime caused by implantation as well as potential pinning from the point defects introduced during implant that block SSFs from expanding

into the epitaxial layer. The various defect mechanisms along with complete statistical analysis will be presented.

[1] P. Bergman et al., Mat. Sci. Forum, **353–356** (2001) 299.

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[3]Agarwal et. al., IEEE Electron Device Lett., **28** (2007) 587.

[4]M. Kato et al., Sci Rep, **12** (1) (2022) 18790.

[5]N. A. Mahadik et al., Appl. Phys. Lett., **100** (4) (2012) 042102.

11:15am **EM-WeM-14 Processing of SiC Pillar Arrays for Quantum and Photonic Applications**, ***Jenifer Hajzus***, *Jose Fonseca, Ignas Lekavicius,* US Naval Research Laboratory*; Samuel Lagasse,* Laboratory for Physical Sciences*; Karl Hobart, Marko Tadjer, Rachael Myers-Ward,* US Naval Research Laboratory

Defects in SiC with optically addressable spin-states (e. g. silicon vacancies, divacancies, nitrogen vacancy centers) have attracted great interest for quantum computing and sensing due to their long spin coherence times, room temperature operation, near infrared emission, and existence in an industrially mature host crystal with wafer scalability, established processing techniques, and exploitable properties such as second order optical nonlinearity and controllable p-and n-type doping. To enhance defect emission and/or improve optical collection efficiency, photonic structures such as nanopillar arrays, solid immersion lenses, and photonic crystal cavities have been utilized [1-3]. Fabrication of these structures in SiC typically involve dry etching in fluorine-based chemistries which can introduce unwanted defects, unfavorable surface states, and roughness on sidewalls and surfaces. Such imperfections have potential to be a source of optical losses, decreased Q-factors, decreased spin coherence times, and high photoluminescence backgrounds [4-6].

This work investigates processing conditions for fabrication of SiC nanopillar arrays, aiming to produce structures with favorable surfaces and morphologies for quantum photonic applications. E-beam lithography is used to define pillars with diameters ranging from 400 nm to 1150 nm in 4° offcut N^+ 4H-SiC substrates. SiC is etched using ICP-RIE in a SF_6/O_2 gas mixture. It is found that the pillar sidewall roughness and morphology are impacted by O_2:SF_6 flow ratio, where a higher O_2:SF_6 ratio produces more vertical sidewalls but increased sidewall roughness. Sidewall roughness can be reduced by modifying the hard mask. A Cr/HSQ hard mask fabricated by an etching process is found to result in smoother sidewalls than a Cr/Ni hard mask fabricated by a lift-off process. Post fabrication annealing is additionally explored as a means to reduce sidewall roughness and reclaim the SiC surface after ICP-RIE. SiC pillar arrays are annealed in hydrogen for a short duration in a SiC CVD reactor. Sacrificial oxidation by annealing in oxygen followed by oxide removal is also performed. The pillars are characterized using SEM, AFM, XPS, and Raman spectroscopy to examine the impact of annealing on surface chemistry, roughness, and pillar array morphology.

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[2] M. Radulaski, et al., Nano Lett., 17, 3, 1782–1786 (2017)

[3] R. L. Myers-Ward, et al., Mater. Sci. Forum, 924, 905–908 (2018)

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[5] M. Scharin-Mehlmann, et al., Adv. Mater. Interfaces, e70525 (2026)

[6] C. Chia, et al., Opt. Express 30, 9, 14189-14201 (2022)

11:30am **EM-WeM-15 Structural and Electrical Characterization of He Ion Implanted 4H-SiC**, ***Ben Sekely***, *Cory Cress, Jeffery Woodward, Daniel Pennachio, Ignas Lekavicius, Jenifer Hajzus, Rachael Myers-Ward,* U.S. Naval Research Lab

He ion implantation has been used in 4H-SiC devices to generate defects and damage the crystal, thus changing the characteristics of the material at the implanted region. This localized implantation has been utilized for the formation of edge termination structures in Schottky barrier diodes [1] and radiation detectors [2] where the impact of implantation of the neutral species on device functionality is observed for a specific He dose. Most characterization studies conducted previously have investigated the behaviors of He-ion-implanted SiC at a dose >1e14 cm^{-2}.

In this study, we widen the scope by studying the structural and electrical properties of 4H-SiC implanted at room temperature with a range of He ion doses from 1e12 – 1e16 cm^{-2}. He implantation is performed at 9.5 keV in unintentionally doped (UID) 4H-SiC homoepitaxially grown by chemical vapor deposition.

High resolution X-Ray photoelectron spectroscopy spectra of the 1s carbon (C1s) peak for three different implant doses are compared to a non-implanted region. The lower-energy C-Si peak diminishes with increasing dose. As those bonds break, more carbon is available to form C-C bonding, increasing the higher-energy peak signal.

Implanted regions are mapped by Raman spectroscopy and compared to non-implanted regions. The 980 cm^{-1} peak intensity attributed to the A1 (LO) mode of SiC shows a dramatic decrease in the implanted region for He doses of 1e15 cm^{-2} and higher. Similarly, the full-width half-maximum (FWHM) of the peak broadens compared to the non-implanted region. The changes in this peak are below the detection limit at lower doses.

High resolution X-ray diffraction was performed at the 4H-SiC (0004) reflection to probe the modification of the crystalline structure due to the He ion implantation dose. The 2θ/ω scans showed broadening in the intensity tail on the low-angle side of the peak at a dose of 10^{15} cm^{-2}, which indicates expansion of the out-of-plane lattice constant.

Electrical characterization of these regions including capacitance-voltage and current-voltage will be presented and correlated with further structural characterization including atomic force microscopy. Additionally, material resistivity will be obtained using circular transmission line measurement structures. Understanding these material properties could make this approach useful for edge termination in high-power devices.

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11:45am **EM-WeM-16 Impact of ZnO Deposition Method on Post-Illumination Charge Trapping and Recovery in Organic Photodiodes**, ***Anna Leonard***, *Neha Chaturvedi, Veena Misra,* North Carolina State University

For organic photodiodes (OPDs) to achieve high sensitivity and operational stability, they must use charge-selective, morphologically stable charge transport layers. ZnO is commonly used as an electron transport layer due to its favorable energetics and solution processability, however, sol-gel ZnO typically contains more defects and structural disorder than films deposited with vacuum techniques. These defects contribute to trap-assisted recombination and persistent photocurrent effects that increase recovery time, making them detrimental to OPD performance. In this work, atomic layer deposited (ALD) and sol-gel ZnO were investigated as electron transport layers to understand the operational stability of PTB7-Th:IEICO-4F OPDs through post-illumination dark current recovery measurements and related structural and electrical characterization. While ALD ZnO has been previously explored in organic optoelectronic devices, its influence on persistent photocurrent effects in OPDs has not been extensively studied.

OPDs were exposed to a controlled light source and dark current density vs. voltage (J_{Dark}-V), capacitance-voltage (C-V), and external quantum efficiency (EQE) were measured before and after light exposure. ALD ZnO devices exhibited improved dark current recovery after light exposure, indicating reduced persistent photoconductivity effects and mitigated trap-assisted charge storage. Differences in post-illumination electrical behavior were further supported by C-V analysis. Grazing incidence X-ray diffraction (GIXRD), atomic force microscopy (AFM), and scanning electron microscopy (SEM) measurements revealed differences in interfacial ordering and morphology between sol-gel and ALD ZnO films.

These results demonstrate that ALD ZnO can mitigate photoinduced trapping in OPDs through improved interfacial quality and reduced metastable charge storage. This work highlights the importance of electron transport layer quality in controlling post-illumination electrical recovery and degradation pathways in organic optoelectronic devices.

12:00pm **EM-WeM-17 Accelerated Data-Efficient Metasurface Simulation Using Deep Learning and Neural-Adjoint Inverse Design**, ***Jack Gude***, *Muhammad Ashar Naveed, Yanan (Laura) Wang,* University of Nebraska - Lincoln

Metasurfaces are ultra-thin nanostructures capable of precise light manipulation for next-generation integrated photonics and quantum technologies. While numerical simulations, such as Finite-Difference Time-Domain (FDTD) provide high-fidelity modeling, the computational cost is significant; optimizing a single 7-parameter geometry can require weeks of simulation time. This bottleneck prevents the rapid iteration required for large-scale design and optimization of metasurface devices. In this work, we

present a neural surrogate model designed to act as a high-speed physics interpolator. Our foundational model successfully reduces simulation time from weeks to milliseconds while maintaining >0.99 R^2 accuracy for Circular Dichroism (CD) spectra predictions.

Building upon this validated surrogate, we introduce an ongoing exploration into novel data encoding strategies to further mitigate the FDTD data generation bottleneck. Standard predictive networks often require massive datasets to predict entire spectra. We present an alternative wavelength-as-input encoding approach. By restructuring the network to accept wavelength as an explicit, continuous input parameter alongside unit cell geometry metrics, we can effectively multiply our dataset size by 121x. We aim to show how this allows for high-fidelity predictions using significantly reduced FDTD sampling.

We will present the comparative performance of this point-prediction encoding strategy against standard spectrum-prediction methods. Preliminary findings regarding the model's ability to maintain high predictive accuracy on constrained datasets will be discussed. Ultimately, refining these neural network strategies and improving data efficiency is a critical stepping stone toward deploying autonomous active learning paradigms, paving the way for real-time inverse design and integrated quantum photonics engineering.

Materials and Innovations for Fusion Energy
Room 321 - Session FUS-WeM

Fusion Materials, Plasma-Facing Components, and Tritium Engineering

Moderators: Dr. Dale Hitchcock, Savannah River National Lab, **Dr. Matthew Sharpe**, The Laboratory for Laser Energetics, The University of Rochester

8:00am **FUS-WeM-1 Water Detritiation: From ML-Guided Selection to Catalyst Synthesis***, **Rashad Ahmadov**, Zachary Robinson, Mark Wittman, Matthew Sharpe,* Laboratory for Laser Energetics

Building on prior validation of a hydrogen-based surrogate unit for water detritiation, this workadvances catalyst development through integrated computational screening and targeted synthesis. The previous study established baseline performance using commercial Cu-Zn catalysts, revealing reaction rates limited by the internal mass diffusion. To identify candidates with potentially improved characteristics, Machine Learning (ML)-accelerated adsorption energy calculations (AdsorbML) were employed to screen a broader alloy design space. A promising composition was selected based on predicted surface energetics favorable for water splitting reaction adsorbates. The candidate catalyst was synthesized and characterized using XRD and XPS to confirm phase composition and surface chemistry. Temperature-programmed reduction (TPR) was performed to determine appropriate activation conditions prior to reactivity testing. The catalyst was then tested in the surrogate reactor under conditions comparable to prior experiments. Preliminary results confirm catalytic activity for hydrogen evolution with oxygen retention. This work demonstrates a computationally-guided pathway for catalyst discovery for thermochemical water detritiation, contributing toward optimized tritium recovery systems for closing the fusion fuel cycle.

This material is based upon work supported by the Department of Energy [National Nuclear Security Administration] University of Rochester “National
Inertial Confinement Fusion Program” under Award Number(s) DE-NA0004144.

8:15am **FUS-WeM-2 Al Intercalation Into C-Vacancy Sites in TiCx for Low-Temperature Synthesis of MAX-Phase Ti_2AlC Hydrogen Permeation Barrier Coatings***, **Isabella Stepanek**,* Georgia Institute of Technology*; Dale Hitchcock,* Savannah River National Lab*; Eric Vogel,* Georgia Institute of Technology

MAX-phase Ti_2AlC thin films were synthesized using PVD magnetron sputtering of a bilayer system that utilizes an Al precursor layer with a subsequent TiAlC layer, followed by vacuum annealing at 650°C for 3h up to 20h. Ex situ XRD of TiAlC only films (no Al precursor layer) reveal that annealing drives Al out of the $Ti_{0.66}Al_{0.34}C$ rocksalt phase present in the as-deposited films, generating additional C-vacancy sites to form $TiC_{0.5}$. No Ti_2AlC was synthesized from these TiAlC only films. With the utilization of an Al precursor layer deposited prior to the TiAlC layer, it was found that the as-deposited bilayer contains spatially distinct $TiC_{0.56}$ and Al phases, establishing the diffusion geometry required for Al intercalation-driven Ti_2AlC formation. This mechanism is initiated via vacuum annealing at 650°C which mobilizes Al both from the $Ti_{0.66}Al_{0.34}C$ phase in the TiAlC layer but also Al from the precursor layer. The resulting upward Al diffusion and intercalation into ordered C-vacancy planes of $TiC_{0.55}$ is identified as the primary mechanism driving low-temperature Ti_2AlC formation in Al/TiAlC films. XRD results also show the formation of Ti_3Al along with the $TiC_{0.55}$ and Ti_2AlC phases, mirroring reported two-step reaction pathways that include the formation of Ti-Al intermetallics and TiC_x that react to form Ti_2AlC. Ex situ XPS depth profiles corroborate this mechanism, showing progressive Al depletion from the precursor layer into the TiAlC layer with annealing time. Associated scans of the Al 2p orbital taken during depth profiles shows binding energy shifts evidencing changes in the Al chemical environment consistent with C-vacancy incorporation and Ti_2AlC synthesis.

These efforts towards low-temperature synthesis of MAX-phase coatings allow for their potential use on low activation structural materials used in fusion reactor blanket components. Ti_2AlC is a particularly promising candidate for this application, as aluminum-containing MAX-phases form a dense, protective Al_2O_3 scale upon oxidation that has been demonstrated to reduce hydrogen isotope permeation through structural materials.

8:30am **FUS-WeM-3 Characterizing Heavy Water Displacement in Molecular Sieve Drying Beds for Practical Trace Tritium Capture Methods***, **Brandon Massett**, Walter Shmayda,* Tritium Solutions Inc.

Tritium plays a crucial role in nuclear fusion power plant designs, and adsorption beds are essential tools for managing tritiated water vapor. A series of tests was performed to investigate whether a saturated adsorption bed preferentially adsorbs heavy water vapor. The design of passive tritium control systems could potentially rely on adsorption beds preferentially trapping heavier isotopologues of water. This work investigates the displacement phenomenon, as well as the effects of carrier gas superficial velocity and heavy water concentration on bed performance. Significant displacement was observed when a humid stream containing heavy water was diverted through a bed pre-saturated with light water, as indicated by changes in the partial pressures of D2O and H2O. Following the capture of heavy water in the bed, the subsequent rise in D2O partial pressure depended on both the superficial gas velocity and the heavy water humidity in the gas stream. Higher superficial velocities and humidities led to faster and steeper mass transfer profiles within the adsorption bed. These heavy water breakthrough curves were fit and compared with theoretical models for adsorption beds operating under standard conditions.

8:45am **FUS-WeM-4 Characterizing the Behavior of Hydrogen Isotopes and Impurity Species on Vanadium Surfaces by Direct Recoil Spectroscopy***, **Feng-Jen Chang**, Antonio Cruz, Mary Alice Cusentino, Robert Kolasinski,* Sandia National Laboratories

Due to their high permeability for hydrogen isotopes (HI), vanadium (V) membranes are being considered for separation of HI from the plasma exhaust of future fusion reactors. Surface effects, particularly the presence of impurities, have a large influence on the performance of such membranes. However, it is often difficult for conventional surface analysis tools to directly observe how HI interacts with other surface species. Ion scattering spectroscopy (ISS) and direct recoil spectroscopy (DRS) offer the advantage of being able to directly detect adsorbed HI by analyzing the energies of scattered and recoiled particles from ion scattering on the surface.

In this study, we use a 2 keV Ne^+ ion beam to probe the surface composition of a polycrystalline V sample while dosing with hydrogen (H) or deuterium (D) with increasing pressure [Fig. S1(a)]. Gas species and surface temperatures (T_s) are varied for comparison, and a gas doser heated to 1100 °C is available for dissociating H_2/D_2 molecules into H/D atoms. DRS peaks of H/D are clearly identified in the ion energy spectra [Fig. S1(b)]. Pressure dependences of the peak intensities can be well fitted by a simple site-blocking model with Langmuir isotherm [Fig. S1(c)], which assumes that adsorbates only interact with each other by competing for empty adsorption sites. Such fittings reveal the change of the adsorption-desorption balance of HI with different surface conditions. The ratio between the adsorption rate coefficient and desorption rate coefficient, $K = k_{ad} / k_{de}$, decreases with increasing T_s, indicating that desorption is stronger at higher T_s [Fig. S1(d)]. K is also higher with atomic H/D dosing than with H_2/D_2 dosing, since atomic species have higher chemical energy to overcome the adsorption energy barrier, and thus result in higher adsorption rates.

In addition, preliminary studies of oxygen (O) adsorption by DRS while dosing the V surface with O_2 have been performed. The DRS O peak intensity growth with increasing O_2 pressure is similar to that measured by X-ray photoelectron spectroscopy (XPS) [Fig. S1 (e)], which validates the DRS results. The ongoing work includes sequentially dosing O_2 and HI to validate the site-blocking model. Finally, investigation of the effect of permeation barrier coatings, such as SiC, W or Al_2O_3, on V and V-alloys with both DRS measurements and density functional theory (DFT) modelling is also underway, and preliminary results from this work will be included in this presentation.

SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

9:00am **FUS-WeM-5 Theoretical and Experimental Study of Hydrogen Super-Permeation in Iron**, ***Masashi Shimada**, Thomas F. Fuerst,* Idaho National Laboratory **INVITED**

Metal foil pumps (MFPs) exploit plasma–driven hydrogen super–permeation to selectively separate and compress hydrogen isotopes (D/T) from helium and impurity species in the fusion exhaust stream, forming a key enabling technology for Direct Internal Recycling (DIR)–based fuel–cycle architectures. Despite their promise, the technical readiness level of MFPs remains insufficient for integration into next–generation fusion systems. Advancing the understanding of hydrogen super–permeation in metallic membranes is therefore essential for developing high–performance pumping components capable of operating under reactor–relevant plasma conditions.

This work presents an integrated experimental and theoretical investigation of deuterium super–permeation in high–purity α–Fe. Plasma–driven permeation experiments conducted in the Tritium Plasma Experiment (TPE) at Idaho National Laboratory demonstrated that a 99.99% α–Fe foil can achieve a maximum pumping throughput of 3.0 L s^{-1} cm^{-2} and a pumping speed of 3.0 m^3 s^{-1} m^{-2} at 523 K under a D_2 pressure of 0.013 Pa. The permeation behavior was found to be strongly governed by the surface sticking coefficient, α, and by the incident D^+ ion energy. Comparison with the Pick–Sonnenberg model showed excellent agreement when using a previously measured $\alpha \approx 1.6 \times 10^{-9}$, with peak pumping performance occurring near an incident ion energy of 10 eV [1]. In contrast, incident energies above 50 eV caused a sharp decline in pumping performance, consistent with sputtering–induced removal of the native oxide monolayer—an effect also reported in prior studies of Nb and Fe.

A complementary theoretical study applied the Pick–Sonnenberg formulation to evaluate hydrogen permeation in candidate group–V membrane materials, focusing on vanadium with an experimentally measured effective permeability influenced by surface oxide and subsurface carbide layers [1]. Modeling showed that even with the reduced permeability, an uncoated 1 mm–thick V membrane can achieve approximately 10% hydrogen permeation at 973 K when operating with $\alpha \approx 10^{-3}$ and ion fluxes near 10^{20} m^{-2} s^{-1}. These findings highlight the potential for high–temperature operation to enable attractive pumping performance without the Pd coatings typically required for group–V metals.

Collectively, these results deepen the mechanistic understanding of hydrogen super–permeation in metallic membranes and provide a physics–grounded basis for optimizing high–flux MFP systems within advanced fusion fuel–cycle concepts.

Reference:

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9:30am **FUS-WeM-7 Development of Tungsten Alloys to Mitigate Impacts of Neutron Irradition on Tritium Inventory**, ***Yuji Hatano**, Qicong Chen, Yuga Kimura, Naoko Oono, Katsuya Suzuki,* Tohoku University, Japan*; Tatsuya Kuwabara,* Aichi Institute of Technology, Japan*; Koji Inoue,* Tohoku University, Japan*; Jing Wang,* Hefei University of Technology, China **INVITED**

While Tungsten (W) is a leading candidate for a plasma-facing material in fusion reactors, neutron-induced displacement damage creates vacancy-type defects that significantly increase tritium retention [1,2]. To mitigate this, we developed W alloys using undersized solute elements like chromium (Cr) and rhenium (Re). These elements promote the annihilation of vacancy-type defects during irradiation at temperatures ≥773 K and reduce the resulting trap density [3-8]. Furthermore, recent findings show these alloying elements enhance defect recovery during post-irradiation annealing at approximately 1473 K, offering a potential pathway for in-vessel trap removal during scheduled maintenance. This presentation explores the mechanisms driving these enhanced annihilation and recovery processes.

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11:00am **FUS-WeM-13 Liquid Metals as Plasma-Facing Components in Fusion Devices: Can They Solve the Power Handling Challenge?**, ***Martin Nieto-Perez**, Calixto Alvarado,* Pennsylvania State University*; Daniel Andruczyk,* University of Illinois at Urbana-Champaign*; Lane Carasik,* Virginia Commonwealth University*; Ama Dahanayakle,* Pennsylvania State University*; Bruce Koel,* Princeton University*; Mike Kotschenreuther,* Exofusion*; Rajesh Maingi,* Princeton Plasma Physics Laboratory*; David Ruzic,* University of Illinois at Urbana-Champaign*; Sergei Smolentsev,* Oak Ridge National Laboratory*; Vlad Soukhanovskii,* Lawrence Livermore National Laboratory*; Xing Wang,* Pennsylvania State University*; Kevin Woller,* Massachusetts Institute of Technology

One of the most daunting challenges on the road to commercial fusion machines is the development of materials and components capable of withstanding the enormous power loads associated with particle leakage from magnetically confined plasmas; in addition to being resilient enough to withstand very high heat loads, these components need to facilitate the recovery of any valuable tritium fuel that reaches them. To satisfy these requirements, plasma-facing component systems based on liquid metals are considered a viable option, but remain at a lower technology readiness level (TRL) than their solid counterparts. To advance the maturity of these technologies, a DOE-funded initiative, Liquid Metals: Advancing the technical Readiness of plasma-facing Materials Operational Response (LM-ARMOR), has been established, spanning multiple federal laboratories and academic institutions. The overarching aim uses a combination of dedicated experiments and targeted calculations to explore and develop different PFC systems based on liquid metals. This collaboration aims to derisk LM technologies by addressing specific scientific and technological gaps that must be overcome to develop next-step integrated fusion test facilities and fusion reactors. The four overarching topics are material compatibility assessments, MHD flows, development of novel liquid metal alloys, and integrated testing. In this talk, efforts to develop the capillary pore system and to study novel metal alloys will be highlighted, emphasizing the need for experimental measurements of critical properties, including wetting, hydraulic permeability, sputtering, and surface segregation.

11:15am **FUS-WeM-14 Atomic Layer Deposition Affecting Gas Retention in Fusion Targets**, ***Mark Bonino**,* University of Rochester

Glow discharge polymer (GDP) is the primary material used as an ablator for spherical, direct-drive laser experiments at the University of Rochester's Laboratory for Laser Energetics. GDP capsules are millimeter-scale hollow spheres with gas permeation time constants of ~1 min for hydrogen isotopes—the gases used for fusion reactions. Gas permeation time constants, however, must be significantly longer (tens of hours) to meet the specified fuel pressure at the time of the laser shot. Most experiments require fuel pressures of 15 atm±10%. Sputter-deposited aluminum has been demonstrated to increase the gas permeation time constant, using layers of around 100 nm. However, sputtered aluminum films often exhibit a broad distribution of time constants, rendering many samples unusable. An alternative to sputter deposition is atomic layer deposition (ALD), where layers of Al_2O_3 are applied using a vapor-phase deposition process to produce a contiguous gas-permeation layer. ALD is an alternative method to increase hydrogen gas retention and is investigated in this study.

The presented work will report gas-permeation time constants on spherical and cylindrical plastic shells from a decay curve measured using a residual gas analyzer. In our time-constant measurement system, the targets are pumped out to high vacuum (10^{-6} Torr) and filled to pressures up to 1000 Torr. Preliminary observations show time constants ranging from 1000s to 2000s, with a dependence on pressure. Changes in the permeation rate as a function of cycling will be investigated. Characterization (using x-ray photoelectron spectroscopy, a scanning electron microscope, and an atomic force microscope) will be performed to observe microscopic changes on the sample surfaces that impact gas retention.

*This material is based upon work supported by the Department of Energy (National Nuclear Security Administration] University of Rochester "National Inertial Confinement Fusion Program" under Award Number DE-NA0004144

Presentation Type: Oral presentation

Presenter: Mark Bonino, mbon@lle.rochester.edu [mailto:mbon@lle.rochester.edu], (585)275-1404 (office)

11:30am **FUS-WeM-15 Measurement of Residual Impurities after a Cryogenic DT Inertial Confinement Fusion (ICF) Implosion***, **Errol Alden**, Zak Robinson, Matt Sharpe,* University of Rochester

In order to gauge the impurities entering the tritium fuel cycle (FC) in an ICF target chamber, we focus on residual target material left after a shot in the forms of ablation coating and gaseous species. The ablation coating, or material left on surface of chamber, was measured by placing sapphire wafers 26 cm away from the target. The gaseous species are measured via Residual Gas Analyzer (RGA) directly mounted on the ICF target chamber. The RGA provides mass information for the major gas species residual in the chamber. After being exposed to an ICF target implosion, the wafers will be separated into two testing groups: one to measure tritium activity and the other to measure surface changes. Tritium surface activity will be measured through etching, while surface changes will be measured by X-ray photoelectron spectroscopy and X-ray reflectivity. The goal is to understand the depth that tritium reaches, surface changes on the wafer, contaminants left on surface, and contaminants left in gas.

This material is based upon work supported by the Department of Energy [National Nuclear Security Administration] University of Rochester "National Inertial Confinement Fusion Program" under Award Number(s) DE-NA0004144; Data were produced by Battelle Savannah River Alliance, LLC under Contract No.89303321CEM000080 with the Department of Energy.

11:45am **FUS-WeM-16 FORGED-PFC High Heat Flux Facility Vacuum Vessel Design Status***, **Jared Tippens**, Ezekial Unterberg,* Oak Ridge National Laboratory

Oak Ridge National Laboratory has partnered with Type One Energy and The University of Tennessee Knoxville to build a world-class High Heat Flux Experimental facility focused on testing and qualifying fusion energy plasma-facing components (PFCs). This facility will utilize two converging high-power electron beams (~1.6 MW total) to heat test articles at fusion-relevant PFC power densities. Heat will be removed from the test articles via a dedicated helium loop with flowrates up to 1 kg/sec at a pressure of 8 MPa. Large components measuring over 1 m x 1 m x 0.5 m can be tested in this facility, enabling sub-component PFCs to be evaluated under representative operating conditions for thermomechanical stress testing and qualification. There are currently no dedicated testing facilities in the Western Hemisphere with these capabilities. Therefore, the FORGED-PFC facility will fill this needed capability and operate as a community resource to accelerate domestic fusion research and deployment of fusion energy systems.

For effective high heat flux testing at this scale, experiments must take place in a vacuum environment at pressures on the order of $1x10^{-4}$ mbar and lower. The two electron beams will be mounted to a relatively large vacuum vessel (~ 10 m^3) that will also house the test articles during experiments. Robust thermal management of the vacuum vessel is required to dissipate up to 1.6 MW of heat from the inner walls, necessitating a jacketed design. In addition, numerous ports are required for diagnostics to enable reactor relevant measurements and support predictive modeling validation. To achieve target pressures and minimize downtime between experiments, a multi-stage roughing pump system is required in tandem with cryopumps. To optimize the layout of the electron beams and diagnostics relative to the test articles, a custom D-shaped vacuum vessel is envisioned for this application.

An overview of the FORGED-PFC project and its current status will be provided, along with design details of this high-performance vacuum vessel and associated pumping system.

Note: This work is supported by the U.S. Department of Energy contract DE-AC05-00OR22725. The views and opinions expressed herein do not necessarily reflect those of Oak Ridge National Laboratory.

12:00pm **FUS-WeM-17 Materials and Deposition Technologies Underlying Target Fabrication for Inertial Confinement Fusion***, **Salmaan Baxamusa**, Sean Hayes, Liam Sohngen, Juergen Biener,* Lawrence Livermore National Laboratory*; Christoph Wild, Tobias Fehrenbach,* Diamond Materials GMBH, Germany*; Casey Kong, Mark Ratledge, Anthony Allen,* General Atomics*; Corie Horwood, Parminderdeep Singh, Alec Schwartz,* Lawrence Livermore National Laboratory*; Loosineh Aghaian,* General Atomics*; Bernard Kozioziemski, Laura Kegelmeyer, Gabrielle Hamza,* Lawrence Livermore National Laboratory*; Nancy Spafford,* Lawrence Livermore National Lab

The demonstration of laser-based inertial confinement fusion (ICF) ignition on the National Ignition Facility (NIF) in 2022 was a triumph of integrated physics and decadal science. This experiment, and the subsequent experiments building up to energy gains >4, are to date the only experimental demonstrations of fusion exceeding the Lawson criterion in the laboratory. Yet underlying this physics result was a complex blend of materials science and vacuum deposition needed to create and field an igniting target. This presentation will cover two aspects of the igniting physics package where vacuum deposition plays a key role: the hollow, spherical fuel capsule that implodes and the cylindrical hohlraum that provides x-ray drive for the implosion.

The capsule used in ignition experiments is CVD-deposited nanocrystalline diamond deposited. This talk will describe improvements to fabrication including machine-learning based diagnostics, Monte Carlo modeling, integrated experiments, and infrared reflectometry to improve coating thickness uniformity to > 99.8% on non-planar, non-stationary substrates.X-ray computed tomography was used to confirm that improvements to coating uniformity did not create additional internal defects.Finally, by controlling the composition along the growth axis we created capsules that stabilized the implosion and resulted in a record gain of >4. We will briefly mention materials science challenges of other capsule materials including boron carbide and glow discharge polymer.

The cylindrical hohlraum that contains the imploding capsule is a high-atomic number material (gold and uranium) that converts incoming laser light into a spherical bath of x-rays that drives the capsule implosion.Despite decades of study, the complex oxidation pathways of uranium are incompletely understood.We observed catastrophic oxide spalling on depleted uranium hohlraums that requires both an oxidant during processing and an environmental trigger. An experimental study confirmed that removing one or the other effectively increased the shelf-life of these components from ~weeks to ~months or years, eliminating a major cause of late-stage target failures for NIF.

LLNL-ABS-2019160. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 and partially within the LDRD program under project 24-ERD-084.

Plasma Science and Technology
Room 315 - Session PS1-WeM

Plasmas for 3D Integration

Moderators: Hiroyuki Fukumizu, KIOXIA, **Dr. Jeffrey Shearer**, TEL Technology Center, America, LLC

8:00am **PS1-WeM-1 Challenges in Plasma Etching for 3D Interconnect Technology***, **Violeta Georgieva**, Jeongsoo Kim, Eoin Jackman, Quyang Lin, Katia Devriendt,* IMEC, Belgium **INVITED**

Three-dimensional (3D) interconnect technology based on die vertical stacking has been attracting increasing attention recently as a key approach to extend system-level performance beyond conventional scaling limits [1]. Through-silicon vias (TSVs), through-dielectric vias (TDVs), and nano-TSVs (nTSVs) used in backside power delivery networks enable high-density vertical electrical signal or power transport in heterogeneous 3D integration.

3D interconnect performance depends not only on interconnect structures but also on upstream processes such as plasma dicing, which ensure die integrity and bonding yield. Reducing wafer thickness and downsizing dies have revealed the limitations of conventional mechanical and laser dicing methods, while plasma dicing offers precise and clean die singulation [2].

This work focuses on the challenges faced by the plasma etching community in delivering high-aspect-ratio processes with tight control of anisotropy at both the macroscale (TSV, TDV, and plasma dicing) and the nanoscale (nTSVs). In addition to profile performance, other important parameters such as high selectivity to photoresist (PR) and hard mask (HM),

as well as endpoint detection in very small open areas with dense layouts, are addressed.

TSVs and nTSVs are both affected by etch-rate suppression and profile distortion due to aspect-ratio-dependent etching [3, 4]. For nTSVs, these challenges are exacerbated by the need for nanoscale precision, especially in TSV-last schemes, where extremely high silicon-to-oxide selectivity is required to preserve thin oxide liners [4].

TDVs introduce additional complexity due to the need to etch multilayer back-end-of-line dielectric stacks while maintaining uniformity and protecting underlying metallization [5]. Furthermore, intrinsically low dielectric-to-PR selectivity and limited HM options remain critical constraints.

Plasma dicing combines many of these challenges, requiring precise etching of silicon, dielectric, and polymer layers within a single process [6].

This presentation reviews current process solutions and innovations addressing these issues and highlights remaining gaps and future directions in plasma etching for advanced 3D interconnect integration.

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This work has been enabled in part by the NanoIC pilot line (nanoic-project.eu).

8:30am **PS1-WeM-3 Low Global Warming Potential (GWP) Gases for Deep Si Etch for Through-Silicon Via (TSV) Applications***, **Richa Agrawal**, Gloria Fraczak, Nathan Marchack,* IBM Research*; Yohei Takakura,* DAIKIN INDUSTRIES, LTD.*; Teodor Todorov, Martin M. Frank, Jaylynn Sheppard, Jose Daboin, Brian Pham,* IBM Research*; Kazunori Horiguchi,* DAIKIN INDUSTRIES, LTD.*; Yasuhiro Nojiri, Hisataka HAYASHI,* DAIKIN INDUSTRIES, LTD., Japan*; ERIC JOSEPH, ROBERT L. BRUCE,* IBM Research

Through-silicon vias (TSVs) are crucial components for three-dimensional (3D) integration technologies. Conventional Bosch processes typically rely on fluorinated gases such as c-C_4F_8 and SF_6, which exhibit high global warming potentials (GWPs) and are increasingly subject to environmental regulations. Given the criticality of deep-Si etch processes for packaging applications, it is of great interest to investigate alternative plasma chemistries to focus on sustainability for future technological node development.

In this work, the applicability of alternative with much lower GWPs for TSV applications at aspect ratios >10:1 with different integration routes, is investigated. The alternative gases show comparable etch profiles to the conventional C_4F_8-SF_6 processes – key performance indices including critical dimensions (CD), anisotropy, etch rates, mask selectivity are compared. Optical emission spectroscopy (OES) is used to assess gas phase species and compare plasma characteristics. Electrical characterization of the integrated TSVs shows similar resistance scaling for C_4F_8-SF_6 processes and alternative gases, with performance governed by TSV geometry, CD, and liner material properties. Exhaust sampling analysis using Fourier Transform Infrared Spectroscopy (FTIR) showed a two to three orders of magnitude reduction in high-GWP emission byproducts with the usage of alternative gases compared to C_4F_8 and SF_6. These results demonstrate a viable alternative pathway to reducing environmental impact while maintaining etch and electrical performance integrity for TSV fabrication.

8:45am **PS1-WeM-4 Multiscale Modeling Approach for Bosch Silicon Etching Process Coupled to Machine Learning, Toward a Fast Etching Process Optimization***, Rim Ettouri,* Nantes Université, CNRS, Institut des Matériaux de Nantes Jean Rouxel (IMN), France*; Fatima-Zahrae Hilal, Valeria Borodin,* IMT Atlantique, CNRS, Nantes Laboratory of Digital Sciences, LS2N, France*; **Ahmed RHALLABI**,* Nantes University, CNRS, Institut des Materiaux de Nantes Jean Rouxel, IMN, France

Deep silicon etching is a major challenge for the development of many electronic devices, such as DRAM memories, integrated 3D capacitors, and MEMS. Developing deep silicon etching processes with minimal morphological defects and a high degree of anisotropy, while avoiding empirical trial-and-error approaches, remains a significant scientific and technological challenge requiring substantial time and resources.

The Bosch process, based on an alternating discharge including an etching phase and a deposition phase, appears to be a particularly suitable solution for meeting these requirements depending on the targeted applications. However, its optimization generally requires long and costly experimental campaigns.

In this context, the development of etching simulators based on a multi-scale approach represents a promising alternative. Such tools could contribute in the understanding of plasma–surface interaction mechanisms and the optimization of the etching processes in a faster time.

In this context, we developed a multiscale approach for a deep silicon etching using the Bosch process with alternating discharges SF_6 for the etching step and C_4F_8 for the deposition step.The model is composed of three modules: a global kinetic model of SF_6 and C_4F_8 ICP plasmas, a sheath model based on the Monte Carlo method, and a 2D etching model based on the cellular Monte Carlo method.The simulator allows the prediction of the temporal evolution of the etched profiles, the surface chemical composition, and the etching rate.Well-known phenomena in the Bosch process, such as scalloping and undercut, are clearly demonstrated.

One of the disadvantages of our multi-physics models is its very long run time.Using machine learning to predict the evolution of silicon etch profiles as a function of the operating conditions (RF power, pressure, gas flow rates, ...) is a good way to significantly reduce the simulation times.The simulations from our multiscale approach serve as training data for the machine learning. This enables to move towards an AI approach that contributes to Bosch process optimization.

The data-driven analysis identified the relative importance of each parameter and their interactions for instance, quantifying how pressure and power jointly affect polymer deposition and SiF_x by-product formation.

9:00am **PS1-WeM-5 Feature-Scale Model of Si Plasma Etching in $SF_6/O_2/SiF_4$ Mixtures***, **Maryam Khaji**,* University of Michigan, Ann Arbor*; Fatima Jenina Arellano, Kouta Kawahara, Noboru Yamaguchi, Taichi Suzuki, Tadamasa Kobayashi, Kenta Doi,* Ulvac Technologies, Inc., Japan*; Mark J. Kushner,* University of Michigan, Ann Arbor

High aspect ratio plasma etching of Si for TSV (through-silicon vias) and packaging applications is primarily performed in fluorine-containing plasmas with feedstock gases containing CF_4, NF_3 and SF_6 [1]. Si etching by F atoms is an isotropic process. Adding gases such as O_2 and SiF_4 produces sidewall passivation which, with moderate substrate biases, enables anisotropy. For comparable F-atom fluxes to the wafer, several studies have reported significantly higher Si etch rates in SF_6-containing plasmas compared to other F-containing plasmas [2]. This enhancement has been attributed to the possible catalytic role of S-containing species, surface sulfidization, which increases the efficiency of fluorination and increases etch yields [1,3]. In this work, results will be discussed from feature-scale modeling of Si HAR etching in an inductively coupled plasma (ICP) source sustained in $SF_6/O_2/SiF_4$ gas mixtures. With the goal of distinguishing the unique aspects of plasma etching in gas mixtures containing SF_6, the surface reaction mechanism includes fluorination, sulfidization, oxidation, and ion sputtering. Reaction probabilities were calibrated against experimental results obtained for different ICP powers, RF bias powers, gas compositions, and pressures. Reactor-scale simulations were performed with the Hybrid Plasma Equipment Model (HPEM), and feature-profile evolution was evaluated using the Monte Carlo Feature Profile Model (MCFPM) [4]. The consequences of plasma properties on feature evolution will be discussed. A brief update on the gas phase reaction mechanism for SF_6 containing plasmas will be provided.

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9:15am **PS1-WeM-6 Transport Gradient Model of Oxygen and Fluorine Flux Ratio in High-Aspect-Ratio Silicon Etching***, **Kenji Ishikawa**, Shuto Tsuchioka, Trung Nguyen Tran, Kenichi Inoue, Takayoshi Tsutsumi,* Nagoya University, Japan*; Thi-Thuy-Nga Nguyen,* nagoya University, Japan

This study presents a quantitative investigation of the bowing mechanism observed in high-aspect-ratio (HAR) silicon etching using SF6/O2 inductively coupled plasmas through a multi-scale simulation framework. By integrating reactor-scale plasma modeling with feature-scale profile evolution analysis, we examine the dynamic balance of reactive radicals at

the etch front and its role in profile formation. In contrast to previous studies relying on qualitative interpretations based on optical emission intensity ratios, this work provides numerical validation of the transport gradient model.

The model demonstrates that the localized oxygen-to-fluorine (O/F) flux ratio, rather than the global gas composition, governs sidewall passivation and etch stability. The local flux ratio incorporates transport physics, including Knudsen diffusion and surface sticking probabilities, which significantly modify reactant distributions. Consequently, gradients in radical flux develop along trench depth, producing spatially varying surface reactions.

Parametric simulations identify a critical threshold in the local O/F flux ratio between 3.5% and 3.6%. Above this threshold, oxygen-rich coverage enables passivation and anisotropic etching. Below it, fluorine-dominant coverage induces a nonlinear increase in etch rate, causing rapid lateral etching and bowing.

This insight explains why a 30% O2 condition maintains verticality at shallow depths, whereas 20% O2 causes immediate bowing as the local O/F ratio falls below the threshold. These findings highlight the importance of transport-limited effects in HAR structures and provide a theoretical basis for optimizing radical flux control in advanced plasma etching processes.

9:30am **PS1-WeM-7 Effects of Discharge Frequency and Precursor Molecule on the Deposition Rate, Film Density, and Residual Stress of a-C:H Hard Masks**, ***Kazunori Koga***, *Shunpei Ohara, Soichiro Yoshida, Ryosuke Kinnami, Shinjiro Ono, Takamasa Okumura, Kunihiro Kamataki, Naho Itagaki, Masaharu Shiratani,* Kyushu University, Japan

Hydrogenated amorphous carbon (a-C:H) films are essential materials for hard masks in high-aspect-ratio (HAR) etching in semiconductor manufacturing. High-speed deposition of high-density and low-stress a-C:H films is strongly demanded for superior plasma etching resistance. Here, a-C:H films were deposited via plasma chemical vapor deposition (plasma CVD) where methane, acetylene, and cumene (C_9H_{12}) were used as precursor gases to evaluate their deposition rate, density, and stress. A parallel-plate plasma CVD system was used with 1 cm^2 Si substrates under Ar-diluted precursors. An RF voltage of 13.56 MHz or 400 kHz was applied. For 400 kHz, the concentration, flow rate, pressure, and Vpp were 5%, 100 sccm, 0.02 Torr, and 1600–2400 V. For 13.56 MHz, the flow rate was 100 sccm, concentration 5–50%, pressure 0.02–0.3 Torr, and Vpp 100 V or 250 V. At 13.56 MHz, acetylene and cumene yielded higher deposition rates than methane. Cumene achieved a 20 nm/min higher rate than acetylene with comparable density and stress (~1.0 GPa). Stress increased with density, reaching 3.8 GPa at 2 g/cm^3. Conversely, 400 kHz conditions—providing higher self-bias and incident ion energy—yielded high density (~2 g/cm^3) and low stress (~1.0 GPa), keeping stress constant independent of density. At 400 kHz, cumene deposited 10 nm/min faster than acetylene. Factors determining density were examined. Raman spectroscopy showed that hydrogen content and density are inversely correlated, independent of discharge conditions or precursors. To clarify ion energy effects, an ion energy index was defined as |Vdc|/pressure/Nc, where |Vdc| is self-bias voltage and Nc is the number of carbon atoms per molecule. Using this index, density peaked at ~5 regardless of precursors or frequencies. This indicates that the sub-plantation model, where incident ion energy is distributed among carbon atoms within a molecule to determine density, holds true even for high-carbon-number cumene. The Raman D/G peak ratio (sp^2/sp^3 bonding ratio) correlated well with density in the low-ion-energy region (13.56 MHz) but deviated in the high-ion-energy region (400 kHz). This deviation suggests a structural difference under high ion energy, explaining why stress remained decoupled from density. Etching measurements confirmed that higher density decreased the etching rate, proving that density governs etching resistance regardless of precursors or deposition conditions.

9:45am **PS1-WeM-8 Impact of HBr/H2 Gas Mixture on Etching of GeSexTe1-x Chalcogenide Thin Films for Reconfigurable and Nonlinear Photonics**, ***Giovanni BEDOUI***, CEA-LETI, France*; Aurélien TAVERNIER, Yoann BRULE, Jean-Baptiste DORY, Pierre MEILLEUR, Jules LAGRAVE, Clémence JAMIN-MORNET, Pierre NOE,* CEA-Leti, France

Chalcogenide materials are alloys composed of one or multiple chalcogen elements (S, Se, Te) and one or multiple alloying elements (Ge, As, ...). They demonstrate a wide transparency window and high linear and non-linear (NL) indices in the near and mid infrared. Some of them exhibit phase-change properties, transitioning reversibly from an amorphous to a crystalline state, with an unusual contrast between the electrical and optical properties of these two states [1,2]. As their properties makes them interesting for micro and nano-photonics applications, one issue impeding their widespread integration is the ability to pattern them without altering their optical properties.[3]

To address this issue, a plasma etching process with minimal impact over morphology and stoichiometry is needed for $GeSe_xTe_{1-x}$ destined to reconfigurable (1.55µm) and NL (2µm) applications. A focus will be made on HBr/H_2 etching gases and H_2/Ar Post-Etching Treatment (PET), expecting low impact on surface roughness (Rq), stoichiometry alteration and non-volatile compound (NVC) formation.[4]

This work involves unpatterned $Ge_{50}Te_{50}$ and $Ge_{50}Se_{50}$ thin film etching with HBr and HBr/H_2 both with and without PET in an ICP chamber. Characterization methods such as 2D Atomic Force Microscopy (AFM) for Rq and X-Ray Photoelectron Spectroscopy (XPS) for atomic composition were used. Figure 1 shows AFM measurement of Rq for both alloys at each gas composition. HBr/H_2 mix induces the lowest Rq and PET decreases Rq for both alloys. Figure 2 shows XPS measurement of both alloys with each gas composition. HBr and H_2 cause stoichiometric shifts by forming volatile GeH_x and NVC $GeBr_x$ in both alloys. For GeTe, PET seems to limit both NVC and volatile by-products. For GeSe, PET induces volatile SeH_x by-products generation.[5] We can conclude that HBr/H_2 + PET etching mix seems the most promising.

To go further, the impact of HBr/H_2 + PET mix over unpatterned and patterned $GeSe_xTe_{1-x}$ thin films will be studied. Characterizations techniques as 3D and 2D AFM for sidewall roughness and Rq measurement, XPS for atomic composition and Scanning Electron Microscopy (SEM) for sidewall angle analysis will be used. The addition of CH_4 gas into the etching mixture could be studied to improve sidewall angle control.[6]

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Plasma Science and Technology
Room 315 - Session PS2-WeM

Plasma Applications in Packaging and Wafer Bonding

Moderators: Prof. Kenji Ishikawa, Nagoya University, Japan, **Dr. Jeffrey Shearer**, TEL Technology Center, America, LLC

11:00am **PS2-WeM-13 Etch Opportunities in Advanced Packaging, Silicon, and Optical Photonics**, ***Brittany Hedrick***, Tokyo Electron America **INVITED**

Advanced Packaging grows more complex as the ever-increasing need for bandwidth, power, and memory persists and drives down feature geometries: from the transistor to the electrical routing line/space, and out to the assembled system through ever-finer plated interconnects and optical interconnects. Interconnect density pitches for conventional electrical interconnects are teetering between the realm of plated micropillars and Cu-Cu bonding down into D2W and W2W pitches enabled by direct Cu Hybrid bonding. Ever thinner HBM layers drive unique TSV integration for ultra thin die and singulation methods to handle these devices with high yield.

Meanwhile Si photonics features have been added to the mix to handle data for long haul and short haul tele-com/data-com and are finding traction in Quantum and AI applications as well.Introducing new materials into standard CMOS flows, Si photonics and Quantum computing devices are driving new tooling applications, novel processes, and research and development activities seeking advances in performance improvement.Waveguide materials and designs, for telecom and datacom, continue to be refined for improved propagation loss performance, and the optical interconnect features themselves are etched, milled, and engineered to reduce insertion loss to as close to 0 as possible.

In the consumer electronics sector personal devices are evolving from cell phones to AR glasses, with top makers looking to bring fashionable, functional, lightweight, and efficient devices to market for mass adoption. Optical photonics now drives glass and SiC wafer device fabrication across traditionally Si wafer/CMOS semiconductor tools.Depositing thin films on

glass, litho, etch, and encapsulation to fabricate optical gratings for AR lenses provide new challenges the industry is rapidly rising to address.

Tokyo Electron (TEL) is working across these spaces to develop processes and equipment to keep pace with the ever-evolving packaging world. Throughout the presentation we will highlight recent process developments and practical adaptations in etch technology that respond to these growing industry applications.

11:30am **PS2-WeM-15 Impact of Surface Activation Plasma Chemistry on AlN - Oxide Wafer Bonding for BSPDN Applications***, **Chetan Jois**, Ryan Allen, Yusuke Suzuki, Andrew Tuchman, Christopher Netzband, Rinus Lee, Ilseok Son,* Tokyo Electron America, Inc.

In Backside Power Delivery Network (BSPDN) process flows, a carrier wafer is bonded to enable wafer thinning and backside access. When the carrier is retained for packaging, the bonding interface plays a dual role as both a mechanical support and a thermal transport pathway. Conventional oxide bonding dielectrics, such as SiO_2, introduce a thermally resistive layer between the carrier and device wafers, motivating the use of alternative bonding materials with improved thermal properties. Aluminum nitride (AlN) has emerged as a promising thermally conductive dielectric for carrier bonding. For integration, bonding interfaces must exhibit bonding energies greater than 1.5 J/m^2 to enable downstream processing and ensure mechanical reliability. However, achieving high bonding energy with AlN based films at low thermal budgets remains a key integration challenge. In this work, we investigate the bonding behavior of a thin AlN based bonding stack consisting of 30 nm PVD AlN capped with 5 nm ALD Al_2O_3, bonded to a thermally grown 100 nm SiO_2 carrier wafer. The surface activation plasma (SAP) process window is systematically studied with direct comparison between O_2 and N_2 plasma chemistries. Bonding energy measurements show a strong dependence on SAP gas chemistry, with O_2 plasma activation yielding higher bond strength than N_2 plasma under comparable process conditions, achieving a bond energy of 2.8 J/m^2 at optimized settings. Surface chemical analysis reveals that O_2 SAP results in a higher concentration of H_2O and hydroxyl related species compared to N_2 activated surfaces, indicating enhanced surface hydration that promotes stronger interfacial bonding. Post–anneal bond energy is found to correlate well with bond propagation speed and surface contact angle, suggesting that improved initial surface adhesion directly translates to increased final bond strength. Finally, the impact of SAP conditions on post–bond lithography overlay (PBLO) is evaluated for BSPDN integration.

11:45am **PS2-WeM-16 Optimization of Dielectric Plasma Activation for Wafer to Wafer Fusion Bonding***, **Christopher Netzband**,* Tokyo Electron America Inc.*,; Andrew Tuchman, Ilseok Son, Angelique Raley,* Tokyo Electron America, Inc.

As logic and memory scaling slows, the demand for higher interconnect density and speed has increased, especially among NAND and DRAM companies. Device performance gains are increasingly achieved in the back end of line using wafer-to-wafer (W2W) hybrid bonding for 3D NAND, CIS, 3D-SoC, and eventually bonded CFET architectures. One major hurdle to achieving bonded CFET structures is the strength and reliability of the bonding interface. If the mechanical strength of the bonding is low the wafers will come apart during grinding or etching, while if the chemical strength is low they will be etched apart during subsequent wet cleans. Most dielectric films have poor mechanical bonding strength as deposited they require plasma activation to enable bonding. This plasma activation breaks the surface bonds enabling hydrogen bonding and condensation to covalent bonds after a post-bond anneal. Unfortunately, just running this activation does not ensure good mechanical or chemical bonding strength as the results can vary based on your incoming film.

In this talk we will discuss what properties are most important for high quality bonding across a range of bonding materials. Examples of film properties that influence plasma parameter selection include exposed metal (hybrid bonding), thickness and density. In the case of hybrid bonding the plasma activation must be very low power and confined to the surface to eliminate the chance of leakage pathways along the bonding interface caused by Cu sputtering. Similar considerations are needed for thin oxides. If the interaction depth of the plasma is too deep can impact underlying layers or, if deposited directly on Si, cause hydrogen gas at the film/Si interface. While it is well known that SiO_2 performs better with N_2 plasma versus O_2 plasma, the degree of the difference between these activation gasses is directly correlated to the porosity of the films. In CVD TEOS the difference in bond strength between the two activation gasses is small and the interface after bonding is void free. Conversely, highly dense thermally grown SiO_2 has a 60% lower bond strength when using O_2 gas for the plasma activation and has small voids at the wafer edge caused by the plasma that further reduce the chemical and mechanical strength of the bond leading to quicker stress corrosion than the N_2 case. By understanding how to adjust plasma activation conditions to obtain high quality bonding with a wide range of materials even more opportunities for hybrid and fusion bonding will emerge in advanced packaging.

12:00pm **PS2-WeM-17 Plasma-Induced Surface Modification of Indium for Improved Bonding***, **Kristen Steffens**,* National Institute of Standards and Technology (NIST)*; Sujitra Pookpanratana,* National Institute of Science and Technology (NIST)*; Junyeob Song, Marcelo Davanco, Tammy Lucas, John Biesecker, Daniel Schmidt,* National Institute of Standards and Technology (NIST)

Bonding between materials plays an important role in advanced microelectronics integration and packaging by bringing together components and devices produced separately.Surface pretreatments on bonding materials have been consistently found to be crucial to achieving a high-quality bond, despite incomplete understanding of why certain treatments have greater success than others.Our project aims to improve understanding of atmospheric plasma pre-treatment effects to provide information to enable more efficient development of bonding protocols.

Indium is a critical material for conductive interconnects for the fabrication of cryogenic low-temperature electronics and optical detectors for infrared and microwave applications. Since indium is a superconducting material which retains its ductility and adhesion properties during thermal cycling, it sees particular use for Quantum Information and Quantum Sensor applications [1].Certain pre-bond plasma treatments increase the success of In-In bond adhesion.We have observed that plasma chemistries such as H_2/He, which do not include N_2 as a plasma gas, promote more successful In-In bonding.To understand why, we investigate the effects of atmospheric plasma exposure on indium surfaces for several plasma chemistries including He/H_2/N_2, He/H_2 and He/N_2.X-ray photoelectron spectroscopy (XPS) and ultraviolet photoelectron spectroscopy (UPS) are used to characterize indium surfaces prior to and after ambient pressure plasma treatment.All plasma treatments decreased the amount of carbon and increased both the amount of In-oxide present as well as the indium oxide/metal ratio as compared to an untreated film.N-$_2$-containing plasmas resulted in the appearance of an additional high binding energy peak in the N 1s XPS spectrum.We postulate that this may be due to nitrate species formed on the indium native oxide surface. Additional experiments were performed on indium foil both prior to and after Ar sputtering for comparison to treated samples.Nitrogen was found to be confined to the surface and reappeared after eleven weeks of exposure to air at room temperature.

UPS measurements showed that all plasma chemistry treatments lowered the work function compared to the non-treated control.Greater spatial variation in work function was observed for chemistries with high N_2 versus those with little to no N_2.This finding possibly correlates with poorer bonding for N_2 containing plasmas.

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Surface Science
Room 305 - Session SS-WeM

Heterogeneous Catalysis

Moderators: Gengnan Li, Argonne National Laboratory, **Joerg Libuda**, Friedrich-Alexander-University Erlangen-Nürnberg (FAU)

8:00am **SS-WeM-1 Molecular Systems for Reversible Hydrogen Storage: Atomistic-Level Insights***, **Swetlana Schauermann**,* Kiel University, Germany **INVITED**

Heterogeneous catalysts based on bimetallic single atom alloys (SAA) play a significant role in numerous technical processes. The fundamental working principles of these systems, however, remain poorly understood, especially the aspects related to the nanoscopic nature of bimetallic particles and the associated structure-reactivity relationships. In this study, we developed well-defined SAA catalysts consisting of Pd atomically dispersed in Cu nanoparticles prepared under ultra-high vacuum conditions on model Al_2O_3/NiAl(110) support.[1] Employing a unique combination of surface sensitive techniques – scanning tunning microscopy (STM), infrared reflection absorption spectroscopy (IRAS), molecular beams – and density

functional theory (DFT) calculations, we performed detailed structural characterization of these systems at the microscopic level. We demonstrate that Pd disperses atomically in Cu nanoparticles and becomes partly negatively charged. Importantly, these Pd/Cu nanostructured systems show an outstanding catalytic performance in selective dehydrogenation of butanol and exhibit 100 % selectivity toward butanal over a broad range of Pd loadings – the property that cannot be reproduced employing simplified single crystalline Pd/Cu(111) counterparts.

In the second part, the catalytic decomposition of 2-propanol to acetone over Co_3O_4(111) catalyst will be addressed with the specific focus on the role of water and its derivatives in the reaction mechanism and the overall catalytic activity.[2] Pre-treatment of this catalyst with water at elevated temperatures (573 K) was shown to result in a substantial increase in the acetone formation rate. Combined STM and IRAS studies revealed that this procedure leads to the formation of isolated hydroxyls involving a lattice oxygen atom, which play a key role in H abstraction, both from molecular 2-propanol and from the propoxy reaction intermediate, leading to efficient formation of the target product acetone. Our results suggest that the isolated O_sH group is substantially more efficient hydrogen acceptor than the adsorbate-free lattice oxygen O_s.

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2. *"Promoting role of isolated surface hydroxyls on selective dehydrogenation of 2-propanol to acetone over Co_3O_4 catalyst: a mechanistic study."*J. Smyczek et al, ACS Catalysis **(2025)** 15, 19268

8:30am **SS-WeM-3 When Interfaces Break Scaling: Metal–Ceria Catalysts for Selective Methane Conversion***, Maria Veronica Ganduglia-Pirovano, Pablo G. Lustemberg, Estefanía Fernández-Villanueva,* Instituto de Catálisis y Petroleoquímica-CSIC, Spain

The selective activation of methane under mild conditions remains one of the central challenges in heterogeneous catalysis. Metal–oxide interfaces, particularly those formed between transition metals and ceria (CeO_2), provide a unique platform to control both activity and selectivity by coupling metal reactivity with the redox flexibility of the oxide support.

In this contribution, we present recent advances in the understanding and design of metal–ceria catalysts for methane conversion, combining DFT+U simulations with operando and in situ characterization (AP-XPS, XRD, XAFS) and catalytic testing. We show that low metal loadings (Ni, Co, Pt, Pd) on ceria generate highly active interfacial sites, where electron transfer to Ce 4f states stabilizes oxidized metal species, enabling methane activation at unusually low temperatures and efficient methane dry reforming under mild conditions. These systems deviate from conventional linear scaling relationships, demonstrating that nanostructured metal–oxide interfaces can overcome intrinsic activity–selectivity limitations.[1]

Building on this concept, we highlight recent results on the direct conversion of methane to methanol under mild conditions. In particular, PdAu/CeO_2 catalysts enable selective methane oxidation using water as the sole oxidant, achieving high methanol selectivity (~80% at 500 K). The alloy–oxide interface plays a decisive role: isolated Pd sites at the PdAu–ceria interface promote methane activation and water dissociation, while Au suppresses over-oxidation pathways leading to methanol decomposition. This synergistic interplay effectively tunes Pd reactivity, balancing activity and selectivity.[2]

These findings establish a unifying picture in which metal–oxide and alloy–oxide interfaces act as tunable active sites that decouple elementary steps and break traditional scaling constraints. This provides a rational framework for designing catalysts capable of selectively converting methane into value-added chemicals under technologically relevant conditions.

This work builds on a close and highly fruitful collaboration with José A. Rodriguez and his team at Brookhaven National Laboratory.

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8:45am **SS-WeM-4 Supported Ni-Cu Catalysts for the Selective Dehydrogenation of Liquid Organic Hydrogen Carriers***, Donna Chen, Nirmal Phuyal, Mengxiong Qiao, Biplab Budhathoki,* University of South Carolina

Hydrogen is a promising source of clean and renewable energy, but a major challenge lies in its storage and transportation. The use of liquid organic hydrogen carriers (LOHC) enables hydrogen storage in organic molecules that are liquids at room temperature and therefore suitable for transportation through existing petroleum infrastructure. The methylcyclohexane (MCH) toluene pair has been used for the catalytic cycle of hydrogenation to store hydrogen and dehydrogenation to release hydrogen. While inexpensive and efficient catalysts are already available for hydrogenation, there is still the need for the development of selective dehydrogenation catalysts that inhibit deactivation due to carbon fouling. In this work, Cu-Ni clusters deposited on a rutile TiO_2(110) support are studied as catalysts for selective dehydrogenation. Methylcyclohexene (MCE) is used as a surrogate probe molecule to investigate the surface chemistry of MCE in ultrahigh vacuum since MCE adsorbs more strongly on Ni surfaces than MCH. Temperature programmed desorption (TPD) experiments for MCE on pure 2 ML Ni clusters show that nonselective decomposition to H_2 and surface carbon is the main reaction pathway; the evolution of CO at high temperature from the recombination of surface carbon and lattice oxygen from the titania support is used to quantify the extent of nonselective decomposition. In contrast, MCE reaction on 2 ML Cu clusters results in little overall dehydrogenation activity although a small amount of toluene is evolved. For 2 ML Ni clusters modified by the deposition of 0.25 ML of Cu, the amount of toluene produced is increased by a factor of 3 compared to pure Cu, but the extent of nonselective decomposition is still comparable to what is observed on pure Ni, indicating that Cu-Ni alloying and site blocking do not completely suppress MCE decomposition. However, the deposition of a small coverage of Ni (0.1 ML) on 2 ML Cu clusters results in 100% selectivity to toluene and a toluene yield that is seven times greater than on pure Cu. Increasing the Ni coverage to 0.25 ML lowers toluene production and leads to the initial onset of nonselective decomposition.The high toluene selectivity for the 0.1 ML Ni on 2 ML Cu clusters is attributed to the formation of a dilute alloy in which the Ni ensembles are not large enough to promote nonselective decomposition, but the desired reaction pathway of dehydrogenation to toluene is facilitated. These results demonstrate that controlling Ni ensemble size in Cu–Ni dilute alloys is an effective strategy for developing selective, coke-resistant dehydrogenation catalysts.

9:00am **SS-WeM-5 Surface Structure, Stability, and Catalytic Reactivity of Metal Nanoparticles Supported on Tantalum Oxide***, Ravi Ranjan, Francisco Zaera,* University of California - Riverside

The surface structure, thermal stability, and catalytic behavior of copper (Cu) and platinum (Pt) nanoparticles (NPs) supported on tantalum oxide (TaO_x/Ta) thin films have been investigated using reflection absorption infrared spectroscopy (RAIRS) and temperature-programmed desorption (TPD), with carbon monoxide (CO) as the probe molecule.

Cu NPs were prepared by vapor deposition at room temperature and under ultrahigh vacuum (UHV) conditions, and characterized by following the adsorption of CO at 77 K. Increasing deposition of Cu led to the growth of nanoparticles exhibiting distinct adsorption sites associated with the metal-oxide interface and different Cu surface facets. The Cu NPs remained stable under both UHV and high-pressure CO environments over a broad range of temperatures.

Pt deposition onto TaO_x/Ta resulted in the gradual formation of NPs with predominantly one major CO adsorption feature. In contrast to the case of Cu, Pt NP growth was less structurally distinct, as indicated by the CO vibrational signatures. Pt nanoparticles remained stable in UHV up to approximately 500 K, above which subsurface migration into the oxide support was observed.

The catalytic properties of the Pt/TaO_x/Ta surfaces were further examined using acrolein hydrogenation as a model reaction. Reaction studies under atmospheric pressures, using a so-called high-pressure cell to directly transfer the surfaces from UHV to the catalytic reactor, revealed the formation of propanal, propanol, and allyl alcohol, demonstrating competing hydrogenation pathways involving both C=C and C=O. These findings provide molecular-level insights into how nanoparticle structure, stability, and metal-support interactions influence catalytic selectivity and

reactivity under catalytic conditions.

9:15am **SS-WeM-6 CO Oxidation on Plasma-Activated Pd and PdAg Surfaces**, ***Pablo de Oliveira***, *Camilla Codeço, Marcos G. Menezes,* UFRJ, Brazil*; J.Anibal Boscoboinik,* BNL

Plasma-assisted surface treatments offer an attractive alternative to conventional sputter/annealing cycles for surface cleaning and activation, particularly in alloyed materials where preferential sputtering or thermal segregation may alter the near-surface stoichiometry. Here, we investigate how sequential oxygen and hydrogen plasma cycles modify the surface chemistry and CO oxidation activity of Pd-based systems. By combining ambient-pressure X-ray photoelectron spectroscopy (AP-XPS), ambient-pressure infrared reflection–absorption spectroscopy (AP-IRRAS), and density-functional theory (DFT) calculations, we compare the reaction pathways on a Pd foil and a PdAg alloy under near-ambient conditions. While both systems exhibit CO oxidation even slightly above room temperature (373 K), they reveal a dependence on the $CO:O_2$ composition. On Pd foil, CO oxidation is mainly observed under balanced feeds ($p_{CO} = p_{O2}$), whereas the PdAg alloy sustains activity even under oxygen-rich conditions ($p_{O2} = 2 \times p_{CO}$). This enhanced tolerance is attributed to the formation of hydride-like Pd species during the in situ, room temperature hydrogen plasma. DFT calculations further confirm that hydrogen dissociation is energetically favored on the PdAg alloy compared to Pd foil. The presence of hydride prevents the formation of PdO layers, enabling alternative low-energy pathways for CO oxidation. These results demonstrate that sequential plasma treatments can do more than clean Pd-based surfaces, actively tuning the active sites that govern CO oxidation in alloy catalysts.

9:30am **SS-WeM-7 Catalysis with Liquid Gallium Alloys**, ***Christian Papp***, Freie Universität Berlin, Germany **INVITED**

Recently, Supported Catalytically Active Liquid Metal Solutions (SCALMS) were shown to surpass conventional alkane dehydrogenation catalysts in both activity and stability, due to their liquid nature and the presence of catalytically active single atom sites. SCALMS consist of a liquid metal matrix (Ga) that dissolves a catalytically active transition metal (Pt, Rh, Pd, Ni). Binary SCALMS systems are the subject of extensive research on the fundamental level with the aim to reach optimal performance.

Here, we present an operando NAPXPS study of the dehydrogenation of simple alkanes on gallium-platinum SCALMS (Supported Catalytically Active Liquid Metal Solutions) catalyst systems. As an industrially relevant test reaction, the dehydrogenation reaction of propane was used. In the study we compare the activity of oxidized GaPt SCALMS and liquid / metallic GaPt SCALMS surfaces, using Near-Ambient Pressure X-ray Photoelectron Spectroscopy. From the study, we conclude that the oxide shows a lower activity as compared to the metallic liquid GaPt SCALMS model systems. Further, the gallium matrix reduces under reaction conditions and coke residues disappear.

Our study thus underscores the practical value of NAPXPS in tracking surface changes and electronic states during catalytic reactions. By exploring these differences, the study sheds light on the role of oxides on the catalytic performance. These findings contribute essential insights for optimizing catalyst design and improving effectiveness, offering a pragmatic approach to catalytic enhancement.

Acknowledgement:

The research is funded by the DFG through SFB 1452 (Project number: 419654270).

11:00am **SS-WeM-13 Ni as a Promotor for Ethylene Epoxidation: Computation, Surface Science, and Reactor Studies**, ***Matthew Montemore***, Tulane University **INVITED**

Single-atom alloys have shown strong catalytic performance for several types of reactions, including hydrogenation reactions and alkane conversion. However, single-atom alloys have not been extensively studied for oxidation reactions, despite the critical importance of these reactions. The possibility that single-atom alloys could easily activate molecular oxygen but bind O relatively weakly makes them intriguing, as weakly bound O is likely to be quite reactive. In this work, we computationally designed single-atom alloys for oxidation, focusing on surfaces that can easily activate O_2 but give relatively weak O binding. We found several Ag-based single atom alloys that are predicted activate O_2 with very low barriers, in some cases near 0, while still binding O relatively weakly. In particular, NiAg stood out as a case with a very low barrier but relatively weak binding. Subsequent experimental synthesis and testing of single-crystal single-atom alloy surfaces shows that NiAg can activate O_2 and create relatively weakly bound O. Characterization with X-ray photoelectron spectroscopy, scanning tunneling microscopy, and temperature-programmed desorption gives strong fundamental insight into the interaction of these materials with oxygen and their state when exposed to oxygen and a reductant. Finally, NiAg nanoparticles were synthesized and tested, and show excellent performance for ethylene epoxidation. This work demonstrates the utility of integrated computational-experimental studies, and opens up the possibility of high-performance single-atom alloy catalysts for many oxidation reactions.

11:30am **SS-WeM-15 Tuning Oxygen Activation on Gold with RhAu Single-Atom Alloys**, ***Dennis Meier***, *Vinita Lal, E. Charles H. Sykes,* Tufts University

Selective oxidation reactions, such as olefin epoxidation and alkane oxidation, are large-scale industrial processes and are key to the more efficient conversion of natural gas into value-added products. Given the ongoing challenge of optimizing industrial chemical processes, there is a great need for highly selective catalysts. We investigated Au, which is known to be exceptionally selective for many oxidation reactions, but whose inability to efficiently activate O_2 limits reaction rates.

Density functional theory (DFT) predicted that small amounts of Rh guest atoms could overcome the low intrinsic activity of Au toward oxygen activation while preserving its high selectivity. We prepared RhAu single-atom alloys (SAAs), in which Rh atoms remain isolated in the Au surface, and probed their reactivity using a combination of temperature-programmed desorption (TPD), scanning tunneling microscopy (STM), and ambient-pressure X-ray photoelectron spectroscopy (AP-XPS). At comparable O_2 pressures and sample temperature, the RhAu systems show a significantly higher amount of Au-associated oxygen than clean Au, providing strong evidence that O_2 is activated at Rh sites and subsequently spills over onto the Au surface, which is the initial step for selective oxidation on Au. We further studied how the coordination environment of the guest atoms influences reactivity by comparing the (111) and (110) facets. The latter forms a (1×2) reconstruction that gives rise to undercoordinated surface sites. Using AP-XPS, we investigated the stability of RhAu SAAs at different temperatures and during exposure to CO and O_2. Together, these findings show that RhAu SAAs can overcome the low oxygen-activation activity of pure Au while retaining the potential for highly selective oxidation chemistry.

11:45am **SS-WeM-16 Reaction Product and Single-Atom Promotion of Acetylene Cyclotrimerization and Cross-Coupling on Ag(111)**, ***Nipun Kahagalla Dewage***, Tufts University*; Santu Biswas,* Tulane University*; Volkan Cinar, Dennis Meier,* Tufts University*; Matthew Montemore,* Tulane University*; Charles Sykes,* Tufts University

Benzene (C_6H_6) and toluene (C_7H_8) are irreplaceable chemical feedstocks used to produce pharmaceuticals, polymers, and materials. These aromatics are currently produced primarily through petroleum cracking and reforming processes, which require high energy input, harsh operating conditions, and lack full selectivity. As hydrocarbon feedstocks increasingly shift from oil to shale gas, alternative catalytic routes for the selective synthesis of aromatics are of significant interest. Acetylene (C_2H_2) cyclotrimerization is one promising pathway because it uniquely produces C_6H_6 with 100% selectivity on Ag(111). However, this reaction requires more than one monolayer (ML) of C_2H_2 on Ag(111) to initiate C_6H_6 formation, necessitating high reactor pressures that limit its practical applicability.

To understand and overcome this limitation, C_2H_2 cyclotrimerization on Ag(111) was investigated using Temperature-Programmed Desorption (TPD), 12 K Scanning Tunneling Microscopy (STM), and Density Functional Theory (DFT). Coadsorption experiments with isotopically labeled benzene (C_6D_6) reveal that C_6D_6 promotes acetylene conversion to 20% at coverages of ≥0.6 ML. STM and DFT show that attractive C_2H_2-C_6D_6 interactions and increased molecular packing stabilize the key C_4 transition state involved in the rate-limiting step, making C-C coupling competitive with C_2H_2 desorption. In addition, coadsorption of C_2H_2 and propyne (C_3H_4) was examined to explore heterocoupling pathways for toluene (C_7H_8) formation. While coupling occurs at ≥1 ML total coverage with higher C_3H_4:C_2H_2 ratios, reaching a maximum at 1.5:1, C_6H_6 remains the dominant product (95%), with C_7H_8 forming only in minor quantities (5%). Guided by mechanistic insights from DFT, we further demonstrate that introducing chromium (Cr) dopant atoms into Ag(111) to form a Cr single-atom alloy dramatically alters the free energy landscape of C_2H_2 cyclotrimerization. This enables C_6H_6 formation at C_2H_2 coverages below 0.1 ML while maintaining the 100% selectivity of Ag(111) at Cr coverages ≤2%.

Together, these findings provide mechanistic insight into product-promoted C_2H_2 cyclotrimerization and C_2H_2-C_3H_4 coupling on Ag(111). They also demonstrate that CrAg(111) single-atom alloys can enable selective aromatic formation, offering a potential pathway for upgrading shale-gas-derived $C_{2,3}$ hydrocarbons into high-value aromatics without requiring high reactor pressures.

12:00pm **SS-WeM-17 Selective Hydrogenation of Styrene to Ethylbenzene Over a Pd/Cu(111) Single Atom Alloy Surface**, ***Mohammad Rahat Hossain***, *Michael Trenary,* University of Illinois - Chicago

Selective hydrogenation of alkynes and alkenes is central to industrial catalysis, yet direct spectroscopic identification of surface intermediates under realistic pressure conditions remains challenging. Here, we investigate styrene hydrogenation on a Pd/Cu(111) single-atom alloy (SAA) surface using polarization-dependent reflection absorption infrared spectroscopy (PD-RAIRS), Auger electron spectroscopy (AES), and kinetic analysis under ambient-pressure conditions. A 0.03 ML Pd/Cu(111) surface selectively hydrogenates styrene to ethylbenzene while suppressing aromatic ring hydrogenation. Time-resolved RAIRS measurements reveal the disappearance of styrene vibrational features at 909, 991, 1018, and 1637 cm^{-1} and the growth of ethylbenzene bands at 1033, 1066, 1329, 1385, and 1462 cm^{-1}, accompanied by aliphatic C–H stretching modes below 3000 cm^{-1}. A transient surface feature at ~1385 cm^{-1} is assigned to a benzylic σ-bound intermediate, consistent with β-selective hydrogenation of the vinyl group. Kinetic measurements show approximately first-order dependence on H_2 and near-zero-order dependence on styrene, supporting a Langmuir–Hinshelwood-type mechanism involving facile styrene adsorption and kinetically relevant hydrogenation steps. Repeated reaction cycles lead to carbon accumulation detected by AES, with carbon coverage increasing from ~45% to ~65%; however, catalytic activity persists despite the formation of a thin carbonaceous overlayer. These findings demonstrate that Pd/Cu(111) SAAs provide atom-efficient and highly selective hydrogenation catalysts while enabling molecular-level insight into hydrocarbon hydrogenation and carbon overlayer formation under elevated-pressure conditions.

Thin Films
Room 317 - Session TF1-WeM
VSHOP Hybrid CVD and MLD

Moderators: Prof. Dr. Sumit Agarwal, Colorado School of Mines, USA, **Prof. Matthias Young**, University of Missouri

8:00am **TF1-WeM-1 Thin-film and Redox-active Polyvinyl Metallocene via Chemical Vapor Deposition**, ***Shadi Motamed***, *Hamidreza Mohajeri Khorasani, Maria Aydt, Mona Bavarian, Siamak Nejati,* University of Nebraska-Lincoln

Metallocene containing polymers such as poly(vinyl ferrocene) (PVF), have gained attention for electrochemical and electronic applications due to the reversible Fe(II)/Fe(III) redox activity of the ferrocene groups in this redox-active polymer. Nonetheless, the current approach to prepare this polymer is mainly based on solution-phase synthesis, limiting the integration of PVF into high aspect ratio electrode architecture for sensing and separation purposes. Herein, to overcome the limitations associated with solution-phase processing of PVF, a solvent-free method was introduced. Thin films of PVF were synthesized by hot filament chemical vapor deposition. The vapor-phase polymerization process enables the direct deposition and synthesis of organometallic polymer coatings while maintaining the ferrocene functionality during film growth. The resulting thin films of PVF deposition on silicon substrate were characterized using scanning and transmission electron microscopy, nuclear magnetic resonance and X-ray photoelectron spectroscopy, along with gel permeation chromatography. The cyclic voltammetry data was used to evaluate the redox activity of the deposited coatings. The results showed Δ*Ep*=0.02V vs. reference electrode and Coulomb efficiency of 94.5% compared to vinyl ferrocene with Δ*Ep*=0.09V vs. reference electrode and Coulomb efficiency of 90%. This indicates a higher reversibility and faster electron-transfer kinetics of PVF when compared to its parent monomer. We report on conditions that led to the successful deposition of PVF thin films through vapor phase and highlight PVF potential as redox-active coatings and electrochemical sensors.

8:15am **TF1-WeM-2 Amine Functionalization of Polydioxanone at Low Temperature By oMLD of Poly(p-phenylenediamine)**, ***Nazifa Z. Khan***, *Nikhila C. Paranamana, Xiaohua Liu, Matthias J. Young,* University of Missouri-Columbia

Polydioxanone (PDO) is a biodegradable aliphatic polyester extensively utilized in biomedical applications due to its flexibility and biocompatibility, and is absorbed by the body within two months post-implantation. However, PDO inherently lacks chemically reactive amino functional groups, thereby preventing its surface modification with peptides or growth factors for tissue engineering applications. In this study, we investigate the application of low-temperature oxidative molecular layer deposition (oMLD) of amino-containing poly-p-phenylenediamine (PPDA) to functionalize PDO. PPDA was deposited using oMLD at a reduced temperature of 90°C to accommodate PDO, considering its melting point is 110°C. Subsequently, PDO was spin-coated with high uniformity, followed by the low-temperature deposition of PPDA on the spin-coated PDO. The linear growth and saturation behavior were assessed using Quartz Crystal Microbalance (QCM). Amine functionalization was characterized through Raman spectroscopy and Fourier Transform Infrared Spectroscopy (FTIR), while the uniformity of thickness was measured using Spectroscopic Ellipsometry (SE). The water stability of the bilayer was evaluated by immersing the samples in water and measuring the thickness vs time, in which the PPDA was found to be unstable in water. QCM results indicated that at lower temperatures, the oMLD growth mechanism produces short-chain polymers, explaining the rapid loss of the oMLD films in water. Raman spectroscopy data also revealed the presence of a polyaniline-type structures within the network at low deposition temperature, contributing to the polymer's dissolution. Following ultraviolet (UV) post-treatment, an amine-containing component of the film remained intact even after >1 week of immersion in water, as confirmed by XPS analysis. This study, illustrates that the oMLD of PPDA at low temperature with UV-posttreatment produces stable surface amine groups on PDO, allowing a potential pathway for subsequent chemical functionalization of PDO for applications such as tissue regeneration.

8:30am **TF1-WeM-3 oCVD Enabled Conjugated Polymer Alloying for Filler-Free High-Capacity Chloride Storage Cathodes**, ***Aqeel Khan***, *Trisha Andrew,* University of Massachusetts - Amherst

Rechargeable chloride ion batteries (CIBs), which utilize Cl^- ions as charge carriers, offer a compelling route to sustainable and biocompatible electrochemical energy storage by combining high theoretical energy density with the natural abundance of chloride resources. p-Doped conjugated polymer electrodes are particularly promising for CIBs, where their chemical tunability, facile processability and compatibility with aqueous operations create numerous pathways for cathode engineering and fabrication. However, a persistent gap remains between theoretically predicted and practically realized capacities of existing polymer-based electrodes, primarily due to the challenge of reconciling the orthogonal design principles for efficient ionic and electronic transport throughout the active electrode volume during cycling. Here, we report a generalizable strategy to fabricate conducting polymer electrodes for CIBs—oxidative chemical vapor deposition (oCVD) enabled controlled phase “alloying”—that allows uniform structural integration of amorphous, swellable, redox-active ionic phases with crystalline, capacitive, electron conducting phases. We describe a representative conducting polymer alloy (CPA) that integrates electron-conductive, crystalline PEDOT:Cl domains within a redox-rich, amorphous PANI:Cl matrix to electronically connect redox-active nitrogen sites in PANI while maintaining its swellable amorphous matrix for reversible Cl- ion insertion and extraction. As a result, the as-prepared CPA film delivers a high specific capacity of 101.5mAh/g over a wide range of film thicknesses, without using conductive fillers or additives. This oCVD enabled polymer alloying strategy can be generalized to any appropriate combination of conjugated polymer structures for designing conducting polymer electrodes for anion batteries. Further, these oCVD-grown conducting polymer interphases can also function as transport mediating and protective layers for existing metal (oxy)chloride salt-based cathode materials, suppressing interfacial dissolution and buffering destructive phase-induced volumetric changes during charge-discharge cycling. Unlike conventional carbon additive-based approaches, vapor-deposited protective layers can be grown directly over the reactive particle surfaces, where dissolution, cracking, and transport bottlenecks originate. By correlating electrochemical behavior with nanoscale interfacial stabilization, this study aims to establish vapor-deposited conducting polymer interphases as a viable route to stabilizing high-capacity Cl^- storage electrodes and improving the durability of the chloride ion batteries under

aqueous operating conditions.

8:45am **TF1-WeM-4 Rational Design of Fluoroalkyl-Free Liquid-Repellent Coatings Accessed via Photoinitiated Chemical Vapor Deposition (piCVD)**, ***Camryn Payne***, *Sejin Choi, Aruzhan Abdikadyrova, Trisha Andrew,* UMass Amherst

Liquid-repellent thin-film coatings are an integral part of multiple high-demand, high-volume products and industries, including food and cosmetics packaging, garments and technical textiles, membranes/separations and microelectronics encapsulation. Until recently, the pervasive molecular engineering paradigm for creating rugged and high-performing liquid-repellent thin-film coatings was to use oligomers and/or polymers formed from long fluoroalkyl chain-containing monomers. Growing knowledge about the destructive long-term health and environmental consequences of fluoroalkyl-containing compounds has motivated broad efforts in developing fluoroalkyl-free coatings for diverse applications. Polymer chemical vapor deposition (CVD) provides multiple compelling options for rugged thin-film coatings, particularly in situations where porous, textured, rough and/or nonplanar substrates need to be coated. Thermally-initiated polymer CVD (iCVD), where thermal decomposition of selected peroxides produces the species that initiates polymer/film growth, is the most common process used for polymer CVD, but it struggles to polymerize monomers containing silicon and/or silicone moieties, which are touted as the most likely contenders for fluoroalkyl-free liquid-repellent coatings. We will describe a photoinitiated chemical vapor deposition (piCVD) process that uses UV-blue light to effect a Norrish Type I/II decomposition of a carbonyl species to initiate polymerization and film growth. We will present our chemically informed framework for monomer, crosslinker, and photoinitiator selection and discuss correlations between reactant properties, polymer/film growth behavior and resulting coating performance. Through systematic variation of monomer structure, crosslinker length, and deposition parameters, the influence of chemical structure on film morphology and performance is evaluated. As expected, monomer identity strongly influences the liquid repellent properties of coatings formed on diverse substrates, including cotton gauze, paper, and glass. A champion hydrophobic coating will be described, created via piCVD using a branched silicone-containing acrylate monomer, that affords a high water contact angle of 112.7o on paper and selected textiles.

9:00am **TF1-WeM-5 Designing Functional Polymer Thin Films via Initiated Chemical Vapor Deposition**, ***Stefan Schröder***, Kiel University, Germany **INVITED**

Functional polymer thin films play an increasingly important role in tailoring surface and interfacial properties for applications ranging from electronics to biomedical systems. Precise control over film thickness, surface chemistry, and coating conformality is essential for engineering functional interfaces at the nanoscale. Solvent-free initiated chemical vapor deposition (iCVD) provides a versatile platform for polymer thin film fabrication by avoiding dewetting and surface tension effects commonly associated with solution-based approaches. The process enables conformal deposition of polymer coatings with nanoscale thickness control on large-area substrates and complex surface geometries, while preserving delicate substrates through room-temperature processing. Particular emphasis will be placed on the relationship between surface chemistry, deposition conditions, and film growth mechanisms, including recent insights into interfacial reaction pathways. The talk further highlights the broad applicability of iCVD-derived thin films in surface functionalization, sensing, biomedical interfaces, and electronic devices.

9:30am **TF1-WeM-7 Kinetically Defined Radical Quenching Window for Area-Selective Photoinitiated Chemical Vapor Deposition (AS-PiCVD)**, ***Junjie Zhao***, Zhejiang University, China

Self-aligned polymer thin-film patterning is increasingly important for heterogeneous device integration, yet vapor-phase radical polymerization often produces nonselective coatings once active species are generated. Our recent efforts have addressed this challenge through confining radical generation on target surfaces. Photocatalytic surface-initiated CVD (PS-iCVD) enabled localized radical formation on photocatalytic TiO_2 surface for area-selective polymer growth[1], while visible-light-initiated CVD (VLiCVD) further demonstrated enhanced selectivity on FeOx surface by reducing monomer photolysis in the vapor phase under 420 nm irradiation[2].

Building on these advances, we report an area-selective photoinitiated CVD (AS-PiCVD) strategy governed by kinetic modulation rather than growth-surface activation alone. Using glycidyl methacrylate (GMA) as both monomer and photolytic radical source under 365 nm irradiation, we established a mathematical kinetic model showing that pGMA deposition follows an apparent second-order dependence on surface-adsorbed monomer concentration. This model links monomer adsorption, photolytic radical generation, chain propagation, and burial-mediated termination, providing a quantitative basis for controlling PiCVD growth. We indentified the kinetic conditions when pGMA growth is sustained on dielectric surfaces while Au suppresses deposition through radical quenching. The resulting AS-PiCVD process achieves self-aligned pGMA patterns on SiO_2/Au, Al_2O_3/Au, and TiO_2/Au substrates, with selectivity over 90% maintained at polymer thicknesses of tens of nanometers. This work advances light-mediated polymer CVD toward kinetically programmed, all-dry, and maskless fabrication of functional polymer patterns.

[1] Y. Shen, X. He, W. Meng, X. Huang, P. Cai, Z. Yang,W. Du, X. Zhang, Y. Luo, J. Zhao. Visible-Light-Driven Sustainable Chemical Vapor Deposition of Polymer Films and Patterns. *Small*, **2025**, *21* (23), 2502586.
[2] Y. Shen, M. Qiu, X. Huang, W. Du, X. He, Y. Luo, Z. Yang, J. Zhao. Photocatalytic Surface Initiation for Area-Selective Chemical Vapor Deposition of Polymer Thin Film. *ACS Materials Letters*, **2024**, *6*, 4058-4065.

9:45am **TF1-WeM-8 Development of Vapor-Imprinted Polymers for Food Spoilage Monitoring via Selective Acetoin Detection**, ***HUIDA DUAN***, *Ze Zong, Jacob Lahne, Rich Helm, Haibo Huang, Sean O'Keefe, Wei Zhou, Yifan Cheng,* Virginia Tech

Real-time monitoring of food spoilage is essential for improving supply-chain management and reducing food waste. Volatile organic compounds released during microbial metabolism and chemical degradation provide molecular signatures of spoilage. However, reliable detection remains challenging because many spoilage-associated volatiles occur at trace levels and coexist with structurally similar interferents. Molecularly imprinted polymers (MIPs) offer a route toward selective vapor recognition, but their solvent-based synthesis and complex post-processing limit their integration into miniature or packaging-compatible sensors. Here, we introduce vapor-imprinted polymers (VIPs) fabricated by initiated chemical vapor deposition (iCVD) as solvent-free, one-pot sensing layers for detection of acetoin, a representative spoilage-related volatile. Acetoin-imprinted poly(ethylene glycol dimethacrylate) films were directly integrated with surface-enhanced Raman scattering (SERS) substrates, enabling vapor-phase molecular recognition without solution processing or template extraction. The binding response of VIPs toward acetoin and the structurally related interferent butanedione was evaluated by SERS and analyzed using principal component analysis (PCA) and partial least squares discriminant analysis (PLS-DA). Compared with non-imprinted polymer controls, VIPs exhibited markedly enhanced recognition of acetoin at 10 ppb, increasing classification sensitivity from 74.4% to 92.4% and specificity from 76.4% to 94.4%. Preliminary interference studies further indicate that VIPs retain a stronger response toward acetoin than non-imprinted controls, including in the presence of butanedione, suggesting improved target recognition under chemically complex vapor environments. This work highlights the potential of VIP–based sensing layers for enabling real–time, selective monitoring of food spoilage in packaging systems.

Thin Films
Room 317 - Session TF2-WeM
VSHOP Applications II, Semiconductor Manufacturing

Moderators: Dr. Jeffrey Elam, Argonne National Laboratory, **Dr. April Jewell**, Jet Propulsion Laboratory

11:00am **TF2-WeM-13 Molecular Layer Deposition of Polyurea Film and their Role in Sidewall Passivation during Reactive Ion Etching in HF Plasmas**, ***Sumit Agarwal***, Colorado School of Mines **INVITED**

Over the last few years, HF-containing plasmas have been widely used for etching of Si-based dielectrics for various applications, including in the fabrication of 3-D NAND memory devices. During SiN_x etching with HF plasma, ammonium fluorosilicate (AFS) forms as a transient byproduct significantly influencing the etch behavior. While AFS formation during SiN_x etching has been known for several decades, the underlying mechanism for its formation and removal remains unclear. In this study, we have used *in situ* attenuated total reflection Fourier-transform infrared spectroscopy to study the changes in the chemical boning on the SiN_x surface during reactive ion etching, along with the AFS formation and removal dynamics. We will show that a thin polyurea layer grown conformally by molecular layer deposition can be used to protect the sidewalls during etching of SiO_2/SiN_x stacks in high-aspect-ratio structures. We will demonstrate the

impact of the MLD film on etching of the underlying SiN_x and SiO_2 films in a direct versus remote HF plasma, and HF gas. We will also show how the polyurea film degrades in a plasma environment and how it influences the formation of AFS.

11:30am **TF2-WeM-15 Realizing Controlled Porosity in Atomic Layer Deposited Metal Oxides**, ***Nicholas Strandwitz,*** Lehigh University

Atomic and molecular layer deposition (ALD, MLD) techniques boast precise control of film thickness, conformal growth, and a wide range of material compositions.Generally, ALD and MLD thin films are non-porous, yet introduction of porosity would enable a wide range of uses ranging from catalysis to low-k dielectrics for electronics.Here, we have examined the purposeful inclusion of organic molecules including bifunctional and monofunctional alcohols during the MLD/ALD process and their subsequent removal using thermal and/or UV treatment to induce porosity.We examined the evolution of various physical and electrical properties with thermal treatment as well as the composition of these films.We found that the density and dielectric constant of these materials are smaller than the parent dense ALD oxides.This strategy is thus promising for tailor made dielectrics based on sequential self-limiting surface reactions characteristic of the ALD and MLD processes.This development parallels other methods for forming porous inorganic oxides such as terpinene inclusion in silicon-based dielectrics or block copolymer templating of inorganic solids.

11:45am **TF2-WeM-16 Coordination-Driven Ambient Infiltration of Silicon and Germanium Precursors for the Synthesis of Polymer–Inorganic Hybrid Materials**, ***Shaghayegh (Poppy) Abtahi,*** Iowa State University

Block copolymer (BCP) self-assembly offers a scalable route to nanoscale pattern generation; however, pattern transfer remains one of the most significant challenges limiting its adoption in semiconductor manufacturing. While self-assembled polymer morphologies can be readily formed, translating these patterns into functional materials typically requires additional steps such as selective polymer removal and metal deposition to generate etch-resistant inorganic features. These approaches often involve elevated temperatures, highly reactive precursors, or multi-step processing, which constrain materials compatibility and process flexibility. Here, we demonstrate a coordination-driven vapor infiltration approach that directly forms inorganic hard masks at room temperature and atmospheric pressure. Poly(4-vinylpyridine) (P4VP) selectively reacts with volatile Group-14 precursors, including chlorosilanes and chlorogermanes, through N→Si coordination, producing polymer–inorganic hybrids without thermal activation or vacuum cycling. Solid-state 29Si NMR, FTIR, and Raman spectroscopy confirm the formation of hypercoordinate silicon species confined within the polymer matrix. This chemistry is applied to PS-b-P4VP block copolymer thin films, where infiltration occurs exclusively within the P4VP microdomains. Selective reinforcement of these domains enables the formation of metalloid-based inorganic hard masks that preserve the native morphology after removal of the organic template. Because the inorganic mask is generated during infiltration, the process simplifies pattern transfer and avoids the thermal budgets and precursor limitations associated with conventional ALD-based infiltration methods.

12:00pm **TF2-WeM-17 Negative-Tone PMMA-InOx Hybrid Resist Prepared by Sequential Infiltration Synthesis**, ***Jiwoong Ham,*** *Minkyung Ko, Young Heon Kim,* Chungnam national university, Republic of Korea*; Hyeong-U Kim,* Korea Institute of Machinery and Materials, Republic of Korea*; Nari Jeon,* Chungnam national university, Republic of Korea

As the semiconductor industry demands ever-smaller critical dimensions, extreme ultraviolet (EUV) lithography has become essential for next-generation patterning. However, conventional organic resists suffer from poor sensitivity under EUV exposure; therefore, hybrid resists have emerged as a promising strategy to address this challenge. In this work, we prepared a hybrid resist via sequential infiltration synthesis (SIS) into poly(methyl methacrylate) (PMMA) using trimethyl indium and trimethyl gallium as metal precursor, with water and ethylene glycol as co-reactants. Due to the scarcity of EUV light sources, electron beam lithography (EBL) was employed as a surrogate tool to evaluate resist performance. Compared to pristine PMMA, SIS resists exhibit improved sensitivity for negative tone behavior and achieve high-resolution patterning down to sub-50 nm linewidth. To investigate the mechanism of improved sensitivity, μ-Raman spectroscopy, μ-X-ray photoelectron spectroscopy, scanning transmission electron microscopy, and electron energy loss spectroscopy were employed. Based on the comprehensive characterization data, we propose molecular-level structural model of the PMMA–InO_x hybrid resist that explains its enhanced sensitivity.

The Future of Temperature Sensing
Room 320 - Session TS-WeM

The Future of Temperature Sensing II

Moderators: Dr. Graham Machin, NPL, **Dr. Stephan Krenek**, PTB

8:00am **TS-WeM-1 Utilizing the SI Redefinition and "NIST on a Chip" to Ensure Readiness Across the United States Air Force, Army, and Navy**, ***Jeremy Latsko,*** United States Air Force Metrology and Calibration **INVITED**

The U.S. military's metrology and calibration programs rely on a complex global calibration chain that is prone to disruption, posing a risk to military readiness. To mitigate these vulnerabilities, the Air Force, Army, and Navy are investing in advanced technologies, particularly Quantum-Based Intrinsically Accurate Technology (QB-IAT). This technology is enabled by the 2019 redefinition of the International System of Units (SI) and the "NIST on a Chip" program. QB-IAT reduces reliance on the traditional calibration chain by providing intrinsic accuracy based on fundamental physical constants. By implementing QB-IAT, the military has the potential to decrease equipment damage, improve measurement confidence, and ensure operational readiness at the point of use. This paper details the military's strategy to integrate these quantum-based technologies, encourages industry partnership for commercialization, and provides an overview of currently funded projects.

8:30am **TS-WeM-3 Air Force Temperature Metrology and Photonic Thermometer Applications**, ***Kaleb Reed,*** Air Force Research Lab

Temperature sensing devices in Air Force inventory are required to be calibrated to ensure operational readiness and effectiveness. To do this there is a long calibration chain of increasingly accurate thermometers providing traceability and accuracy. Existing platinum resistance thermometers (PRTs) are a key part of that chain. However, they are fragile, prone to drift, and require labor-intensive calibrations.

Photonic thermometers could be able to match PRT accuracy while being more robust, stable, and having longer calibration intervals. The successful introduction of photonic thermometer technology would reduce or eliminate the calibration chain for thermometers in the USAF. This presentation will discuss how the USAF Temperature Metrology Program could benefit from accurate, stable, and more robust thermometers to increase readiness.

8:45am **TS-WeM-4 The Standard Photonic Thermometer (SPoT) program at NIST**, *Pavan Challa, Michal Chojnacky, Kevin Douglass, Thinh Bui, Klaus Quelhas, Daniel Barker, Nazanin Hoghooghi, Franklyn Quinlan,* ***Nikolai Klimov,*** National Institute of Standards and Technology (NIST)

Temperature underpins modern technology, and resistance thermometers remain the primary means of realizing the SI kelvin. However, their inherent limitations – most notable calibration drift over time and the resulting need for frequent recalibration – have motivated the search for alternative approaches such as integrated photonic thermometry.Photonic thermometry offers a compelling alternative, but practical adoption has been limited by the lack of packaged, infrastructure–compatible systems that combine SI–traceable interrogation, a rigorous uncertainty framework, and millikelvin–level performance. Achieving this combination is necessary for photonic sensors to serve as viable metrological replacements for resistance standards.

Building on these needs, The Standard Photonic Thermometer (SPoT) program at NIST is developing a chip–scale, SI–traceable temperature standard that overcomes the drift, fragility, and calibration burdens of resistance–based thermometry. SPoT leverages integrated silicon photonics to realize narrow linewidth resonant structures whose temperature–dependent optical frequency response provides a stable and reproducible thermometric signal. This presentation will provide an overview of the SPoT program, including device–level design, advanced packaging approaches, and the frequency–metrology framework that defines the absolute frequency scale for SPoT thermometry.

9:00am **TS-WeM-5 From SPRT Comparison to SI-traceable Photonic Thermometry with SPoT**, ***Michal Chojnacky,*** *Pavan Challa, Kevin Douglass, Thinh Bui, Klaus Quelhas, Frank Quinlan, Alessandro Restelli, Nikolai Klimov,* National Institute of Standards and Technology (NIST)

Photonic thermometry offers a promising alternative to resistance-based temperature sensing, but its adoption for precision metrology requires an SI-traceable relationship between optical frequency and temperature. We present the initial metrological evaluation of the Standard Photonic Thermometer (SPoT), a fully packaged silicon microring-resonator thermometer designed for use in conventional thermometric baths and

fixed-point-cell infrastructure. Using four months of side-by-side measurements with a calibrated standard platinum resistance thermometer (SPRT) over 10 °C to 90 °C, we developed SI-traceable calibration functions relating SPoT resonance frequency to temperature and evaluated the uncertainty contributions associated with the comparison. The SPoT resonance frequency was measured using two independent interrogation methods: resonance scanning and offset-sideband laser locking. The uncertainty framework includes contributions from the SPRT reference measurement, bath stability and uniformity, frequency-axis determination, resonance peak fitting, and offset-lock noise, yielding combined standard uncertainties of 1.67 mK and 2.61 mK for resonance scanning and offset-sideband locking, respectively. The uncertainty budget identifies key limitations from both the reference temperature environment and the offset-lock readout, highlighting clear pathways for improvement through fixed-point-cell measurements, frequency-comb-based metrology, and alternative interrogation systems. This work establishes the calibration-function and uncertainty-analysis framework that supports ongoing efforts toward practical, deployable, SI-traceable photonic temperature measurement.

9:15am **TS-WeM-6 Optical Frequency Comb Metrology for Assessing the Ultimate Stability of SPoT in a Water Triple-point (WTP) Cell**, ***Thinh Bui***, *Pavan Challa, Michal Chojnacky, Kevin Douglass, Nikolai Klimov,* NIST-Gaithersburg

Reliable and long-term measurement of SI-traceable temperature is a fundamental challenge due to drifts in standard, calibrated resistance-based thermometers. The Standard Photonic Thermometer (SPoT) is a chip–scale, SI–traceable thermometry platform that has potential to achieve long-term stability and high accuracy. Using an optical frequency comb stabilized to an ultra-stable cavity reference, we determine the ultimate temperature accuracy and precision of SPoT, only limited by the stability of the water triple-point (WTP) cell rather than the optical reference. We report on SPoT's long-term stability and reproducibility in a WTP cell using our frequency comb-based methodology.

9:30am **TS-WeM-7 Dual Mode-Locked Comb Readout Method for Chip-Scale Silicon Photonic Thermometer**, ***Nazanin Hoghooghi,*** NIST-Boulder*; Pavan Challa, Nikolai Klimov,* NIST-Gaithersburg

We present a dual mode-locked laser comb-based readout method for Standard Photonic Thermometer (SPoT), a chip-scale silicon photonic thermometer platform. In this work, we demonstrate how fiber mode-locked frequency combs enable a tunning-free, SI-traceable optical readout method for SPoT devices with no moving parts. The broad bandwidth and high resolution of the combs allow precise detecting of SPoT resonance-frequency shifts over a wide temperature range and with high sensitivity.

In our experiments, two self-referenced fiber frequency combs centered at 1550 nm, with slightly different repetition rates, are used to probe and track the SPoT resonance transmission spectrum. Light from fiber mode-locked combs is optically filtered and coupled into a fiber-coupled SPoT device. The SPoT chip is hermetically sealed in a miniature metal capsule and placed in a drywell capable of providing a stable temperature environment. Using the dual-comb readout system, we track SPoT resonance-frequency shift over -25°C to 140°C range. The dual–comb readout exhibits sensitivity at ≈ 200 MHz–level; however, in the present setup the achievable temperature–measurement resolution is primarily limited by the drywell stability (≈ 20 mK), rather than by the SPoT device or the comb–based readout.

9:45am **TS-WeM-8 Developing Portable Tools for Photonic Thermometry**, ***Kevin Douglass***, NIST-Gaithersburg*; Michal Chojnacky, CH. S. S. Pavan Kumar, Thinh Q Bui, Nikolai Klimov,* NIST

As part of the photonic thermometry program at NIST we are developing a Standard Photonic Thermometer (SPoT) as a drop-in replacement for resistance-based thermometry devices.One of the major challenges of this program is to make the system portable and to minimize costs.To achieve this goal, we are developing new optical readout tools based on high accuracy optical frequency metrology to interrogate the temperature dependent frequency shifts of the SPoT.We have combined a broadband rapidly sweeping laser with a gas cell and etalon to provide an absolute frequency axis with high precision.We demonstrate measurement repeatability over a range of 20 °C to 80 °C of nearly 10 mK.This approach also gives us the ability to track multiple modes of the ring resonator simultaneously, which can be used to determine the free spectral range and group index, n_g, as a function of temperature. Recent results will be reported along with potential pathways to further improve the accuracy and precision of the portable readout methodology.

11:00am **TS-WeM-13 A Lighter Footprint: The Evolution of Ring-Resonator Thermometer Design at NRC**, ***Sergey Dedyulin***, *Siegfried Janz, Dan-Xia Xu, Ross Cheriton, Shurui Wang, Martin Vachon, John Weber,* National Research Council Canada **INVITED**

Over the past decade, ring-resonator thermometers have emerged as promising candidates for high-accuracy temperature metrology, offering small footprint, resistance to electromagnetic interference, and on-chip photonic integration. At the National Research Council Canada, our work over the past several years has focused on evaluating the metrological performance of these devices and on understanding how resonator design and packaging influence measurement accuracy and long-term stability.

This presentation traces the evolution of silicon ring-resonator thermometer design at NRC, from early prototype characterization to the development of smaller and lower-uncertainty implementations. During this time, we characterized the short- and long-term stability of the ring-resonator thermometer in a stirred liquid bath between 20 °C and 80 °C, investigated various packaging options, measured the influence of self-heating, optimized the interrogation methods, tested the resolution and time response, varied the gas atmosphere, and created the full uncertainty budget for the packaged RR thermometer. The combined 10-mK standard uncertainty was found to be consistent with the repeatability reported previously for an unpackaged device and includes a long-term stability component evaluated over the course of 3 years. The presentation draws parallels with the development of the platinum resistance thermometer and concludes with an outlook on the remaining challenges toward routinely achieving millikelvin-level accuracy.

11:30am **TS-WeM-15 Chip-Based Photonic Thermometers: In-Situ Calibration and Si Traceability**, ***David Pabst***, *Daniel Schmid, René Eisermann, Bruno Rohloff, Stephan Krenek,* Physikalisch-Technische Bundesanstalt (PTB), Germany

Highly integrated lab-on-a-chip applications such as on-chip optical clocks or ion traps require integrated temperature sensors, as many of these applications are sensitive to temperature, so accurate temperature control is essential for high-level scientific and industrial applications. Yet conventional electronic thermometers based on platinum resistance or thermocouples face fundamental limitations in mechanical stability and immunity to electromagnetic interference. Chip-based photonic temperature sensors, which exploit the temperature dependence of the resonance wavelengths of ring resonators and Bragg gratings, are emerging as a compelling alternative in many applications. Lab-on-a-chip applications in particular require integrated temperature sensors, as many of these applications are influenced by temperature and therefore require temperature-dependent corrections.

A major factor in the practical implementation and design of ring resonator and Bragg-grating-based photonic thermometers is the development of a data acquisition and processing method that combines accurate in-situ determination of the circuit's resonance wavelengths
with a high acquisition speed in a small form factor. Additionally, traceability to the International System of Units (SI) is required to guarantee long-term comparability and absolute accuracy. This requires very stable wavelength determination schemes or in-situ calibration with each measurement. As part of the pan-European PhoQuS-T project, we designed and manufactured Si- and SiN-based photonic integrated circuits as temperature sensors. They were packaged for use with the temperature calibration infrastructure of the PTB (the German National Metrology Institute). We developed novel techniques based on a multi-peak fit model, with which we achieve accurate in-situ calibration over a span of 100 nm while maintaining a high acquisition speed. This includes SI traceability to different reference gas cells, as well as advanced data analysis for temperature determination.

In this work, we will present our findings on the implementation of these methods and compare them with current state-of-the-art approaches under realistic thermometer calibration conditions.

11:45am **TS-WeM-16 Band-Edge Optical Microthermometers for Ultrahigh-Resolution Temperature Sensing**, ***Alex Shoghi Tekmedash***, *Amin Reihani,* Rutgers University

Ultrahigh-resolution thermometry at room temperature is critical for emerging applications in bio-calorimetry, bolometry, infrared imaging, and characterization of electronic, optoelectronic, and quantum devices. In this presentation, we discuss the development and future scaling of optical

microthermometers based on semiconductor band-edge thermoreflectance. We first present a GaAs band-edge microthermometer that utilizes the strong temperature dependence of optical absorption near the semiconductor band edge. Using a suspended asymmetricFabry–Pérot resonator and a wavelength-stabilized probe laser, the device achieves at hermoreflectance coefficient exceeding 30 K^{-1}, enabling a thermometry noise floor ofapproximately 60 nK.Hz $^{-1/2}$ and sub-100 nK temperature resolution at room temperature. We then discuss how multilayered nanostructures can further miniaturize band-edge thermometers while simultaneously enhancing sensor sensitivity. These advances establish new opportunities for high-resolution thermal metrology at the microscale.

12:00pm **TS-WeM-17 Quantitative Temperature Mapping with Nanometric Resolution***, Rituparna Mohanty,* ***Amin Reihani,*** Mechanical and Aerospace Engineering, Rutgers University

Quantitative nanoscale thermal imaging is critical for understanding energy transport and dissipation in emerging technologies, including nanoelectronics, plasmonics, quantum systems, and high-frequency microelectronics. In this presentation, we discuss recent advances in scanning thermal microscopy (SThM) techniques that enable quantitative mapping of both lattice and electron temperature fields with nanometric spatial resolution under practical operating conditions. First, we present Contact Resistance-Resolved Scanning Thermal Microscopy (CR-SThM), a technique capable of quantitatively mapping unmodulated surface temperature fields while simultaneously resolving the local tip–sample thermal resistance. Using custom-fabricated scanning thermal probes with integrated heater/thermometers and sharp tips (~25 nm radius), the approach achieves ~7 nm spatial resolution and ~50 mK temperature resolution in a 1 Hz bandwidth. By introducing a modulated heat input to the probe and measuring both AC and DC thermal responses, CR-SThM enables accurate thermometry even in the presence of strong topography-dependent variations in thermal contact resistance. We then present Electron-Scanning Thermal Microscopy (E-SThM), a novel technique for imaging nonequilibrium electron temperature distributions on conductive surfaces. The method employs a metal–insulator–metal tunneling junction formed using a Pt-coated thermal probe with an ultrathin Al_2O_3 tunneling barrier. Variations in electron temperature modify the tunneling current through broadening of the Fermi–Dirac distribution, enabling nanoscale mapping of hot-electron transport with sub-kelvin sensitivity. Together, these techniques provide powerful new capabilities for probing coupled thermal and electronic nonequilibrium phenomena at the nanoscale.

2D Materials
Room 304 - Session 2D-WeA
Surface-Sensitive Techniques for 2D Materials Characterization

Moderators: Qiong Ma, Boston College, **Dr. Chris Jozwiak**, Advanced Light Source, Lawrence Berkeley National Laboratory

2:15pm **2D-WeA-1 Exploring and Manipulating Charge Density Textures in Tas2 with NanoARPES***, **Chris Jozwiak**,* Advanced Light Source, Lawrence Berkeley National Laboratory **INVITED**

The ability to directly probe electronic structure in energy-momentum space with surface sensitivity makes ARPES a critical spectroscopic tool for studying 2D materials. Adding spatial resolution capabilities to its arsenal greatly expands the range of material systems and phenomena that can be impacted by nanoARPES. I will give an overview of this technique at the MAESTRO beam line at the Advanced Light Source, where we aim to maximize impact across the 10 um to 100 nm scales by enabling various *in operando* measurements. I will present measurements of 1T-TaS_2, a prototypical quasi-2D transition metal dichalcogenide that hosts a series of charge density wave phases and associated electronic phenomena. Although a classic target of ARPES experiments for decades, this scale of spatial resolution enables insights into the electronic textures in real- and momentum-space that form in this system. I will discuss these, with a particular focus on measurements of the metastable “hidden” state that can be created with electrical currents and ultrafast optical pluses.

2:45pm **2D-WeA-3 Visualization of Tunable Electronic Structure of Monolayer $TaIrTe_4$***, **Sandy Adhitia Ekahana**, Aalok Tiwari,* Carnegie Mellon University*; Souvik Sasmal,* Argonne National Laboratory*; Zefeng Cai, I-Hsuan Kao, Ravi Kumar Bandapelli,* Carnegie Mellon University*; Jian Tang,* Boston College*; Chenbo Min,* Carnegie Mellon University*; Tiema Qian,* UCLA*; Kenji Watanabe, Takashi Taniguchi,* NIMS (National Institute for Materials Science), Japan*; Ni Ni,* UCLA*; Qiong Ma,* Boston College*; Chris Jozwiak, Eli Rotenberg, Aaron Bostwick,* ALS-LBNL*; Simranjeet Singh, Noa Marom, Jyoti Katoch,* Carnegie Mellon University

The advent of *in operando* angle-resolved photoemission spectroscopy (ARPES) has unlocked new capabilities for dynamically tuning and visualizing electronic band structures. The success of this progress has been largely coupled by the recent advancements in the van der Waals heterostructure device stacking. Among the diverse transition metal dichalcogenide (TMDC) family, monolayer $TaIrTe_4$ is of particular interest due to previous transport measurements suggesting it hosts a dual quantum spin Hall state [1]. Here, we present *in operando* ARPES measurements on monolayer $TaIrTe_4$ devices, revealing an asymmetric electronic response to electrostatic gating. Hole doping via a negative back-gate voltage exhibits expected behavior by depleting the states near the Fermi level. Conversely, inducing electrons via positive gating does not result in the anticipated filling of the monolayer $TaIrTe_4$ upper band. Further intentional electron doping through *in situ* alkali surface dosing reveals further resistance to this Fermi level rigid shifts stems from an intrinsic band gap in monolayer $TaIrTe_4$, as suggested by our density functional theory (DFT) calculations utilizing the HSE hybrid functional [1]. We observe that this gap gradually closes as the electron concentration increases, pointing to strong electron interactions that dynamically modify the band structure. In conclusion, this study demonstrates that the conventional single-electron picture of rigid band shifting is insufficient to describe the complex band evolution observed during *in operando* ARPES.

[1] S. A. Ekahana *et al.*, "Visualization of tunable electronic structure of monolayer $TaIrTe_4$," *arXiv preprint*, arXiv:2601.11504 (2026)

3:00pm **2D-WeA-4 Substrate Driven Electronic Reconstruction in Bilayer Graphene***, **Aalok Tiwari**,* Carnegie Mellon University, USA, India*; Sandy Adhitia Ekahana, Souvik Sasmal,* Carnegie Mellon University, USA*; Liangtao Peng,* Washington University, St. Louis*; Pratik Saud,* Carnegie Mellon University, USA*; Syeda Faiza Rubab Sherazi,* University of Central Florida*; Ravi Kumar Bandapelli,* Carnegie Mellon University*; Duy Le,* University of Central Florida*; Rahul Rao,* Air Force Research Laboratory, Materials and Manufacturing Directorate, USA*; I-Hsuan Kao,* Carnegie Mellon University, USA*; Chris Jozwiak, Eli Rotenberg, Aaron Bostwick,* Advanced Light Source, Lawrence Berkeley National Laboratory*; Talat S Rahman,* University of Central Florida*; Simranjeet Singh,* Carnegie Mellon University, USA*; Shaffique Adam,* Washington University, St. Louis*; Jyoti Katoch,* Carnegie Mellon University, USA

The electronic and optical properties of two-dimensional van der Waals material systems are intimately tied to stacking configuration and sublattice arrangement. Interface engineering through substrate interactions, layer alignment and twist angle, offers a powerful route to design and manipulate electronic correlations. In this talk, I will use angle-resolved photoemission spectroscopy with micron sized spatial resolution (microARPES) to present direct evidence that substrate interactions and twist angle can dramatically modify the electronic band structure of bilayer graphene (BG). First, I will discuss our result of tuning the electronic structure of BG when interfaced with two distinct van der Waals substrates: hexagonal boron nitride (hBN), a wide-gap semiconductor, and α-$RuCl_3$, a Mott insulator, on the same sample. In the pristine heterostructure, differential charge transfer in the BG/hBN and BG/$RuCl_3$regions induces spatially modulated doping, forming an atomically sharp lateral p–p† junction. We observe a flattened valence band tip in BG on hBN, while BG on $RuCl_3$ exhibits strong hole doping. Upon electron doping via alkali-metal deposition, we access the conduction band in the heterostructure and observe that BG on hBN develops a ~0.4 eV band gap, while BG on $RuCl_3$ retains robust semimetallic in-gap states. These findings establish that substrate interactions modify BG's intrinsic ground state. Next, I will explore what occurs when graphene or BG is aligned with hBN at 0° or 30° along the high-symmetry Γ–K direction. At specific alignments, we observe flat bands away from the Fermi level whose dispersion is tunable via perpendicular electric field and strongly dependent on graphene–hBN relative orientation. These results demonstrate that substrate selection and layer alignment together provide a powerful basis for achieving correlated electronic phases in graphene-based heterostructures, opening pathways toward functional quantum devices in interface-tunable van der Waals systems.

3:15pm **2D-WeA-5 Interpreting Strain in X-Ray Photoelectron Spectroscopy Measurements of Two-Dimensional Materials***, **Muhidul Chaman**, Nargol Jalali, Michelle Becerra, Joy Roy, Joslin Prasanna,* The University of Texas at Dallas*; Paul Bagus,* The University of North Texas*; Rafik Addou, Cormac Toher, Kevin Brenner,* The University of Texas at Dallas

Strain is a common modification to two-dimensional (2D) materials. Their atomic thinness allows them to be strained from growth, interactions with substrates, and virtually all processing steps used to fabricate them into devices. As such, it is important to properly interpret strain in almost all characterizations of 2D materials. While the effects of strain are well understood for vibrational or valance electron spectroscopies, they are not well understood for core electron spectroscopies like X-ray photoelectron spectroscopy (XPS). In fact, the effects of strain on XPS measurements have been a longstanding challenge for many materials. This is partially due to the extreme difficulty in quantitatively computing core electron binding energies (BEs) compared to vibrational and electrical dispersions. This is problematic as the interpretation of XPS measurements requires reference peaks. As such, the lack of experimental and computational insights into the relationships between strain and core BEs significantly hinders the application of XPS measurements to 2D materials. We present the first XPS measurements that directly investigate the relationships between strain and core BEs in 2D (monolayer) MoS_2. These XPS measurements applied controlled strain by bending MoS_2 on a flexible substrate. The strain was then quantified using Raman spectroscopy and photoluminescence. We found the Mo $3d_{5/2}$ BE shifted by 0.19 eV and the S $2p_{3/2}$ BE also shifted by 0.11 eV in position per percentage of applied strain. These shifts are both significant (comparable to shifts from other physical and chemical phenomena) and counterintuitive to a simple electrostatic model that would predict opposite shifts. This suggested that there are changes in the core orbital distributions that offset the electrostatic effect. These shifts were investigated with density functional theory and proposed to arise from strain changing the bond distances, which changes the crystal and

ligand fields acting on the core orbitals. These measurements provide insights into the fundamental relationships between strain and core BEs and enable better interpretation of XPS measurements of 2D materials where strain is prolific.

3:30pm **2D-WeA-6 Electrical-XPS: A Novel Research Tool for Organic and Biological Materials**, ***Hagai Cohen***, The Weizmann Institute, Israel

XPSapplications to bio/organic systems encounter critical inherent challenges, in particular with those structural nuances that enrich functional diversity in biology. However, surprisingly effective answers can be gained by probing the electrical properties of specimens using an XPS-based technique, the chemically resolved electrical measurements (CREM). [1,2] A recent review focuses on this branch of electrical-XPS applications. [3]Challenges and their proposed answers are discussed, including specimens' limited stability, charging artifacts and, importantly, the typical XPS 'blindness' to key features of organic architectures. Among the unique capabilities demonstrated are the evaluation of monolayers' integrity, hydrogen-bond formation and structure-function relationships. Starting from small molecules up to relatively large supramolecular sugars and proteins, the CREM-XPS approach offers particularly attractive capabilities and a template for advanced characterization strategies.

References

1. I. Doron Mor et al., "Controlled Surface Charging as a Depth Profiling Probe for Mesoscopic Layers", *Nature* **406**, 382 (2000).
2. H. Cohen, "Chemically Resolved Electrical Measurements using X-ray Photoelectron Spectroscopy", *Appl. Phys. Lett.* **85**, 1271 (2004).
3. M. Miali et al., "Electrical XPS Meets Bio: In-Situ Chemo-Electrical Sensing and Activation of Organic Materials", *Phys. Chem. Chem. Phys.* **27,** 19591 (2025).

4:15pm **2D-WeA-9 Scanning Probe Microscopy of Engineered Bound States on Semiconductor Surfaces**, ***Victor Brar***, University of Wisconsin - Madison **INVITED**

I will present recent scanning probe microscopy (SPM) measurements of synthetic defects with deep in-gap energy levels in semiconducting 2D materials. It will be shown how charged impurities on the surface of WSe_2 can be manipulated to form artificial "nuclei" with deep, long-range two-dimensional Coulomb potentials that trap quasiparticles in hydrogenic-like orbits. These states persist to high quantum numbers, with binding energies exceeding 600 meV, such that the lowest level changes its occupation. Using multiple SPM modalities in combination with theoretical modeling, these experiments provide chemical insight into color centers in 2D materials and enable the creation of localized states with exotic properties.

4:45pm **2D-WeA-11 Interplay of Silver-Mean Quasiperiodicity and Weyl Semimetallicity in WTe_2**, ***Daejin Eom***, *So-Dam Sohn, Ja-Yong Koo, Chang-Youn Moon,* Korea Research Instutue of Standards and Science (KRISS), Republic of Korea

Quasiperiodic potential modulation in topological materials has attracted growing interest due to the intriguing interplay between the disorder effects associated with quasiperiodicity [1,2] and the topological invariance of these materials [3,4]. However, experimental studies on this topic remain scarce. Here, we employ the scanning tunneling microscopy (STM) to investigate the formation of an intercalation layer in WTe_2, a three-dimensional Weyl semimetal. The intercalant molecules are long-chain aliphatic *n*-alkanes dissolved in an epoxy resin. During thermal treatment, these molecules intercalate into the WTe_2 crystal and self-assemble into an atomically flat lamellar layer. Notably, the intercalation layer exhibits slight topographic variations in the STM images, characterized by two distinct heights, denoted as *L* and *H*. This variation forms a self-similar, quasiperiodic pattern, which is best described by the Pell sequence associated with the silver mean, although the coherence is occasionally disrupted by phason defects. Furthermore, the quasiperiodic potential modulation induced by the intercalation layer enhances the surface conductance near the Fermi level while preserving the semimetallic nature of WTe_2. This finding provides a direct experimental verification of theoretical predictions regarding the effects of quasiperiodic potential modulation on topological Weyl semimetals.

[1] C. Janot, *Quasicrystals: A Primer* (Oxford University Press, New York, 1994).[2] *Quasicrystals*, edited by T. Fujiwara and T. Ogawa (Springer, Berlin, 1990).[3] M. Z. Hasan, and C. L. Kane, Colloquium: Topological insulators, Rev. Mod. Phys. **82**, 3045 (2010).[4] X.-L. Qi and S.-C. Zhang, Topological insulators and superconductors, Rev. Mod. Phys. **83**, 1057 (2011).

5:00pm **2D-WeA-12 Emergent Superparamagnetism in TiS_2 Induced by Atomic-Scale Defects**, *Thomas Pekarek, Patrick Keeney, Kyle Taylor, Cole Ratkus, Jason Haraldsen,* ***Paula Mariel Coelho***, University of North Florida

Defect engineering has emerged as a powerful route to induce and control magnetism in otherwise nonmagnetic two-dimensional materials [1]. Titanium disulfide (TiS_2), a layered transition metal dichalcogenide traditionally studied for energy storage and electronic applications, is nonmagnetic in its pristine form, making it an ideal platform to explore defect-driven magnetic behavior [2]. Here, we report the observation of superparamagnetism in bulk 1T-TiS_2 arising from clusters of intrinsic defects. In a comprehensive scanning tunneling microscopy (STM), superconducting quantum interference device (SQUID) magnetometry, and density functional theory (DFT) study, we identify Ti adatoms as the primary source of local magnetic moments [3]. SQUID measurements reveal a pronounced paramagnetic response, and a Brillouin fit yields an effective spin of 4. This surprisingly large magnetic response is consistent with cooperative clustering of Ti adatoms forming superparamagnetic centers. Atomically resolved STM images show a high surface concentration of point defects and well-defined triangular clusters, while DFT calculations confirm that both isolated Ti adatoms and small Ti clusters generate localized magnetic moments and enhanced collective magnetic responses. These results establish TiS_2 as a defect-tunable magnetic material, highlighting its potential for future application in spintronics.

[1]P.M. Coelho, J. Phys.: Condens. Matter **36** 203001 (2024)

[2]P. J. Keeney et al Nanomaterials **15**, 1435 (2025)

[3]T.M. Pekarek et al., under review (2026)

Advanced Microelectronic Materials and Devices Mini-Symposium
Room 318 - Session AM1+EM+TF-WeA

Industry Perspective

Moderators: Dr. Robert Grubbs, IMEC Belgium, **Dr. Sarah Lynch**, TEL Technology Center, America, LLC, USA

2:15pm **AM1+EM+TF-WeA-1 Memory Centric AI and the Role of Advanced Materials in Future Semiconductor Technologies**, ***Shivani Srivastava***, Micron Technology **INVITED**

The rapid growth of artificial intelligence (AI) is shifting system design from compute-centric to memory-centric architectures, where bandwidth, capacity, and energy efficiency increasingly determine performance. For AI workloads, the resulting memory bottleneck is creating new demands on semiconductor materials, processes, and integration schemes.

This talk will examine how these demands are influencing the future direction of advanced DRAM, High Bandwidth Memory (HBM), 3D and emerging nonvolatile memory technologies.

In DRAM, continued scalingis increasingly associated with efforts toward leakage reductions, variability minimization, and the exploration of novel integration schemes to optimize performance.

In parallel, industry trends toward increasing 3D DRAM layer counts are driving the need for high aspect-ratio etch and gap fill, conformal deposition, and high-quality epitaxial growth approaches.

While HBM, advanced CMOS integration, and heterogeneous packaging are becoming essential to reducing the compute-memory gap, thermal-mechanical reliability, power efficiency, and co-packaged optics are expected to play an increasing role in improving system-level performance.

Across these platforms, thin-film process control, conformality, interfaces, defect management, thermal-mechanical reliability, and system-level co-optimization are emerging as central levers for overcoming the AI memory wall.

2:45pm **AM1+EM+TF-WeA-3 Angstrom-Era Logic: From Nanosheets to Hybrid Bonding**, ***Biswajeet Guha***, Intel Corporation **INVITED**

Advanced microelectronics scaling has entered an era in which performance and density gains can no longer come from transistor miniaturization alone. Innovation now spans two tightly coupled fronts—front-end device architecture and advanced heterogeneous packaging—unified under the emerging paradigm of System Technology Co-Optimization (STCO). This talk presents a material-centric perspective on both, highlighting opportunities for the AVS community to contribute foundational research.

At the transistor level, the transition from FinFET to gate-all-around (GAA) nanosheet architectures, exemplified by angstrom-class nodes such as 18A, restores electrostatic control while introducing demanding materials challenges in high-k interfaces, work-function metals, and inner-spacers. Backside power delivery further reshapes the device stack, imposing new requirements on wafer thinning, through-silicon contacts, and thermal management, while contact and interconnect resistance remain critical bottlenecks demanding novel liner/barrier schemes and interface engineering.

Equally consequential are the materials challenges in advanced packaging, where scaling has shifted to the system level through heterogeneous integration. Fine-pitch hybrid bonding makes void-free Cu–Cu and dielectric–dielectric joining a surface-science problem governed by oxidation control, CMP dishing, and surface activation. Stacked high-power dies intensify the need for advanced thermal interface materials and careful management of CTE mismatch, while fine-line redistribution layers, low-loss dielectrics, underfills, and interposers each present challenges in adhesion, stress, and warpage.

By framing transistor and packaging innovation together through an STCO lens, this talk argues that the future of microelectronics depends on co-optimizing materials, processes, and architectures across the entire system—offering fertile ground for the surface- and materials-science community.

3:15pm **AM1+EM+TF-WeA-5 Epitaxial CVD Ruthenium for High-Performance Interconnects at A7 and Beyond**, ***Gyana Pattanaik,*** Tokyo Electron America

Ruthenium is projected to replace Cu in A7 node or beyond, likely bringing back subtractive integration that Cu replaced with damascene almost 3 decades ago. To enable this transition, integration of Ru interconnect metal lines and vias with lower resistivity need to be demonstrated. Ru thin films with very low resistivity (~8 μΩ-cm at 30nm; bulk =7.4 μΩ-cm) has been reported [1], by depositing epitaxial PVD Ru on Si (111) with buffer layers like AlN (001). Layer transfer approach has been proposed for integration of such epitaxial Ru [1]. PVD epi-Ru can be suitable for interconnect metal lines through patterning and direct metal etch. However, it may not be ideal for via, even though some integration approaches explore to use it. CVD via filling remains an attractive integration approach for via metal [2]. Here we demonstrate epitaxial CVD Ru for selective via filling (Fig 1).

In this study, we used epitaxial PVD Ru (6 and 8 nm)/AlN (001)/Si(111) as substrates for CVD Ru experiments conducted in a CVD reactor. A series of preclean steps was applied to eliminate surface oxides and refresh the surface before CVD Ru growth under different deposition conditions. Powder XRD patterns (2θ-ω scans) show only Ru (*00l*) peaks, indicating CVD Ru film growth along *c*-axis. Representative CVD Ru film growth is shown in Fig 2. Laue oscillations at the bottom of Ru (002) peak are signature of epitaxial film growth. The Ru (101) Φ-scans collected at c=61.3^{0} show six-fold symmetry (Fig 3), like the underlying PVD epi-Ru, further confirming epitaxial CVD Ru film growth [1]. This paper will summarize systematic studies of CVD Ru film growth on PVD epi-Ru and characterizations including microstructure and electrical properties.

References:

1. C. Adelmann et.al, Epitaxial Ruthenium for Advanced Interconnects, IITC (2025) P32.
2. M. H. van der Veen, et. al, Selective Deposition and Ruthenium Superfill Exploration Beyond A10 Node Interconnects, VLSI Symposium (2025), T18-3.

Keywords: Interconnects, Ruthenium, Epitaxy, CVD

Advanced Microelectronic Materials and Devices Mini-Symposium

Room 318 - Session AM2+EM+TF-WeA

Devices I

Moderators: Dr. Devika Choudhury, ASM, **Dr. Philip Lee**, University of Kentucky

3:30pm **AM2+EM+TF-WeA-6 Beyond Binary Erasure: Harnessing a Constrained RESET Operation for Analog Synaptic Plasticity in ReRAM**, ***Marius Orlowski,*** Virginia Tech

Neuromorphic computing overcomes von Neumann bottlenecks by co–locating memory and processing. Filamentary ReRAM and CBRAM are promising synaptic candidates due to compactness, non–volatility, and analog tunability, but conventional binary SET/RESET offers coarse control over conductance. This work reports a novel regime in Cu/TaO_x/Pt CBRAM—constrained RESET—where a compliance–limited RESET strengthens rather than ruptures the filament. For high–resistance filaments (R_{on} > 1 kΩ), constrained RESET reduces resistance up to tenfold, while robust filaments are unaffected, making the effect self–limiting and most useful for fragile states. The reconstruction of the Cu atom filament leads to reduced electric fields, reduced Joules heat, and reduced resistance, rendering this mechanism self-limiting. Electrostatic simulations show that a weak filament (truncated cone) concentrates electric field at its narrow tip (>1.6×10^{6} V/cm) under negative bias, driving Cu^{+} electromigration toward the constriction and forming a stable hourglass (double–cone) morphology. To harness this for analog weight control, we integrate the memristor with a series transistor operating in saturation, providing tunable compliance current (I_{cc}). Using pulse trains, we implement two programming techniques: (i) Incremental Step Pulse with Verify Algorithm (ISPVA), modified to stay below the rupture threshold, and (ii) Incremental Gate Voltage with Verify Algorithm (IGVVA), where gate voltage (hence I_{cc}) is incremented with fixed programming pulses. The three control parameters (ramp rate, compliance current, stop voltage) map to biological learning mechanisms, enabling precise, linear, symmetric synaptic weight updates. This work addresses three persistent challenges: instability of high–resistance states, asymmetry between potentiation/depression, and lack of linear analog control. The constrained RESET operation, implemented with transistor–based compliance control, provides stable, fine–grained weight updates. It is fully compatible with existing ReRAM stacks, adds no fabrication complexity, and improves retention and variability, accelerating commercialization for edge AI, robotics, and autonomous systems. The advantages of the new potentiation technique include: (i) Precise and stable analog resistance control for reliable synaptic weight updates, (ii) Non-destructive constrained RESET enabling symmetric and linear weight modulation, (iii) High-resistance state stabilization for improved memory retention and device reliability.

4:15pm **AM2+EM+TF-WeA-9 Epitaxial β-Ga_2O_3 Thin Films on Mica Integrated with Copper Heat-Dissipating Electrodes for High-Power Devices**, ***Ping-Hsien Wu,*** *Ying-Hao Chu,* National Tsing Hua University, Taiwan

Gallium oxide (Ga_2O_3) has recently attracted significant attention as an ultra-wide-bandgap semiconductor for next-generation high-power electronic devices. In high-power applications, device operation generally relies on high voltage and low current to reduce conduction losses. However, conventional device design faces a trade-off between reducing on-resistance and maintaining high breakdown voltage, as thinner drift layers lower resistance but also degrade voltage endurance. To address this limitation, materials with high critical electric fields are essential. Ga_2O_3 offers a significantly higher critical electric field than conventional semiconductors such as Si and SiC, enabling high breakdown voltage operation even at reduced thickness, thereby improving power efficiency. Nevertheless, its low thermal conductivity remains a critical challenge due to heat accumulation and potential thermal breakdown. In this work, high-quality Ga_2O_3 thin films with a rocking curve full width at half maximum (FWHM) of approximately 0.3° were achieved, indicating excellent crystalline quality. The Ga_2O_3 films were epitaxially grown on two-dimensional artificial mica substrates and subsequently transferred onto high-thermal-conductivity copper foils to enhance heat dissipation. In addition, a pn heterojunction composed of 600 nm-thick Ga_2O_3 and NiO was fabricated, exhibiting a breakdown voltage exceeding 500 V. The proposed structure simultaneously preserves high-voltage capability and improves thermal management, demonstrating a promising approach for high-power Ga_2O_3-based electronic devices.

4:30pm **AM2+EM+TF-WeA-10 Ultra-thin nickel films for 4H-SiC Schottky barrier diode**, ***Renato Beraldo,*** UNICAMP, Brazil

4H-SiC Schottky barrier diode (SBD) devices were fabricated on n-type 4H-SiC substrates using an ultrathin nickel film of 2 nm as the Schottky contact layer, deposited via electron-beam evaporation. First, the ohmic contact was formed using 100 nm of nickel, and the samples were annealed at 950 °C for 5 minutes. Subsequently, 2 nm of Ni was deposited, and the devices were subjected to various annealing temperatures. To create the metallic contact, 300 nm of Al was deposited by thermal evaporation and patterned into pads of 2 mm diameter without any shielding structure. The influence of annealing temperature on electrical performance and interface quality was evaluated. Electrical characteristics were measured using a parameter analyzer, and surface morphology was analyzed by atomic force microscopy

(AFM). For comparison, reference SBDs with a conventional 100 nm Ni film were fabricated and characterized under identical conditions.

A set of samples was annealed at temperatures ranging from 500 to 700 °C in 50 °C steps for each sample. After the annealing treatment, the final thickness was approximately 8 nm, as measured by AFM. Electrical measurements showed that diodes were obtained at all annealing temperatures, but the best electrical performance was achieved at 650 °C, with devices annealed at 500 °C and 700 °C showing inferior rectifying behavior. For comparison, a reference Schottky diode with a 100 nm thick Ni film was fabricated. The results revealed that the 2 nm diodes exhibited a Schottky barrier height (SBH) of 1.2 eV compared to 1.6 eV for the 100 nm diodes. However, the 2 nm diodes showed a rectification ratio two orders of magnitude larger and a leakage current of 22 pA compared to 3.2 nA at -200 V. Leakage current was also measured as a function of temperature from 25 to 175 °C. From 25 °C to 50 °C, the leakage current was approximately five times lower for the 2 nm devices compared to the 100 nm devices. Finally, the density of interface states was extracted from the 2 nm device, yielding a value of $10^{12}cm^{-2}eV^{-1}$, while the 100 nm device showed values around 10^{13} $cm^{-2}eV^{-1}$.

For future analysis, devices with lateral shielding will be fabricated to compare the breakdown voltage. Additionally, HRTEM and XPS characterization will be performed to verify the silicide composition stoichiometry and the presence of undesirable carbon clusters.

4:45pm **AM2+EM+TF-WeA-11 GaN Nanoscale Vacuum-Channel Transistors*, Huu Nguyen,*** *George Wang, Keshab Sapkota,* Sandia National Laboratories

Field-emission-based nanoscale vacuum-channel transistors (NVCTs) can combine the robustness of vacuum devices with state-of-the-art lithography techniques enabling low operating power, on-chip integrability, energy efficiency, and high-performance stability in extreme environments such as high temperatures and high radiation. By scaling device channels to be below the electron's mean-free path in air, the NVCTs can be operate in air while maintaining the ballistic electron transport characteristic of vacuum. Here, we report experimental and modeling results of top-down fabricated, single emitter gallium nitride (GaN) lateral NVCTs. We used electron beam lithography along with dry and wet etching to fabricate GaN NVCTs with device channel lengths less than 60 nm. The devices exhibited stable high field-emission current up to 100 nA, with tuning on/off ratio greater than 10^3. Minimal leakage current from the gates was observed to be less than 0.1 nA. Finite-element (COMSOL) modeling showed strong electric field penetration of GaN emitter led to emission current modulation by the gate voltage. This study elucidates the operation of field emission based lateral gated devices and provides important understanding in the design and operation of these new class of devices. *Sandia National Laboratories is managed and operated by NTESS under DOE NNSA contract DE-NA0003525. This work was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. Department of Energy, Office of Basic Energy Sciences user facility. This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.*

5:00pm **AM2+EM+TF-WeA-12 Atomic Layer Etching of Yttrium Orthovanadate Using Sequential Exposures of H_2 and SF_6/Ar Plasma*, Mariya Ezzy,*** *Emanuel Green, Will Pajak, Andrei Faraon,* California Institute of Technology*; Joonhee Choi,* Standford University*; Austin Minnich,* California Institute of Technology

Yttrium orthovanadate (YVO) is a promising host crystal for rare-earth ion (REI)-based quantum devices, such as quantum memories and quantum transducers. The long optical lifetimes of REIs require coupling to optical resonators for faster single-photon emission and for enabling single-ion control. Such resonators are currently fabricated through focused ion beam (FIB) milling, which can leave rough, defect-rich surfaces that can degrade optical and spin properties, such as spectral diffusion. Atomic layer etching (ALE) has the potential to mitigate these fabrication-induced defects through precise, nanometer-scale etching and its surface smoothing effect. Here, we report the first ALE process for YVO in a home-built plasma etcher using an H2 plasma modification step followed by an SF6/Ar plasma removal step. Preliminary results indicate an etch rate of 0.35 Å per cycle. The etch rates, surface morphology, and surface chemical composition are characterized using atomic force microscopy and X-ray photoelectron spectroscopy (XPS).

Atomic Scale Processing Mini-Symposium
Room 316 - Session AP+2D+EL+EM+PS+TF-WeA

Atomic Scale Processing to Enable 2D Materials

Moderators: Dr. Robert Bruce, IBM Research, T. J. Watson Research Center, **Prof. Dr. Cristina Satriano**, University of Catania

2:15pm **AP+2D+EL+EM+PS+TF-WeA-1 Chemistry (and Some Physics) of Atomic Layer Deposition of Two-Dimensional Metal Dichalcogenides*, Miika Mattinen,*** University of Helsinki, Finland **INVITED**

Two-dimensional (2D) materials are of interest for a range of applications from microelectronics to sensing to energy storage and production. One of the most prominent group of 2D materials are metal dichalcogenides, some of which are semiconductors, such as the prototypical MoS_2, while others are (semi)metals such as TiS_2 and TaS_2.[1] Deposition of 2D materials with desired properties on large, often temperature-sensitive, and complexly shaped substrates is a key challenge for practical applications. Atomic layer deposition (ALD) can fulfill these requirements, but unlocking the full potential of ALD requires understanding of precursor chemistry, nucleation, substrates, and film characteristics, among other factors.[1,2]

I will discuss chemistries for deposition of a range of 2D metal dichalcogenides including MoS_2,[3] SnS_2,[4] ReS_2,[5] WS_2,[6] HfS_2 and ZrS_2[7] using thermal ALD. I will cover precursor challenges related to reactivity, thermal stability, and etching reactions. Controlling crystallinity and morphology and continuity at low thicknesses are also key challenges encountered in ALD of 2D materials. To this end, I highlight the role of substrate choice and the use of a two-step SnS_2 process where the deposited amorphous film is crystallized with mild-post deposition annealing.[4,8,9]

Plasma-enhanced ALD (PEALD) can help overcome some of the challenges encountered in thermal ALD, such as limited reactivity of many precursors. For example, few thermal chemistries are available for direct deposition on low-cost plastic substrates for flexible applications (T ≤ 150 °C). To this end, I will discuss PEALD of TMDCs including MoS_2, TiS_2, and WS_2 at record-low temperatures down to 100 °C by controlling plasma chemistry[10] I will also describe advanced ABC type processes with two plasma steps, where both the plasma chemistry (reactive radicals) and physics (low-energy ions) are used to control film growth and properties.[11]

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2:45pm **AP+2D+EL+EM+PS+TF-WeA-3 First-Principles Survey of Molybdenum ALD Precursors for MoS_2 Thin Films*, Ian Kerby,*** *Ashlee Riedinger, Lan Li,* Boise State University

Transition metal dichalcogenides, such as molybdenum disulfide (MoS_2), are promising candidates for various semiconductor applications. A crucial requirement for these applications is the controlled and conformal deposition of a monolayer film. Chemical vapor deposition (CVD) and atomic layer deposition (ALD) techniques are key to achieving thin films at commercial scale. Towards this end, the reactions of a variety of precursor chemicals with another variety of surfaces need to be understood. A reaction between a surface and a precursor can be difficult to study in-situ and ex-situ, making computational modeling a valuable tool for addressing this challenge. The work presented here is a survey of common and proposed molybdenum precursors for use in atomic layer deposition of MoS_2 films. Our work in modeling nucleation of these precursors includes various surfaces with the primary aim of determining the role of surface morphology and chemistry during deposition. We have conducted thermodynamic surveys using density functional theory (DFT) for spontaneity of proposed reaction pathways for the precursors to interact and nucleate on the surfaces. To generate and account for the inherent variability in the amorphous substrate, we have utilized ab-initio molecular dynamics (AIMD), enabling a more comprehensive exploration of the complex energy landscape. We have also investigated the formation of reaction residues on surfaces. Our studies lay the groundwork for future

kinetic analyses. The stable intermediate states identified along the reaction pathways can be used in nudged elastic band (NEB) calculations to determine the associated energy barriers during nucleation. These insights may further help guide and inform experimental efforts.

3:00pm **AP+2D+EL+EM+PS+TF-WeA-4 Thermal and Plasma-Enhanced ALD of MoS_2 using $MoO_2(THD)_2$, *Ryan Weiland,*** University of Michigan, Ann Arbor*; Ian Campbell,* IMEC*; Pierre Morin, Benjamin Groven,* IMEC Belgium*; Ageeth Bol,* University of Michigan, Ann Arbor

Field effect transistors (FETs) are foundational components of modern electronics. For these applications, scalability is as important as device performance. Two-dimensional MoS_2 exhibits a direct band gap and enables high fidelity electrostatic control due to its reduced dimensionality and the absence of dangling-bonds at the surface. MoS_2 is therefore an ideal channel material for future FETs. Atomic layer deposition (ALD) is a promising technique for scalable, conformal, and back-end-of-line compatible MoS_2 deposition. While promising, the electrical performance of ALD grown 2D MoS_2 does not meet expectations when compared to the electrical properties of mechanically exfoliated MoS_2, due its polycrystalline nature. Polycrystalline MoS_2 contains grain boundaries that act as scattering centers, trap-rich regions, and structural discontinuities, that degrade its desirable electronic properties. In this work, ALD processes were developed using a novel molybdenum precursor, $MoO_2(THD)_2$. $MoO_2(THD)_2$ contains bulky organic ligands, which could impose steric hindrance during surface reactions, thus limiting surface chemisorption density and favoring formation of larger crystal grains.

First, $MoO_2(THD)_2$ volatility and decomposition behavior were studied by thermogravimetric analysis (TGA). TGA showed sublimation beginning at 120°C with 100% mass loss at 300°C. Next, plasma and thermal ALD processes were developed at 400°C. A mixed H_2S/Ar co-reactant was used for both plasma and thermal ALD. The effects of precursor and co-reactant dosing times, co-reactant ratios, as well as purge conditions were systematically investigated using in situ ellipsometry. The growth per ALD cycle (GPC) was measured to be 0.07 Å/cycle for the thermal recipe and 0.15 Å/cycle for the plasma process. The resulting films were characterized by X-ray photoelectron spectroscopy (XPS), Raman spectroscopy, and atomic force microscopy (AFM). XPS indicates near-stoichiometric MoS_2. Raman spectra confirm MoS_2 vibrational modes and film crystallinity for both processes, while AFM reveals smooth, continuous films without out-of-plane features, with an RMS roughness of ~0.5 nm.

Overall, this work establishes $MoO_2(THD)_2$ -enabled thermal and plasma-enhanced ALD at 400 °C as a scalable route to smooth, continuous, and crystalline MoS_2 thin films. These results lay the groundwork for integrating conformal, large-grain MoS_2 channels into back-end-of-line compatible process flows, with ongoing grain-size quantification and electrical testing expected to link microstructural improvements to device performance.

3:15pm **AP+2D+EL+EM+PS+TF-WeA-5 Low Temperature Magnetized Plasmas for Processing of Two-Dimensional Materials, *Yevgeny Raitses,*** Princeton Plasma Physics Laboratory*; Stanislav Musikhin, Yerbolat Ussenov,* Princeton University Plasma Physics Lab*; Satya Butler, Saien Xie,* Princeton University*; Nirbhav Chopra,* Princeton University Plasma Physics Lab

INVITED

Low-temperature magnetized plasmas generated by electron beams or non-thermal electrons offer new opportunities for atomic-scale materials processing relevant to microelectronics and quantum technologies.[1-3] Operating at low pressures (0.1–10 mTorr), the applied magnetic field enables spatial separation between a high-density plasma generation region (~10^{11}–10^{12} cm^{-3}, electron energies >10 eV) and a peripheral processing region characterized by lower plasma density (<10^{9} cm^{-3}) and electron temperatures (<1 eV).[4] Substrates placed in this region are primarily exposed to low-energy ion fluxes ($\lesssim$ a few eV), enabling damageless processing of two-dimensional materials or processing with a controllable defect formation of such materials. However, plasma instabilities can drive anomalous cross-field transport and increase ion fluxes and energies at the surface.[5] We present experimental results on instability mitigation in ExB plasma systems[4] and demonstrate improved low-damage processing of graphene and transition metal dichalcogenides. Quantitative defect characterization in plasma-treated monolayered WS_2 films is presented and benchmarked against conventional RF inductively coupled plasma processing. A focus will also be made on the effect of vacuum conditions in the plasma reactor chamber on the defect formation (e.g. sulfur vacancies). Applications to hydrogen and nitrogen surface passivation of diamond for quantum devices are also discussed.[2]

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Acknowledgement

This work is supported by the U.S. Department of Energy, Office of Science, Fusion Energy Sciences and Basic Energy Sciences, as part of the Extreme Lithography & Materials Innovation Center (ELMIC), a Microelectronics Science Research Center (MSRC) through the Plasma-enabled 2D Materials project at the Princeton Plasma Physics Laboratory (PPPL), under contract number No.DEAC02-09CH11466.

4:15pm **AP+2D+EL+EM+PS+TF-WeA-9 Impact of Fluorination and Oxygenation Sources on the Thermal Atomic Layer Etching of Crystalline MoS_2, *Spencer Smith,*** *Steven M. Hues, Elton Graugnard,* Boise State University

Atomic layer etching (ALE) has emerged as a transformative technique for atomic-scale processing of two-dimensional (2D) materials, including molybdenum disulfide (MoS_2), a promising semiconductor due to its high carrier mobility in monolayer form. Precise etching of MoS_2 films offers a pathway for tuning electrical and optical properties through controlled thickness. Previous studies have explored alternative fluorination and oxygenation chemistries for thermal ALE of amorphous MoS_2, including oxygen sources such as H_2O and O_3 and fluorine sources including HF/pyridine and MoF_6. In this work, we investigate the application of these alternative chemistries to the thermal ALE of MOCVD-grown and ALD-grown MoS_2 films. Preliminary work on ALE of crystalline MoS_2 indicates that etching occurs at defects and grain boundaries. This study aims to correlate etching behavior with changes in surface topography and defect density. Etching effectiveness will be characterized by atomic force microscopy, Raman spectroscopy, and photoluminescence spectroscopy. This study seeks to further expand the capabilities of ALE for precise processing of 2D materials relevant to next-generation semiconductor devices.

4:30pm **AP+2D+EL+EM+PS+TF-WeA-10 Atomic Layer Etching of Tungsten Disulfide in O2/Ar and BCl3/Ar Remote Plasmas, *Jeremy J. Mettler,*** University of Houston*; Jaehong (Russell) Kwon, David. B. Graves,* Princeton University*; Vincent M. Donnelly,* University of Houston

Transition-metal dichalcogenides (TMDs) are a class of 2D materials consisting of covalently bonded sheets. Multi-layers are held together by cross-plane van der Waals forces. While these materials hold promise in future semiconductor applications, processes for manufacturing using TMDs are in the early stages of development. One challenge is obtaining uniform, monolayer growth of TMD films over large areas. Chemical vapor deposition results in the formation of multilayer islands. Etching of TMD films will also be required, if for no other reason than to thin multilayers to single layers. Atomic layer etching (ALE) is likely to be called upon for etching steps. TMDs are easily damaged by high temperature and energetic species bombardment, making thermal or plasma-assisted etching challenging. We have explored ALE of WS_2, a promising TMD 2D material. A remote plasma supplied reactive radicals. A switchable magnetic field allow low energetic ion bombardment to be turned on or off while having little effect on radical density. ALE of WS_2 was achieved in a two-step process. Vacuum-transfer x-ray photoelectron spectroscopy (XPS) was used to characterize the chemical composition and thickness of the remaining film at various stages in the process. Sulfur-terminated multilayer films of WS_2 were exposed to O atoms downstream of an Ar/O_2 inductively coupled plasma (ICP). Without ion bombardment thermal O atoms removed S from the surface and formed a tungsten oxide layer 1-2 monolayers thick, with a composition of roughly WO_4. These results agree favorably with parallel molecular dynamics simulations. In the presence of low energy ions (~15 eV) at a flux of ~3 x $10^{15}cm^{-2}$, the etching rate increased several-fold and the W-oxide stoichiometry was not changed. The Ar/O_2 plasma was followed by Ar/BCl_3 plasma to selectively etch the tungsten oxide layer relative to the underlying WS_2. This step required low energy ion bombardment to remove the WO_4 film and expose the next WS_2 layer. A detailed analysis of the film at various stages in the ALE process was carried out by using the high-resolution W(4f), S(2p), B(1s) and Cl(2p) in the film as well as the Si(2p) from the underlying substrate and O(1s) in the WS_2 film and underlying interfacial native oxide layer on Si. A complete picture of the stoichiometry of the film during ALE was obtained and will be presented.

This material is based upon work supported by the U.S. Department of Energy, Office of Science, Fusion Energy Sciences and Basic Energy Sciences, as part of the Extreme Lithography & Materials Innovation Center (ELMIC), a Microelectronics Science Research Center (MSRC), under contract No. DEAC02-09CH11466.

4:45pm **AP+2D+EL+EM+PS+TF-WeA-11 Investigation of Layer-by-Layer Etching of MoS_2 by Atomic Oxygen and XeF_2**, ***Sei-won Chung***, *Daniel Cho, Jane Chang,* University of California, Los Angeles

As semiconductor devices continuously scale down, the demand for channel materials of field effect transistors (FETs) with high mobility at low dimensions has increased. 2D transition metal dichalcogenides (TMDs) have gained interest due to relatively consistent mobility at 5 nm of body thickness compared to conventional silicon channel. However, non-uniform large area synthesis has been a challenge in integration. To improve device performance, non-uniform adlayers should be removed layer-by-layer to realize a uniform and large-area TMD films.

To investigate layer-by-layer etching of MoS_2, thermochemical analysis suggests thermodynamic feasibility of using oxygen and fluorine chemistries for MoS_2 etching. Individual and synergistic effects of Ar^+, O radical (produced by a coaxial waveguide microwave source) and XeF_2 (3Torr) were studied in the molecular beam where each species can be independently controlled in flux and energy. The as-received MoS_2 has S/Mo and Si/Mo ratios of 1.6 and 1.0. Neither O nor XeF_2 spontaneously reacted with the as-received MoS_2. Ar^+ ion beam (200V, 0.5mA, 10s) was used to remove surface contamination prior to etching, resulting S/Mo and Si/Mo ratios of 0.94 and 0.18 respectively. Following in-situ Ar^+ ion beam cleaning, O radical was shown to oxidize MoS_2 decreasing S/Mo from 0.94 to 0.46, while XeF_2 removes MoS_2 increasing Si/Mo from 0.18 to 7.1. It showed surface fluorination (~3%), corresponding to formation of $MoOF_x$ and CF_x.

Finally, the sequential process consisting of Ar^+ ion bombardment, O radical introduction, and XeF_2 vapor exposure (0.5T, 10 pulses) was applied which could enable surface activation, self-limiting oxidation and removal of modified layer by forming oxyfluorides. After XeF_2, O atomic composition decreased and S atomic composition increased indicating removal of MoO_3 with surface fluorination (~3%) of MoF_x and $MoOF_x$. Increasing number of pulses to 20 increases S/Mo from 1.1 to 1.4 while reducing the MoO_3 content. This research reveals the individual and combination effects of Ar^+ ion beam, O radicals and XeF_2 on MoS_2 etching and potentially applied to investigating mechanism of layer-by-layer etching of MoS_2.

This research is supported by the U.S. DOE, Office of Science, as part of the ELMIC MSRC through the Plasma-enabled 2D Materials project at PPPL, under contract No. DEAC02-09CH11466.

5:00pm **AP+2D+EL+EM+PS+TF-WeA-12 Width Reduction and Edge Smoothing of 2D MoS_2 Nanoribbons by Lateral Thermal Atomic Layer Etching**, ***Janine Wyand***, University of Colorado at Boulder; *Tara Pena, Eric Pop,* Stanford University; *Steven George,* University of Colorado at Boulder

Atomic layer etching (ALE) of 2D MoS_2 nanoribbons is important for the fabrication of MoS_2 channel transistors. E-beam lithography and conventional dry etching processes face problems when etching MoS_2 films. These disadvantages include delamination for nanoribbon widths < 25 nm and inability to control line edge roughness. ALE methods may bypass these limitations and produce narrower width MoS_2 channels with smoother edges that may have better electrostatic control and on/off switching.

Narrowing the width of 2D MoS_2 nanoribbons requires lateral etching in the 2D plane. Our earlier work on the thermal ALE of 2D MoS_2 showed that sequential exposures of O_3 and $SOCl_2$ produced lateral etching by either "outside-in" or "inside-out" mechanisms. In this study, the "outside-in" lateral etching of 2D MoS_2 crystalline nanoribbons was utilized to reduce the widths of 2D MoS_2 nanoribbons. O_3 (ozone) was used for MoS_2 oxidation to MoO_3 and $SOCl_2$ (thionyl chloride) was used for the volatilization of MoO_3 as MoO_2Cl_2. The studies were performed using high quality 2D MoS_2 nanoribbons on silicon coupons. The MoS_2 nanoribbons were prepared from monolayer 2D MoS_2 films using e-beam lithography and dry etching.

The etching of the 2D MoS_2 nanoribbons was examined by atomic force microscopy (AFM) at 150°C. The lateral etching could be quantified by returning to the same nanoribbon after various numbers of etching cycles and measuring the nanoribbon width using AFM. **Figure 1** shows that the width of the nanoribbons decreases progressively versus number of etching cycles. The AFM images indicate that the etching cycles also smooth the nanoribbon line edge roughness.

The AFM images were consistent with lateral etching at the edges of the 2D MoS_2 nanoribbons. The AFM measurements determined that the 2D lateral etching rate was ~3.9 Å per etching cycle at 150°C as displayed in **Figure 2**. This lateral etch rate represents ~1 MoS_2 units removed per etching cycle at the step edge of the 2D MoS_2 crystalline domains. Additional AFM measurements revealed that nanoribbon widths < 25 nm were possible using this thermal ALE process.

Applied Surface Science
Room 319 - Session AS-WeA
ToF SIMS in Applied Surface Science

Moderators: Dr. Jean-Paul Barnes, CEA-LETI, France, **Dr. Tanguy Terlier**, Rice University

2:15pm **AS-WeA-1 Enhancing Industrial Problem Solving with ToF-SIMS**, ***David Carr***, *Stacy Hanson,* 3M **INVITED**

Working in a central research laboratory within a large corporation presents both exceptional opportunities and unique challenges. The surface analysis facility supports every stage of product development, from fundamental research and early-stage innovation to scale-up and manufacturing troubleshooting, across an extraordinarily diverse portfolio of materials and products that extend far beyond the familiar Post-it® notes and Scotch® tape that many people associate with 3M. Because there are rarely "standard" analyses, success depends on combining technical depth with creative problem solving.

Among the available analytical techniques, time-of-flight secondary ion mass spectrometry (ToF-SIMS) is particularly valuable because of its ability to generate highly sensitive surface chemical maps and provide insight into composition both at and beneath the outermost surface of a material. These capabilities make ToF-SIMS a powerful tool for addressing a wide range of industrial materials questions, including failure analysis, process optimization, contamination identification, and structure–property investigations.

This presentation will highlight a range of topics with practical advice on methods to apply ToF-SIMS for industrial problem solving.

2:45pm **AS-WeA-3 Capabilities and Challenges of Dual-Beam Depth Profiling at Ultra-Low Sputter Energies**, *Derk Rading, Julia Zakel,* ***Thomas Grehl***, *Philipp Brüner, Wolfgang Paul, Ewald Niehuis,* IONTOF GmbH, Germany

For the majority of TOF-SIMS users, inorganic dual beam depth profiling [1] is one of the key modes of operation, particularly in the semiconductor industry where its versatility and flexibility are essential for its success. With current instrumentation, routine analyses are typically performed at 500-1000 eV sputtering energy, while the lowest energies used are in the range of 250-350 eV. The dual beam principle, with separate sputtering and analysis ion beams, enables independent optimization of the lateral resolution, mass resolution, and detection limit (high energy beam), as well as the sputtering conditions. The latter determine depth resolution, transient regime, and chemical signal enhancement. However, the dual beam mode also comes with a trade-off: to prevent the high-energy beam from degrading the depth resolution while maximizing detection sensitivity, the fluence ratio of the two beams must be carefully controlled [2].

To the best of our knowledge noextrapolation has yet been performed below 250 eV, so experiments are needed to verify the usefulness of dual beam depth profiling at these ultra-low sputtering energies. Our results show that dual beam depth profiling even at sputtering energies < 250 eV follows the trends from previous studies very nicely and no unexpected deviation is found. This study expands the knowledge beyond the currently practical energy range by identifying the fluence ratio limit required for silicon-based materials to maintain optimum depth resolution. It also examines how this limit varies with the choice of primary species and energy. Additionally, we assess the impact of different primary species on the sensitivity at the critical fluence ratio for a given sputtering energy.

The experiments were conducted on well-defined model samples, extending previous work to lower energies. Finally, we demonstrate the practical applicability of the extended energy range and optimized analytical conditions in TOF-SIMS depth profiling on a relevant real-world sample.

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3:00pm **AS-WeA-4 Ultraviolet Picosecond Laser Ablation of Agar Films Evaluated by SEM and ToF-SIMS***, **Anna Karagiannakis,*** University of Illinois at Chicago*; Anton V. Ievlev, Gabriel D. Parker,* Oak Ridge Natinal Laboratory*; Mehak Verma, Reyhane Shavandi, Luke Hanley,* University of Illinois at Chicago

Laser ablation with mid-infrared femtosecond laser pulses is used for rapid depth profiling in soft materials, but the use of ultraviolet picosecond lasers for ablation requires investigation of potential sample damage. The surface sensitivity and gaseous cluster ion beam depth profiling capability of time-of-flight secondary ion mass spectrometry (ToF-SIMS) make it ideal for tracking potential surface modification. Picosecond UV laser ablation (213 nm, 30 ps) was used to etch craters in dried agar films loaded with known metabolites on either optical grade glass slides or polished silicon wafers. Ablation crater morphology was assessed by scanning electron microscopy (SEM) across multiple power levels to identify the optimal fluence to be ~80 mJ/cm^2 for uniform and reproducible material removal on both substrates, a prerequisite for meaningful depth-resolved chemical interpretation. Higher fluences produced non-uniform crater morphologies with mechanical fracturing of the agar film, including cracking and delamination at crater edges, rendering them unsuitable for depth profiling. Negative-ion ToF-SIMS spectra were then used to compared ablated and non-ablated regions: non-ablated surfaces, representing the outermost film layer prior to ablation, were dominated by inorganic salt ions accumulated during drying: F^- (*m/z* 19), Cl^- (*m/z* 35), CN^- (*m/z* 26), CNO^- (*m/z* 42), PO_2^- (*m/z* 63), and PO_3^- (*m/z* 79), co-existing with detectable agar polysaccharide fragment ions, establishing the chemical baseline before ablation. Following ablation at the optimized power, inorganic salt signals were markedly reduced while agar-associated fragments — OH^-, C_2HO^-, $HCOO^-$, $C_2H_3O_2^-$, $C_3HO_2^-$, and $C_3H_3O_2^-$ — were retained at comparable intensities, demonstrating that ablation exposed a chemically distinct subsurface layer in which the organic matrix was preserved but the salt-enriched surface was removed. These results demonstrated the chemical changes that ablation induced through the surface of a dried agar film. Additional characterization is ongoing to further validate these findings across substrates and loading conditions. Ongoing experiments seek to determine the distribution of a metabolite doped within the agar matrix via ToF-SIMS depth profiling.

3:15pm **AS-WeA-5 3D Characterization of High-Aspect-Ratio Trench Using SIMS***, **Dimitry Kouzminov,*** *Vikram Bhosle, James Cournoyer, David Barrett, Cuiyang Wang,* Applied Materials Inc.

Achieving precise conformal doping in **high-aspect-ratio trench (HART)** structures like CMOS image sensors, 3D NAND and 3D DRAM is becoming increasingly important for next generation device performance. 1.5D SIMS has been used to characterize sidewall *dopant dose conformality* for 2 decades. This technique was developed mostly in application to FinFet transistor where trench depth typically doesn't exceed 200-300 nm and trench width is of the order of 100-150 nm[1]. 1.5D SIMS measurement, however, does not provide information on sidewall dopant concentration which is crucial for contact manufacturing in 3D DRAM process.

1.5D SIMS analysis requires a-Si trench backfill, and there are adverse effects associated with it. One of them is the loss of sidewall dopant [2].Another effect is specific to the HART itself: unfilled void in the middle of the trench due to the "bottleneck" forming at trench top during a-Si CVD deposition process. The presence of this void results in SIMS measurement artifact which appears as modulation in dopant distribution. The nature of this artifact will be discussed in the paper. To eliminate this problem, we developed primary beam trench auto-filling technique resulting in artifact-free 1.5D SIMS analysis. This technique will also be discussed in detail in the current paper.

Besides adverse effects associated with backfill void formation, HART dimension measuring from 5 to 30-40 um in depth presents a possibility for the *through-sidewall SIMS dopant distribution measurement* [3]. We call this technique ***Lateral SIMS***. This technique is introduced and in-detail discussed in the current paper. Combined analyses using combination of *Lateral SIMS* and 1.5D SIMS comprise ***3D HART dopant characterization***. Sidewall dopant distribution obtained by *Lateral SIMS* is corroborated by the correlative APT analysis which is also presented in the current paper

References:

1. J. Mody et al, J. Vac. Sci. Technol. B **28**, C1H5 (2010); https://doi.org/10.1116/1.3269755
2. D. Kouzminov et al, *Microscopy and Microanalysis*, Volume 25, Issue 2, 1 April 2019, Pages 511–516
3. D. Kouzminov, V. Bhosle et al, Patent Number: US12575379

3:30pm **AS-WeA-6 In-situ Gas Cluster Ion Beam Cryo-Sectioning to Enable Subcellular Cryo-ToF-SIMS Imaging***, Claire Seydoux,* Univ. Grenoble Alpes, CEA, IRIG-MEM, Current address: ESRF – The European synchrotron, France*; Bérangère Moreau,* Univ. Grenoble Alpes, CEA, IRIG, MEM, France*; Michel Boujard,* Univ. Grenoble Alpes, CEA, Grenoble INP, IRIG-Pheliqs, France*; Eric Gauthier,* Univ. Grenoble Alpes, CEA, Grenoble INP,IRIG-Spintec, France*; Pierre-Henri Jouneau,* Univ. Grenoble Alpes, CEA, IRIG-MEM, France*; **Jean-Paul Barnes,*** Univ. Grenoble Alpes, CEA, Leti, France

Time-of-flight secondary ion mass spectrometry (ToF-SIMS) is capable of label-free molecular imaging at lateral resolutions below a micron, but the analysis of biological samples is contingent on adequate sample preparation. Conventional fixation or dehydration alters morphology and induces analyte relocation, while cryo-transfer systems are costly and not always available. We present an in situ cryo-etching approach using a gas cluster ion beam (GCIB) and a custom sample holder with a flat titanium ridge mask, enabling the sectioning of frozen specimens directly inside the ToF-SIMS instrument [1]. To illustrate the potential of this method produced flat, artifact-free surfaces suitable for subcellular imaging without chemical treatment or cryo-transfer we used Arabidopsis thaliana seeds as a model system. ToF-SIMS secondary ion images indicated that the tissue architecture was not modified by the sample preparation and distinct subcellular compartments were visible at a lateral resolution of ∼1 µm. Secondary ion mass spectra contained intact molecular ion peaks up to 1000 Da This is in stark contrast to air-dried cryosections of the same model seed sample, that suffered from structural collapse and analyte delocalization. This in-situ cyo etching approach provides a practical and accessible route for cryo-ToF-SIMS analysis of hydrated biological materials, combining structural fidelity with molecular integrity. It offers an interesting alternative to conventional cryo-transfer methods for high-resolution chemical imaging and opens up the possibility for 3-D imaging by modifying the height of the mask and performing several etching and imaging cycles.

This work was carried out on the Platform for Nanocharacterisation (PFNC) of CEA-Grenoble, supported by the "Recherche Technologique de Base", "3D-Lipid" InterCarnot Project between CEA-Leti et 3BCAR institutes and "France 2030 - ANR-22-PEEL-0014" programs of the French National Research Agency (ANR).

[1] C. Seydoux et al. J. Am. Soc. Mass Spectrom. 2026, 37, 1132−1139

4:15pm **AS-WeA-9 Advancing TOF-SIMS Workflows for Automated Mineral Grain Identification in Complex Samples***, **Jacob Schmidt,*** *Siddhartha Ghosh,* Physical Electronics USA*; Susana Brito e Abreu,* University of Queensland, Australia

In mineral exploration and processing, the surface chemistry of individual mineral particles plays a critical role in separation efficiency and process performance, particularly for complex ores. Time of Flight Secondary Ion Mass Spectrometry (TOF-SIMS) provides a unique capability to probe this chemistry at the scale of individual grains. However, the practical application of TOF-SIMS to large, heterogeneous mineral samples is limited by the time and effort required to locate, analyze, and identify particles of interest, which restricts throughput and statistical representativity. This work is part of a collaborative effort with the University of Queensland to advance TOF-SIMS toward a more scalable analytical approach for mineral processing applications.

To address these limitations, we have leveraged AI-assisted software development to rapidly prototype automated TOF-SIMS workflows for the identification of regions of interest. Large area Mosaic imaging is used to systematically survey samples and identify grain scale regions containing minerals of interest. Spectra from these regions are then extracted and compared to curated reference data to support mineral identification, reducing reliance on manual interpretation while improving consistency across large datasets. This approach enables particle-specific surface chemistry measurements across statistically meaningful populations, including fine and sparsely distributed target phases. These developments support the practical use of TOF-SIMS for mineral processing and contribute toward its adoption as a routine tool for studying surface chemistry drivers in complex mineral systems.

4:30pm **AS-WeA-10 Rapid Large-Area Mapping of Rare Earth Elements and Mineral Phases in Geological Samples Using ToF-SIMS**, ***Zihua Zhu***, *Xin Zhang, Xiaoxu Li, Yifu Feng, Vaithiyalingam Shutthanandan, Odeta Qafoku,* Pacific Northwest National Laboratory

Rare earth elements (REEs) in geological drill core samples typically occur at trace concentrations within heterogeneous mineral hosts, creating significant challenges for rapid, phase-resolved characterization during exploration workflows. This study demonstrates that time-of-flight secondary ion mass spectrometry (ToF-SIMS), owing to its exceptional sensitivity, enables rapid, large-area mapping of REE distributions and associated anion clusters directly on polished core sections. Importantly, its high mass resolution effectively resolves spectral interferences that commonly hinder energy-dispersive X-ray spectroscopy (EDX) and synchrotron-based mapping approaches. Large-area surveys quickly identify localized REE-enriched regions, while high-resolution imaging reveals co-localization with diagnostic phosphate fragments (e.g., PO_x^-), allowing discrimination of REE host phases such as apatite and xenotime. Applied to altered Yellowstone rhyolite, ToF-SIMS reveals microscale REE enrichments that remain undetected by conventional bulk analytical and electron/X-ray-based techniques. By combining high sensitivity, minimal sample preparation, and rapid analytical throughput (<2 hours per sample), ToF-SIMS offers a powerful complementary method for rapid screening and phase-resolved REE characterization, supporting more informed early-stage exploration decisions and enabling more targeted downstream analyses.

4:45pm **AS-WeA-11 Determination of Relative Sensitivity Factors for Mg, Co, B, Be, K, and Si in Various Oxide Matrices Using Quadrupole SIMS.**, ***M. K. Indika Senevirathna***, Clark Atlanta University*; Jacob Steele, Seungmin Lee, Anna Park, Kathy Azizie,* Cornell University*; Michael D Williams,* Clark Atlanta University*; Darrell Schlom,* Cornell University, Kavli Institute at Cornell for Nanoscale Science, Leibniz-Institut für Kristallzüchtung

Complex oxide semiconductors are of considerable interest for emerging electronic and functional device applications due to their wide range of tunable structural, electronic, and defect-related properties, which can be engineered through composition, doping, and processing conditions. In this work, matrix-dependent Relative Sensitivity Factor (RSF) behavior will be investigated using quadrupole Secondary Ion Mass Spectrometry (SIMS) in different oxide matrices, including $(Al_xGa_{1-x})_2O_3$, SnO, Al_2O_3 and Ga_2O_3, implanted with Si, Mg, Co, B, Be, and K ions. Depth-resolved SIMS profiling will be performed to examine impurity incorporation, elemental distribution, and matrix effects on secondary ion yield for quantitative analysis.

The results will show pronounced variations in RSF values as a function of both implanted species and host oxide matrix. Significant differences in secondary ion intensities, depth profile shapes, and sensitivity behavior will be observed across the investigated materials, indicating strong matrix-dependent ionization and sputtering effects. Further analysis will reveal that cobalt implantation exhibits distinct behavior compared to light and alkaline-earth species, reflecting the influence of local bonding environment and matrix composition on SIMS quantification. These findings provide important information on RSF variability across $(Al_xGa_{1-x})_2O_3$, SnO, Al_2O_3, and Ga_2O_3 systems and improve the accuracy and reliability of quantitative quadrupole SIMS analysis for the doped oxide matrices studied.

5:00pm **AS-WeA-12 In-situ thermal analysis of Pyrolyzed Polyacrylonitrile Film using operando ToF-SIMS**, ***Tanguy Terlier***, Rice University, Department of Chemical & Biomolecular Engineering, Shared Equipment Authority*; Khalid Alkandery, Sibani Lisa Biswal,* Rice University, Department of Chemical & Biomolecular Engineering

Emerging technologies increasingly depend on complex multifunctional materials whose performance and reliability are strongly governed by their chemical composition, interfacial chemistry, diffusion behavior, degradation pathways, and thermally induced transformations. Understanding these mechanisms is essential for both fundamental research and industrial implementation; however, the structural and chemical complexity of advanced materials remains difficult to probe using conventional characterization techniques.

Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) has become a powerful surface analytical technique capable of providing highly sensitive elemental and molecular information from surfaces, interfaces, thin films, and three-dimensional architectures. Recent advances in ToF-SIMS instrumentation now enable operando investigations under realistic reaction environments, offering new opportunities to directly monitor dynamic thermal and chemical processes in functional materials.

In this work, we present an operando thermal analysis methodology based on ToF-SIMS for investigating thermally driven reactions through controlled in-situ heating during analysis. As an initial demonstration, a reference polystyrene film is annealed to illustrate how operando thermal SIMS can probe both physical and chemical transformations. We then investigate pyrolyzed polyacrylonitrile (pPAN) films, a conductive binder widely used in lithium-ion batteries. Owing to its high elasticity, pPAN has shown significant potential for silicon-based anodes. Here, we examine the evolution of aromatic and aliphatic secondary ion fragments as a function of temperature and demonstrate how their relative intensity ratio can be used to monitor the pyrolysis behavior of the material under various annealing conditions. The ToF-SIMS results are correlated with thermogravimetric analysis/differential scanning calorimetry (TGA/DSC) and Fourier-transform infrared spectroscopy (FTIR) to validate the operando thermal analysis approach.

Materials and Innovations for Fusion Energy
Room 321 - Session FUS-WeA

Materials for Fusion Fuel Containment

Moderators: Dr. Eric Dombrowski, Commonwealth Fusion Systems, **Dr. Matthew Sharpe**, The Laboratory for Laser Energetics, The University of Rochester

2:15pm **FUS-WeA-1 MAX Phase Materials for Hydrogen Permeation Barriers**, ***Eric Vogel***, *Moses Nnaji,* Georgia Institute of Technology*; Dale Hitchcock,* Savannah River National Lab **INVITED**

Hydrogen isotope permeation is a critical materials challenge for fusion and other nuclear technologies, where tritium loss, inventory control, and degradation of structural alloys must be managed under high temperature and radiation. Conventional ceramic barriers such as Al_2O_3 can provide large permeation reduction factors, but brittleness, thermal-expansion mismatch, radiation sensitivity, and high processing temperatures limit integration with engineering alloys. This talk will present Ti_2AlN MAX phase thin films as radiation-tolerant hydrogen isotope permeation barriers. MAX phases combine ceramic stability with metallic transport, radiation damage tolerance, oxidation resistance, and the ability to form protective alumina scales.

The presentation will focus on low-temperature vapor deposition routes for MAX phase Ti-Al-N coatings, especially two-stage reactive magnetron sputtering. Ti-Al-N precursor films are deposited near ambient temperature and then annealed to drive solid-state reactions and Ti_2AlN crystallization. By controlling precursor architecture, composition, and modulation period, the formation pathway can be shifted from conventional high-temperature synthesis toward substrate-compatible processing. XRD, DSC-TGA, STEM show that Ti/AlN and TiN/TiAl multilayers follow distinct reaction pathways, with Ti/AlN enabling Ti_2AlN formation at lower temperatures. Trace Ti_2AlN was observed after extended annealing at 475 °C, an unusually low synthesis temperature for Ti-based MAX phase films by sputtering, while higher-temperature anneals produced crystalline Ti_2AlN coatings for permeation testing.

Deuterium permeation measurements on coated Grade 91 steel demonstrate substantial flux reductions relative to uncoated steel. The best Ti_2AlN coatings produced permeation reduction factors from tens to more than 1000, depending on temperature, pressure, film texture, and surface condition. Strong basal texture, improved crystallinity, and reduced high-angle grain-boundary content were correlated with improved barrier performance, consistent with anisotropic diffusion in layered MAX phase structures. Non-ideal behavior, including surface-limited dissociation, trapping, residual Ti-rich layers, oxide/carbon-rich surfaces, and pressure-induced flux changes, will be discussed. Together, these results identify processing-structure-property relationships that can guide radiation-hard, substrate-compatible MAX phase permeation barriers.

2:45pm **FUS-WeA-3 Atomic Layer Deposition on Novel Fusion-Relevant Substrates**, ***Zachary Robinson***, The Laboratory for Laser Energetics, The University of Rochester*; Soren Bentley,* UKAEA, UK*; Jeffrey Woodward,* NRL*; Alexander Kozen,* University of Vermont*; Thomas Cochran, Rashad Ahmadov, Joshua Ruby, Mark Wittman, Matthew Sharpe,* The Laboratory for Laser Energetics, The University of Rochester

Atomic layer deposition (ALD) is an ideal technique for deposition of films on arbitrarily-shaped containers such as those used to contain tritium for fusion applications. The substrates required for such containers generally differ from common ALD substrates, which have historically been primarily

semiconductors. In this talk, I will give an overview of a custom ALD system built to deposit permeation barrier films on substrates and components relevant for various fusion and fusion fuel-cycle applications.

The primary benefit of our ALD system is the ability to deposit films on arbitrarily-shaped surfaces, such as the interior walls of tubing and canisters used to contain tritium. Initially, we deposited thermal ALD alumina films on both silicon wafers and planar copper foil substrates. Characterization with ellipsometry yielded ALD growth rates of ~1.1 Å/cycle for temperatures between 100 °C and 210 °C on Si witness samples. X-ray photoelectron spectroscopy (XPS) on both the Cu foils and Si substrates indicates stoichiometric Al_2O_3. To quantify the permeation reduction factor (PRF) of the of the ALD films, the permeability of deuterium through 25µm-thick Cu-foils coated with 10 nm of alumina was measured. We found that thin ALD films have a PRF of ~25 at permeation temperatures between 275 °C and 350 °C.

Finally, we discuss the difficulty of achieving a high quality ALD-stainless steel 316 (SS316) interface, which is complicated by the complex surface chemistry and the interactions with vapor-phase metalorganic species. The native oxide on SS316 substrates is reactive with TMA, and forms an AlOH layer, as evidenced by XPS measurements. To prevent this interfacial hydroxide formation, substrates were polished and conditioned in the ALD reactor. Following these steps, linear growth rates of 1.2Å/cycle were achieved. The ALD films on steel substrates resulted in orders of magnitude reduction in hydrogen permeation.

Current efforts include developing new materials in our ALD reactor, including a fundamental study of ALD bilayer and nanolaminate performance as a hydrogen-permeation barrier.

This material is based upon work supported by the Department of Energy [National Nuclear Security Administration] University of Rochester "National Inertial Confinement Fusion Program" under Award Number(s) DE-NA0004144.

3:00pm **FUS-WeA-4 Passivation of Stainless Steel for Tritium Service**, ***Dale Hitchcock,*** Savannah River National Lab

Austenitic steels are generally preferred for hydrogen/tritium service due to their low hydrogen isotope permeability and relative resistance to hydrogen-isotope embrittlement. In applications where high purity gas is needed the surfaces in contact with hydrogen isotopes must be passivated to maintain gas composition. Passivation serves to minimize the surface features that catalyze isotopic exchange and to form a barrier against the ingress of impurities from the bulk. The passivation process generally includes an electropolishing step designed to minimize surface area by removing surface roughness and control surface chemistry followed by vacuum firing to both remove solubilized hydrogen from the bulk and also further modify the surface chemistry. Previously multiple vendors have supplied passivated components to the DOE, however, procuring "well" passivated components has become more difficult. This presentation will outline current efforts at SRNL to both evaluate the performance of vendor passivated material and also develop a robust passivation process inhouse.

3:15pm **FUS-WeA-5 Measurement of Hydrogen Isotopologues and Contaminant Species Within a Canister Coated with Alumina by Atomic Layer Deposition**, ***Matthew Sharpe,*** *Thomas Cochran, Zachary Robinson,* University of Rochester

The interaction of tritium with pristine metallic surfaces catalyzes the formation of various hydrogen molecular isotopologues (HD, HT, DT, etc.). Additionally, because these surfaces have not been exposed to tritium, protium (H) native to the surface will enter the gas phase by isotope exchange with tritium. For many Fusion applications, this dilutes the gaseous tritium concentration, thereby contaminating the gaseous tritium with undesired isotopes. Furthermore, protium present within the bulk structure of the metal can act as a source of additional contamination. Finally, any trace organics present on the surface may also enter the gas phase as tritiated compounds. These organic molecules may poison other tritium technologies or become a health or environmental risk. Mitigating this contamination may be possible by use of atomic layer deposition (ALD) of low permeable materials.

In this work, we show the results of an aging study of a stainless-steel (type 316) canister coated with an alumina layer deposited on the interior surface by ALD. The canister was mounted in a custom ALD system designed for deposition on arbitrarily-shaped and fusion-relevant components. In a series of measurements performed to evaluate the deposition in a canister similar to those used in this study, a 10% variation in film thickness was observed between the inlet and outlet of the canister. Films of > 10 nm were used for this study, deposited at a temperature of 150°C.

Once the ALD-coated canisters were prepared, several similar canisters were prepared with pre-treatments including solvent surface cleaning and vacuum baking. After pre-treatment or ALD coating, the canisters are exposed to tritium gas. Assessment of the effectiveness of various treatments is done by periodically sampling the gas phase and measuring with gas chromatography (GC). The GC method utilized allows for simultaneous injection of a sample into two columns. One column allows for measurement of common impurities (CH_4, CO_2, CO, O_2, N_2, Ar), while the second allows for discrimination of hydrogen isotopologues (H_2, HD, HT, D_2, DT, T_2).

This material is based upon work supported by the Department of Energy [National Nuclear Security Administration] University of Rochester "National Inertial Confinement Fusion Program" under Award Number(s) DE-NA0004144.

3:30pm **FUS-WeA-6 Native Protium Content in Stainless Steel Pipework**, ***James Pittard,*** *Kyle Shipman, Zhiheng Wu, Tshepo Mahafa, Rosemary Brown, Gowri Karajgikar, Iryna Bennett,* UKAEA, UK

Stainless steel pipework is used extensively for transporting gases, ranging from laboratory-scale experiments up to larger scale facilities. Such pipework is known to contain non-negligible amounts of native protium [J. Vac. Sci. Technol. A 21(1) (2002) 167–174], outgassing of which can limit the achievable vacuum and contaminate gas streams. For fusion applications, protium contamination could add additional requirements to an isotope separation system with the potential to change both the concentrations and speciation of isotopologues within gas flows. To assess the impact of native protium outgassing, an understanding of both the total inventory and the desorption energetics is required. This information can also be used to indicate potential tritium retention and transport through stainless steel components. Therefore, a series of thermal desorption spectroscopy (TDS) measurements have been carried out on samples taken directly from various pieces of SS316 pipework to give a value for inventory and an estimate for the variation between different pieces of pipe. TDS spectra consisted of a single broad peak which gave total inventory values of the order of 1018 H atoms g-1 (101 mol H atoms m-3). Spectra were fitted with a simple Fickian diffusion model using FESTIM [Int. J. Hydrogen Energy 63 (2024) 786–802] giving an activation energy for diffusion of 0.55 eV which aligns well with expected values. Some samples were measured twice, with the first measurement at a lower temperature meaning a desorption peak in the second measurement could still be seen. The model was able to reproduce desorption spectra for both initial and secondary measurements, whilst its simplicity would aid integration into larger, system scale models.

Plasma Science and Technology
Room 315 - Session PS1-WeA
Machine Learning for Plasma Processes

Moderators: Dr. Robert Bruce, IBM Research, T. J. Watson Research Center, **Joseph Vella**, TEL

2:15pm **PS1-WeA-1 Machine Learning-Assisted Plasma Process Monitoring and Optimization**, ***Fatima Jenina Arellano,*** *Kenta Doi, Fumito Ootake, Tadamasa Kobayashi, Kenta Tanino, Tzuan Chou, Yutaka Nishioka, Kouta Kawahara, Hanna Taku,* ULVAC, Inc., Japan **INVITED**

Advanced packaging is becoming an increasingly important part of AI-era semiconductor scaling alongside continued transistor scaling, as modern computing systems increasingly rely on heterogeneous integration, larger-format packaging, high interconnect density, and package-level thermomechanical reliability to achieve higher bandwidth, lower latency, improved power efficiency, and greater compute density. In both wafer and panel-level packaging, plasma-based etching must operate across increasingly diverse material systems including organic build-up films, dielectrics, polymers, metals, and deep silicon structures, while maintaining tight requirements in uniformity and reliability over larger substrates. In these systems, plasma nonuniformity and substrate warpage become major challenges that impact process stability and yield. To help address these challenges, we explore the use of machine learning techniques such as transfer learning, artificial neural networks, and Hidden Markov models alongside conventional plasma simulations, diagnostics, and process development tools. Target applications include correlating wafer-scale (often axisymmetric) plasma simulation behavior with panel-scale experimental results; improving endpoint detection and plasma process

monitoring for the etching of organic materials and deep silicon structures; bridging experimental and prediction gaps in electron temperature and electron density estimation from optical emission spectroscopy; and accelerating plasma process and tool optimization.

2:45pm **PS1-WeA-3 Autonomous Determination of Plasma Reaction Rates Using Plasma-Physics-Informed Machine Learning**, ***Yusuke Ando,*** *Takayoshi Tsutsumi, Kenichi Inoue, Kenji Ishikawa,* Nagoya University, Japan

The inherent complexity of plasma reaction fields has long hindered precise control of process outcomes. The lack of reaction databases often results in discrepancies between simulations and experiments and delays the implementation of new gas chemistries. The direct application of previously proposed methods for calculating reaction rates or cross sections, such as the transition state theory, remains challenging due to the vast number of reactions and nonequilibrium plasma fields where reactive species often deviate from the Maxwell-Boltzmann distribution. Consequently, data-driven approaches have recently attracted increasing attention as alternative analysis tools for process development [1]. In addition, previous studies have demonstrated that neural networks can virtually reproduce conventional liquid-phase chemical reactions [2].

In this study, we propose a plasma reaction neural network (PRNN) as a framework for the simultaneous analysis of plasma reactions. The neural network, designed based on plasma physics, consists of a single hidden layer with an exponential activation function and is capable of simulating the entire reaction network, where each node represents an elementary reaction. Given densities and temperatures of electrons, ions and neutral species at a certain time, the PRNN predicts the temporal evolution of each reactive species. This plasma-physics-informed machine learning architecture incorporates several physically meaningful parameters, particularly reaction rate coefficients. To validate the proposed model, time-resolved quadrupole mass spectrometry and Langmuir probe measurements were performed under various conditions with varied gas mixtures, pressures, and RF powers to train the PRNN. After fitting the model to the experimental dataset, the stoichiometric coefficients and reaction rate coefficients were extracted from the edge weights and node biases, respectively. The proposed methodology enables direct experimental acquisition of reaction rates with significantly reduced time and resources, regardless of the energy distributions of reactive species. Furthermore, the PRNN is applicable to other complex plasma systems, paving the way for efficient data acquisition for new gas chemistries and the realization of digital twins for plasma processes.

[1] Y. Ando et al., Diam. Relat. Mater. **151**, 111687 (2025) [2] W. Ji, S. Deng, J. Phys. Chem. A **125**, 1082 (2021)

3:00pm **PS1-WeA-4 Machine Learning Enhanced Kinetic Modeling of Plasma Processing Reactors**, ***Andrew Tasman Powis,*** Princeton Plasma Physics Laboratory*; Alexander Khrabry,* Princeton University*; Melanie Huynh,* University of California Berkeley*; Salman Sarwar,* Princeton University*; Domenica Corona Rivera, Edward Startsev,* Princeton Plasma Physics Laboratory*; Ali Mesbah,* University of California Berkeley*; Igor Kaganovich,* Princeton Plasma Physics Laboratory

For plasma processing, there is a need to simulate large plasma devices via kinetic means, since the Electron Velocity Distribution Function in these devices is non-Maxwellian and therefore fluid treatment is insufficient to accurately capture the physics. Even on modern GPU accelerated high-performance computing systems, such simulations can take days or even weeks to deliver engineering relevant insights. Machine Learning (ML) offers many possibilities for accelerating kinetic plasma simulation or developing reduced order models which can provide insights at speeds that could enable rapid computer aided engineering of plasma reactors. We will discuss three recent approaches, including (1) using convolutional neural networks to provide improved initial conditions for PIC simulations which can reduce runtime by nearly 20x [1], (2) development of a hierarchical-embedding autoencoder with predictor (HEAP) architecture which can accurately model the multiscale nature of plasma dynamics [2], and (3) generalizable and interpretable symbolic regression models for ion flux within a capacitively coupled plasma discharge [3]. Together, these methods demonstrate how ML can bridge the gap between high-fidelity kinetic simulation and the fast, predictive modeling needed for practical plasma reactor design.

[1] A. T. Powis, D. Corona Rivera, A. Khrabry, and I. D. Kaganovich, Phys. Plasmas 33, 013902 (2026).

[2] A. I. Khrabry, E. A. Startsev, A. T. Powis, and I. D. Kaganovich, Phys. Fluids 38, 045138 (2026).

[3] M. T. Huynh et al., submitted to Mach. Learn.: Sci. Technol. (2026).

3:15pm **PS1-WeA-5 Machine Learning Applications and Challenges in Low Temperature Plasma Systems**, ***Kallol Bera,*** Applied Materials, Inc.*; Abhishek Verma,* Applied Materials Inc.*; Sathya Ganta, Shahid Rauf,* Applied Materials, Inc. **INVITED**

Low-temperature plasmas (LTPs) are widely used in the semiconductor industry, where plasma modeling plays significant roles for chamber design and process optimization. However, physics-based plasma simulations are computationally expensive due to their multi-dimensionality, nonlinear behavior, multi-physics coupling, complex chemistry, plasma-surface interactions and wide spatio-temporal scales (nm to m, ns to s). These limitations hinder their use in applications requiring rapid and repeated computation. Machine learning (ML), particularly deep learning–based nonlinear model order reduction, is increasingly used to accelerate plasma modeling. ML enables fast design exploration, real-time control, and process optimization. Operator learning techniques help accelerate key solvers in multi-physics simulations. For complex plasma chemistries involving many species and reactions, methods such as principal component analysis, graph neural networks are used for mechanism reduction and identification of dominant pathways. Bayesian optimization is developed for real-time reactor control and multi-objective optimization. ML-based interatomic potentials further enable accurate and efficient modeling of plasma–surface interactions. Advances in machine learning for LTP systems are demonstrated through several examples. Deep neural networks trained on simulation data have been used to accurately predict plasma variables across operating conditions in inductively coupled plasmas. A neural network with long short-term memory (LSTM) predicts well the time evolution of electrode current from unseen voltage sequences in RF hollow cathode discharges using substantially lower computational cost within the training range and outside the range. Applications of Fourier neural operators (FNOs) and Physics informed neural network (PINN) for coupled PDEs describing capacitively coupled plasmas are also illustrated. Despite these advances, key challenges remain. High-fidelity training data whether generated using computational plasma modeling or experimentation, is scarce and expensive. ML models typically interpolate well but struggle to extrapolate. Exploring different gas chemistries and new reactor configurations are extremely challenging. LTP systems, being multiscale and strongly coupled across multiple physics, are difficult to learn. Purely data-driven models may also violate physical constraints. Physics-informed approaches, such as PINNs, aim to incorporate conservation laws into ML, improving reliability. Such hybrid ML models, combined with experimental data, offer a promising pathway toward digital twins for plasma-based semiconductor processes

Plasma Science and Technology
Room 315 - Session PS2-WeA

Low Global Warming Potential and Sustainability in Plasma Processing

Moderators: Phong Nguyen, Air Liquide, **Prof. Dr. Necip Uner**, Middle East Technical University

4:15pm **PS2-WeA-9 Impact of Low-GWP GST Etch Chemistries on PCM Device Performance and Reliability**, ***Luxherta Buzi,*** IBM Research*; Yohei Takakura, Kazunori Horiguchi,* DAIKIN INDUSTRIES, LTD.*; Aya Kagimura,* DAIKIN INDUSTRIES, LTD., Japan*; Asit Ray, Amlan Majumdar, Lynne M. Gignac, Matthew BrightSky, Jaylynn Sheppard,* IBM Research*; Yasuhiro Nojiri, Hisataki Hayashi,* DAIKIN INDUSTRIES, LTD., Japan*; Eric Joseph, Robert L Bruce,* IBM Research

PCM is an emerging non-volatile memory technology for AI and Storage Class Memory applications due to its low power consumption, high density, and fast switching capability. Optimization of GST etch chemistry and process integration while minimizing structural and compositional damage is critical for reliable PCM device operation and long-term endurance. GST is commonly etched using halogen-based plasmas, where hydrofluorocarbons are often employed for sidewall passivation and profile control. However, due to the ongoing phase-out of high global warming potential (GWP) gases, development of low-GWP alternatives is becoming increasingly important for future PCM manufacturing.

In this work we report on the development and integration of GST reactive ion etch (RIE) processes using DIN01, a proprietary low-GWP chemistry, combined with Xe and Ar gas mixtures with and without passivating additives. DIN01/Xe and DIN01/Ar processes demonstrated good elemental

composition and were successfully implemented on integrated PCM hardware. Electrical characterization showed excellent wafer yield, strong within-chip yield, fast SET speed, and high cycling endurance. PCM etch processes using DIN01/Xe gas mixtures exhibited superior electrical performance over DIN01/Ar mixtures.

Transmission electron microscopy (TEM) and chemical analysis were performed on DIN01/Xe etched devices and compared to a conventional PCM etch gas mixture. After approximately 20 programming cycles, similar electrical behavior and chemical evolution were observed for both process schemes without evidence of significant trace of gas residue. However, optimization is required to address poor etch selectivity to the SiN hard mask that leads to tungsten redeposition and oxidation in DIN01-patterned structures.

These results demonstrate that DIN01-based GST etch processes can successfully enable integrated PCM device operation and high yield while maintaining structural integrity and long-term device reliability.

4:30pm **PS2-WeA-10 A Low-GWP Molecule for High-Performance Plasma Etching**, ***Phong Nguyen***, *Nathan Stafford, Xiangyu Guo,* Air Liquide

In recent years, several countries and semiconductor manufacturing companies have announced targets for net-zero carbon emission by 2050 or earlier. Plasma etch processes are responsible for a high percentage of a semiconductor manufacturer's scope 1 emissions. Dielectric plasma etch applications are pervasive in the manufacturing process, and are a significant contributor to these scope 1 emissions. These processes typically employ high global warming potential (GWP) fluorocarbon gasses such as C4F8. . Not only is C4F8 a high GWP gas, in addition hard to abate high GWP chemistries such as CF4 maybe formed in the plasma fragmentation process.

To address this challenge without sacrificing process capabilities, we introduce a novel low-GWP molecule (intrinsic GWP ~0) designed as a robust alternative to legacy etchants. This alternative chemistry is engineered to permit advanced plasma etch performance while providing a friendly abatement profile that substantially reduces overall direct CO2-equivalent emissions, whether evaluated post pump with no dedicated PFC abatement technology or post abatement systems designed to abate a portion of the PFC.

Characterization of the etch characteristics is done using an Ellipsometer for thickness and selectivity assessment. Furthermore, the plasma etch chamber emission gas stream is analyzed and quantified by Fourier Transform Infrared Spectroscopy (FTIR). Complementary to FTIR analysis, Quadrupole Mass Spectrometry (QMS), is implemented to help identify emission species in the chamber through studying the positive ion fragments present inside the plasma.

Results demonstrate that this novel molecule matches legacy etching rates while delivering improved selectivity to amorphous carbon (a-C) mask materials. The combination of analysis via QMS and FTIR gives us a better understanding of the etching process, confirming that this novel molecule yields beneficial deposition-promoting positive ions and crucially lacks the CF3 fragmentation pathways responsible for excessive CF4 generation. In addition, this novel chemistry has shown improved etch performance with lower CO2 equivalent emission than the current baseline.

4:45pm **PS2-WeA-11 Machine-Learning-Assisted Investigation of CF_3–X (X=H, I) Plasma Kinetics In Semiconductor Manufacturing for Etch Effectiveness and Environmental Sustainability**, ***Chi-Yun Lin***, *Jane Chang,* UCLA

Hydrofluorocarbons (HFCs) gases are commonly used in semiconductor manufacturing to etch silicon dioxide, an essential insulator in integrated circuits, either from chamber wall deposits or patterned features. CHF_3 plasma is utilized for its high etch rate (ER), comparable to CF_4, and favorable anisotropic etching characteristics, though its high global warming potential (GWP_{100}) of 12400 and long atmospheric lifetime (LT) of 222 have prompted its phasedown by the EPA. CF_3I has a lower atmospheric lifetime (<0.005) and GWP_{100} (<1), which are 4-5 orders of magnitude smaller than those of HFCs, making it a promising alternative gas.

This work investigates CF_3X-based plasmas (where X = H, I) in etching SiO_2 with a focus on machine learning to extract meaningful kinetic parameters for modeling. $CHF_3/O_2/Ar$ plasma was first used to evaluate the reduce and abate strategies. O_2 serves a dual role: process-gas additive to reduce the usage of CHF_3 for improving SiO_2 etching and abatement reactant for reducing high-GWP fluorocarbon emissions. The experimental and modeled SiO_2 etch rate increased with measured emission of SiF_4 (kg-CO_2e) and the modeled ratio of fluorine flux to oxygen flux (Γ_F/Γ_O), reaching above 150 nm/min under selected conditions. The corresponding downstream composition was converted to $MMTCO_2e$ for CHF_3, CF_4, and C_2F_6. After introducing O_2 to downstream abatement, the modeled $MMTCO_2e$ decreased by approximately a few orders of magnitude relative to the untreated emission.

$CF_3I/O_2/Ar$ was evaluated as a lower-GWP alternative. A differentiable surface-kinetic model was developed to infer the unknown iodine adsorption and abstraction probabilities, using experimental SiO_2 etch rates as the ground truth, while modeled ion fluxes and etch rates served as known inputs. Descriptor information from CF_3X (X = F, Cl, Br, and I), including C–X bond dissociation energy, Si–X bond strength, and electronegativity, was used to define physically reasonable bounds for the unknown iodine-related surface kinetics. Automatic differentiation through the ODE solver reduced the average absolute percent error from 23% for the initial assumption to 12.5% after applying new surface kinetic by AI/ML inference. As the SiO_2 etch rate increases from 50–80 nm/min to above 100–130 nm/min, the corresponding measured and modeled emission for CF_3I and CF_4 decreases by an order of magnitude in $MMTCO_2e$.

Overall, selected $CF_3I/O_2/Ar$ operating conditions showed the SiO_2 etch rate increased by approximately 70% while the estimated emission impact reduce by an order of magnitude, indicating that higher etch performance can be achieved with lower greenhouse-gas-equivalent emissions.

5:00pm **PS2-WeA-12 A Low GWP and Low Emission Gas for Trench and Hole SiO_2 Etching**, ***Scott Biltek***, *Nathan Stafford, Phong Nguyen, Angéla Christin,* Air Liquide

Over the past few years, numerous countries and semiconductor manufacturing entities have unveiled their commitments to achieving net-zero carbon emissions by 2050 or even sooner. A substantial fraction of direct emissions (as CO_2e) in semiconductor manufacturing stems from plasma etch processes. Standard gases for dielectric etching such as C_4F_8, CH_2F_2, CHF_3 or CF_4 typically have high global warming potential (GWP) or emit high GWP byproducts after plasma fragmentation and recombination processes. While low GWP etch gases exist, it is challenging to find alternative gases that provide comparable etch process performance, with limited recipe development, that significantly decreases the direct CO_2e etch process emissions.

In previous work we have presented a novel low GWP etching gas as a replacement for C_4F_8 in high power, high aspect ratio etching[1]. In this work we revisit that gas as a replacement for C_4F_8 in lower power SiO_2 etches for both trench and contact hole applications. In both applications, we once again demonstrate matching etch performance with minimal recipe modification (simply replacing C_4F_8 flow with an appropriate replacement gas flow rate). Due to the high efficiency in the dissociation of the replacement gas, this etch performance is achieved at a significantly lower flow rate relative to C_4F_8. In addition to the low intrinsic GWP_{100} of the low GWP gas (<50) compared to C_4F_8 (~10,200), we also show significant (~80%) reduction in GWP_{100} of the final post plasma exhaust emissions as measured via fourier transform infrared spectroscopy (FTIR). In combination with past results, this strongly indicates the broad compatibility of this low GWP gas with current C_4F_8 plasma etch processes.

[1] - Biltek, Scott, et al. "Low GWP and Low Emission Gases for High Aspect Ratio Etching." AVS 70th International Symposium & Exhibition, Nov. 2024, Tampa, FL. Conference Presentation.

Surface Science
Room 305 - Session SS-WeA
Somorjai

Moderators: David Castner, University of Washington, **Prof. Jeong Park**, Korea Advanced Institute of Science and Technology (KAIST)

2:15pm **SS-WeA-1 Professor Somorjai's Impact on the Evolution of Surface Science**, ***Miquel Salmeron***, Lawrence Berkeley National Laboratory **INVITED**

The surface of materials usually exhibits unique chemical and electronic properties determined by their atomic structure, which is largely determined by their interaction with the external phases of vacuum, gas, liquid or solids. The current scientific foundation of the field of Surface Science was the result of the work of several Pioneers of which Professor Somorjai was a prominent one, who provided new concepts on the role of the surface structure that determine their properties. andthe development of new instruments. In this review I will highlight the evolution of surface

science in the last 40 years, and the important role of the development of new instruments and the discoveries they brought, to the scientific and engineering communities.

2:45pm **SS-WeA-3 Professor Somorjai's Impact on my Journey from Single Crystals to Biomaterials**, ***David Castner***, Depts of Bioengineering & Chemical Engineering

Surface science plays an important role in a wide range of research and development areas such catalysis, biomaterials, microelectronics, clean energy and corrosion. The toolbox of surface scientist allows us to easily move across research topics and make significant impacts in both industrial and academic settings. The typical surface scientist is an expert in multiple techniques, surface modification, sample preparation/handling and instrumentation. We have all benefited from the significant and numerous advances that have occurred in the past 50 years in terms of improved instrumentation, introduction of new techniques and development of sophisticated data analysis methods, which has allowed us to perform detailed analysis of increasing complex samples. I am extremely grateful for the training I received during my PhD studies with Professor Somorjai as well as his continued mentorship and support throughout my career. This talk will discuss my adventures as a surface scientist starting from chemisorption and reactivity studies of small molecules on single crystal surfaces at UC Berkeley followed by industrial catalysis research at Chevron and eventually moving to biomedical surface analysis at the University of Washington. It has been an exciting journey and I will use it to provide some examples of the multidisciplinary nature of surface science embraced by Prof. Somorjai and his students, post-docs and staff. For example, comprehensive analysis of surfaces and surface immobilized molecules with modern surface science instrumentation provides an unprecedented level of detail about the immobilization process and the structure of the immobilized molecules. However, even with the advances that have been achieved with these powerful surface science techniques, there remain many significant challenges for surface scientist. These include characterizing the surface chemistry and structure of nanoparticles, determining the atomic level structure of complex molecules bound to surfaces, 3D imaging of samples, and improved sample preparation methods that maintain materials in a relevant state when using ultra-high vacuum-based analysis techniques.

3:00pm **SS-WeA-4 Surface Chemistry at the Sliding, Solid-Solid Interface**, ***Wilfred Tysoe***, University of Wiscosin-Milwaukee

Somorjai realized that the action of lubricants was inherently a surface science problem and, in 1995, was instrumental in launching Tribology Letters. The focus of the journal was to be on the science, rather than the engineering, of tribology, the study of friction and wear, and this is still its guiding principle today. Furthermore, the ultrahigh vacuum approach to understanding surface chemistry pioneered by Somorjai can be adapted to studying sliding-induced reaction pathways and this approach is illustrated here by studying a simple model tribochemical reaction consisting of the lubrication of copper by dialkyl disulfides. For example, this approach identifies a tribochemical reaction cycle, analogous to a catalytic reaction mechanisms, which includes shear-induced adsorbate decomposition and a mixing processes that causes adsorbates to be transported into the subsurface region to form a friction-reducing film. These model systems are sufficiently simple so that they are amenable to being analyzed using first-principle density-functional theory calculations that allow a deep understanding of the physical principles that underpin stress-induced reactions on surfaces to be obtained.

3:15pm **SS-WeA-5 Structural Evolution and Stability of Rh/TiO_2 Catalysts under CO_2 Hydrogenation Conditions**, ***Simon R Bare***, SLAC National Accelerator Laboratory; *Greg Barber,* Penn State University; *Xiaobo Chen, Judith Yang,* Brookhaven National Laboratory; *Robert Rioux,* Penn State University

At low temperatures (< 400°C), single atoms of Rh supported on rutile TiO_2 ($rTiO_2$) are responsible for the formation of CO during the reverse water gas shift (RWGS), while methane production is associated with the Rh-TiO_2 interface due to the observed correlation between methane formation rates and the volume-averaged Rh nanoparticle diameter.As the temperature is increased to >540°C, there is a notable increase in CO selectivity as the methane production rates tend towards zero.At 600°C and > 4 h time on stream, the catalytic behavior becomes completely agnostic to the initial Rh structure as well as weight loading, and the catalysts are highly selective for the RWGS reaction.Post-reaction HR-TEM image analysis confirms Rh nanoparticles crystallize/order during the reaction; at 400°C, most of the Rh particles are disordered, while at 600°C, they are more ordered. Infrared spectroscopy of CO adsorption on Rh nanoparticles supports the appearance of defined facets after annealing in nitrogen at high temperatures.will be referenced to the pioneering research of Gabor Somorjai in the 1980's where he showed the ability of Rh(111) surfaces and the Rh(111) terraces of stepped Rh single crystal surfaces to dissociate CO_2.

3:30pm **SS-WeA-6 Origins of Lipid Asymmetry in Supported Biomembranes**, ***Paul Cremer***, *Ruofei Wang, Ella Gregory,* Penn State University

Biological membranes show remarkable asymmetry in living systems. Phospholipids, such as phosphatidylethanolamine (PE) and phosphatidylserine (PS), primarily reside on the inner leaflet, while others, like phosphatidylcholine (PC) and sphingomyelin (SM), are more abundant on the outer leaflet. While maintaining this asymmetry in vivo requires significant energy from ATP-hydrolyzing enzymes, we show—using a novel lipid bilayer unzipping assay—that an uneven lipid distribution exists at equilibrium solely due to differences in the hydrogen-bonding environments between the leaflets. Specifically, a remarkable degree of asymmetry was generated using planar glass supports rich in hydrogen-bond acceptors that form stronger hydrogen bonds with PE and PS lipids than with water. Protein-coated substrates yielded nearly identical results. These findings have important implications for in vivo systems, where distinct hydrogen-bonding gradients naturally exist between the inner (cytoskeletal) and outer (glycocalyx) leaflets.

4:15pm **SS-WeA-9 Behavior of Cu-Pt Single-Atom Alloy Catalysts Under Realistic Conditions**, ***Francisco Zaera***, Dept. Chemistry **INVITED**

There has been some recent interest in the use of so-called single-atom catalysts, whereby one catalytic metal is isolated within a second to add a key but otherwise unavailable functionality, to control selectivity during the hydrogenation of organic reactants. We have recently shown that metal alloys consisting of Pt single atoms diluted within Cu nanoparticles selectively promote the hydrogenation of C=O bonds in unsaturated aldehydes, a reaction of interest in fine chemical manufacturing. Our rationale, that Cu surfaces may favor C=O over C=C hydrogenation steps with atomic hydrogen but may require Pt sites to promote the initial activation of molecular hydrogen, was corroborated by kinetic catalytic experiments. However, fundamental surface-science studies and quantum mechanics calculations showed a more nuanced picture. Specifically, IR titration experiments using carbon monoxide failed to identify Pt atoms accessible on the surface of the catalysts, suggesting that their catalytic contribution may involve indirect electronic changes on neighboring Cu atoms. Additional *in situ* x-ray absorption (XAS) data have indicated a preference for the Pt atoms to locate at the metal/support interface. DFT calculations also support the preference for the Pt atoms to be placed at the metal nanoparticle/silica boundary, and explain how they can still facilitate H_2 activation, remotely. These results have led us to reinterpret the way that single-atom alloy catalysts operate.

4:45pm **SS-WeA-11 Plasmonic Hot Carrier-Driven Catalytic and Photoelectrochemical Processes**, ***Jeong Y. Park***, Department of Chemistry, Republic of Korea

The detection of hot electrons and understanding the correlation between hot electron generation and surface phenomena are challenging questions in the surface science and catalysis community. The earlier works in Berkeley indicate hot electron flow generated on a gold thin film by photon absorption (or internal photoemission) appears to be correlated with localized surface plasmon resonance. In addition, it has been found that the hot electron flux generated under photon absorption and exothermic chemical reaction is the major mediator of energy conversion process [1-3]. In this talk, I highlight the research direction to attempt to detect the surface plasmon driven hot carrier at the nanometer scale by using scanning probe microscopy. To detect and utilize the hot electron flows at the macroscale level, the metal-semiconductor nanodiodes were constructed. At the nanometer scale, we utilized photoconductive atomic force microscopy to observe photoinduced hot electrons on a triangular Au nanoprism on n-type TiO2 under incident light. This is the direct proof of the intrinsic relation between hot electrons and localized surface plasmon resonance. We observed surface plasmon induced hot hole by using the system of Au nanoprism on p-type GaN [4]. I will discuss the impact of hot carriers in the photocatalytic activity under photoelectrochemical water splitting by using Au-based plasmonic nanostructures [5] an AuPd bimetallic nanoparticles [6]. Plasmon-driven hot carriers provide new mechanistic insight into light–matter interactions at catalytic interfaces and offers a pathway toward designing highly efficient plasmonic energy conversion systems.

References

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5:00pm **SS-WeA-12 2D Ising Model for Enantiomer Adsorption on Achiral Surfaces: L- and D-Aspartic Acid on Cu(111)***, **Andrew Gellman**,* Carnegie Mellon University, USA

The 2D Ising model is well-formulated to address problems in adsorption thermodynamics. It is particularly well-suited to describing the adsorption isotherms predicting the surface enantiomeric excess, *ees*, observed during competitive co-adsorption of enantiomers onto achiral surfaces.

Herein, we make the direct one-to-one correspondence between the 2D Ising model Hamiltonian and the Hamiltonian used to describe competitive enantiomer adsorption on achiral surfaces. We then demonstrate that adsorption from racemic mixtures of enantiomers and adsorption of prochiral

molecules are directly analogous to the Ising model with no applied magnetic field, i.e., the enantiomeric excess on chiral surfaces can be predicted using Onsager's solution to the 2D Ising model. The implication is that enantiomeric purity on the surface can be achieved during equilibrium

exposure of prochiral compounds or racemic mixtures of enantiomers to achiral surfaces.

Thin Films
Room 317 - Session TF-WeA
Far from Equilibrium Thin Films and Processes

Moderators: Dr. Saeed Almishal, Pennsylvania State University, **Prof. Lauren Garten**, Georgia Institute of Technology

2:15pm **TF-WeA-1 Frustration and Function in Single Crystal Compositionally Complex Oxides***, **Zac Ward**,* Oak Ridge National Laboratory **INVITED**

High entropy materials open vast compositional phase spaces inaccessible in conventional binary and ternary systems. Stabilizing single-crystal films comprising five or more principal cations in increasingly complex and reduced-symmetry crystal structures is creating new opportunities for discovering unexpected and exotic phenomena. Recent work has demonstrated that these systems can exhibit unique combinations of structural, thermal, and chemical robustness alongside continuously tunable electronic, magnetic, and optical properties relevant to next-generation computing and sensing architectures. The ultrashort quench times intrinsic to laser ablation are ideally suited to trapping these compositions as homogeneous, randomly mixed solid solutions. Here we discuss ongoing efforts using nonequilibrium pulsed laser deposition to synthesize perovskite, spinel, and Ruddlesden–Popper single crystal high entropy oxides. Observed functionalities are interpreted through many-body effects driven by inherent frustrations among coupled spin, charge, and lattice order parameters. Finally, we describe how these science drivers are motivating the development of autonomous synthesis platforms integrated with multimodal characterization and AI/ML-guided closed-loop optimization. These capabilities aim to accelerate the construction of reproducible defect–structure–function maps and to deliver experimentally grounded datasets essential for data-driven discovery.

2:45pm **TF-WeA-3 Designing Altermagnetism and Topological States in Ultrathin Multiferroic $BiFeO_3$***, **Lucas Caretta**,* Brown University **INVITED**

Magnetoelectric multiferroics - materials in which electric polarization and magnetic order are intrinsically coupled - offer a platform for ultralow-power switching, nonvolatile memory, and energy-efficient transduction. Yet practical deployment demands ultrathin films down to the atomic limit, where both orders typically degrade. Maintaining both order parameters at the thinnest scales in complex oxides remains a tremendous challenge, as uncompensated bound charge drives nanoscale depolarization in most ferroelectrics, while off-stoichiometry, reduced anisotropy, and charge transfer can produce magnetic dead layers in ultrathin oxides at substrate interfaces. Here, we realize a metastable multiferroic phase of $BiFeO_3$ (BFO) that not only sustains both order parameters at room temperature with no dead layer in the four unit cell, ultrathin limit, but also exhibits signatures of emergent altermagnetism. This second-order, thickness-driven phase transition gives rise to new multiferroic topological textures, where electric and magnetic symmetries become intertwined in previously unobserved ways. Additionally, we show pathways to design altermagnetism and topology at thicker length scales, where at domain boundaries, we uncover a rich hierarchy of noncollinear topological magnetoelectric structures, including polar bi-merons, polar vertices coupled to magnetic cycloid disclinations, and topological cycloidal knots, whose stability and dynamics are intimately linked to the underlying crystal symmetry. These findings establish a pathway to stabilize multi-order topology at device-relevant thicknesses and reveal emergent magnetic symmetry. Collectively, they reframe scaling limits in oxide multiferroics and open the door to emergent topological phenomena and ultralow-energy functionalities in correlated quantum materials.

3:15pm **TF-WeA-5 Chemical Disorder in Improper Ferroelectrics***, **Billy Yang**, Jeffrey Hodgson, David Sanchez, Sai Venkata Gayathri Ayyagari, Saeed S. I. Almishal, Nasim Alem, Jon-Paul Maria,* The Pennsylvania State University

Among rare-earth oxide derivatives, hexagonal manganites h-$RMnO_3$ (where R = Sc, Y, Dy-Lu) stand out as particularly interesting for exploring their geometrically driven improper ferroelectricity by exhibiting a polar phase with a space group of $P6_3cm$ below the Curie temperatures of approximately 1250 K. These materials further demonstrate multiferroic behavior below 100 K, with antiferromagnetic order occurring in the Mn sublattice. In this study, we report the synthesis of a high-entropy rare-earth manganite ($Y_{0.167}Gd_{0.167}Dy_{0.167}Ho_{0.167}Er_{0.167}Yb_{0.167}MnO_3$) in both bulk and thin-film forms, with X-ray diffraction (XRD) confirming that both forms stabilized as a hexagonal single-phase structure. Thin films with a targeted thickness of 80-100 nm were deposited by pulsed laser deposition (PLD) onto YSZ substrates and conductive bottom electrodes of Pt and ITO films for ferroelectric testing. Polarization-electric field measurements confirmed robust ferroelectric hysteresis loops at room temperature with a remanent polarization of ~2 μC/cm^2. Structural characterization via scanning transmission electron microscopy (STEM) reveals a polar structure accompanied by the rare-earth displacements and captures the domain structures. Preliminary magnetic measurements indicate non-negligible saturation magnetization values both in-plane and out-of-plane below 50 K. Furthermore, we investigate the influence of the growth atmosphere and discuss the associated defect chemistry in relation to the improper ferroelectricity. Ultimately, this work provides a detailed discussion of potential A-sites (e.g., Gd and Eu, which are traditionally orthorhombic-stabilizing species) and B-site disorder (e.g., Fe and Ga, for potential magnetic ordering tuning), and presents the first thorough investigation of improper ferroelectricity in a complex high-entropy system. These results demonstrate that the geometrically driven improper ferroelectricity remains remarkably robust against extreme local chemical disorder and defects, leading to a new design principle for novel multiferroic materials.

3:30pm **TF-WeA-6 Magnetic Exchange Bias Control in Kinetically-Arrested High-Entropy Oxide Heterostructures***, **Joseph Petruska**,* The Pennsylvania State University*; Timothy Charlton,* Oak Ridge National Laboratory*; John Heron,* University of Michigan*; Jon-Paul Maria, Saeed Almishal,* The Pennsylvania State University

High-entropy oxide (HEO) thin films grown under far-from-equilibrium conditions uniquely combine extreme chemical disorder with exceptional crystalline coherence. In this talk, we demonstrate predictive control of this anomalous crystalline state through the kinetic arrest of metastable macrostates. Specifically, aliovalent cation substitution, tightly controlled substrate temperature, and high adatom kinetic energy during growth enable deterministic programming of the out-of-plane lattice parameter in coherent rock salt HEOs while preserving in-plane epitaxial pinning to MgO. Using this approach, multilayer heterostructures sustaining lattice strains exceeding 5% can be stabilized, where the defect chemistry is dominated by trivalent cations compensated by cation vacancies, producing valence interfaces across which the Co valence evolves from predominantly Co^{2+} to a mixed Co^{2+}/Co^{3+} state. These chemically disordered yet coherent valence interfaces give rise to emergent magnetic phenomena that we interrogate using magnetic hysteresis measurements and polarized neutron reflectometry.We will highlight two exemplar pseudomorphic heterostructures:500°C (Sc,Mg,Co,Ni,Cu,Zn)O/300°C(Sc,Mg,Co,Ni,Cu,Zn)O(JSc/JSc)and500°C(Sc,Mg,Co,Ni,Cu,Zn)O/300°C(Cr,Mg,Co,Ni,Cu,Zn)O(JSc/JCr) where the abrupt,

exceptionally large coherent strain and valence interface generates emergent magnetic macrostates inaccessible in equilibrium analogs.

4:15pm **TF-WeA-9 Probing Disorder and Metastability in Complex Oxide Thin Films with X-ray Absorption Spectroscopy**, ***Christina Rost***, Virginia Tech **INVITED**

X-ray absorption spectroscopy (XAS) has become an indispensable tool for understanding materials systems that exist far from equilibrium, particularly high entropy oxide and metastable thin films where conventional diffraction techniques often fail to capture the complexity of the local atomic structure. In these systems, functional behavior is frequently governed not by the average crystal structure, but by distributions in local coordination environments, oxidation states, and short-range chemical ordering that emerge from configurational disorder, strain, and kinetic stabilization during synthesis. XAS provides element-specific sensitivity to local bonding, coordination geometry, and electronic structure, enabling direct interrogation of chemically distinct local environments even in highly disordered or nanostructured films.Our work leverages synchrotron-based XAS to investigate the local structural evolution of compositionally complex oxide thin films synthesized under far-from-equilibrium growth conditions using pulsed laser deposition. These studies focus on understanding how compositional complexity, strain, and metastability influence local bonding environments and electronic structure in functional oxide systems. XAS enables direct probing of non-equilibrium valence states, local distortions, and chemically distinct coordination environments that are inaccessible through conventional crystallography alone. By combining XANES and EXAFS measurements with complementary electrical, ferroelectric, magnetic, and structural characterization, this approach establishes experimentally grounded links between local disorder and emergent functional behavior. These studies demonstrate that XAS is uniquely positioned to resolve the local structural complexity that underpins next-generation functional oxide thin films designed through disorder, metastability, and non-equilibrium synthesis.

4:45pm **TF-WeA-11 Epitaxial Strain Engineering of Correlated Electronic States and Crystal Structure in Thin Film Nickelates**, ***Abigail Jiang***, Harvard University*; Maria Bambrick-Santoyo,* Massachusetts Institute of Technology*; Lopa Bhatt,* Cornell University*; Kyeong-Yoon Baek,* Harvard University*; Yi-Feng Zhao,* Arizona State University*; Dan Ferenc Segedin, Ari Turkiewicz, Jenna Hatmin, Grace Pan,* Harvard University*; Suchismita Sarker,* Cornell University*; Donald Walko,* Argonne National Lab*; Charles Brooks,* Harvard University*; Berit Goodge,* Max Planck Institute for Chemical Physics of Solids, Germany*; David Muller,* Cornell University*; Hua Zhou,* Argonne National Lab*; Antia Botana,* Arizona State University*; Julia Mundy,* Harvard University

Since the discovery of high-temperature superconductivity in cuprates, there have been long-standing efforts to understand and engineer the underlying electronic and crystal structure in superconducting materials. A new family of high-temperature superconductors was recently discovered in the *n=2,3* Ruddlesden-Popper (RP) nickelates [1,2]. When bulk crystals of these nickelates are placed under large hydrostatic pressures, superconductivity is stabilized concomitant with suppression of correlated density wave states, and also concomitant with crystallographic symmetry raising [1,2]. Thus far, compressive epitaxial strain has been demonstrated to mimic effects of pressure in *n=2* RP nickelates, leading to ambient-pressure superconductivity and equivalent structural changes in compressively-strained thin films [3,4]. However, ambient-pressure superconductivity and other analogous effects of strain have not yet been demonstrated in the *n=3* compound. Here, we use reactive oxide molecular beam epitaxy (MBE) to synthesize a series of *n=3* RP nickelate ($La_4Ni_3O_{10}$) thin films across a wide range of epitaxial strains [5]. Combining electronic transport, picoscale electron microscopy, and synchrotron X-ray diffraction techniques, we develop a strain-dependent electronic and structural phase diagram for *n=3*. Critically, we identify a structural distortion and corresponding crystal symmetry not present in *n=3* (or *n=2*) bulk crystals, highlighting key distinctions within the RP nickelate family towards engineering more robust superconducting materials, and demonstrating the unique capability of epitaxial synthesis to stabilize new metastable states in complex oxides.

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5:00pm **TF-WeA-12 Optimizing Interfaces in High Entropy Carbides for Ultra High Hardness**, ***Nestor Marquez Rios***, *Tainara de Carvalho, Jon-Paul Maria,* The Pennsylvania State University

High chemical disorder compositions like high entropy transition metal carbides display potential for materials with high mechanical properties, high stability in extreme conditions and low synthesizability cost compared to the gold standard C-BN and diamond. These materials have shown the ability to impinge dislocation nucleation and dislocation motion at the nanoscale due to a non-uniform energy landscape; hardening the materials. A second mechanism that enhances hardness in materials is the interface addition in a multilayer system to impinge dislocation motion at the microscale. To tackle these two mechanisms, we have synthesized carbide films with high chemical disorder, (Ti Zr Hf Nb Ta) C, and multilayer them with TiC using 2 bipolar high-power impulse magnetron sputtering (HiPIMS) with methane gas as a carbon source.To determine the effect that synthesis parameters have on thin film crystalline structure, morphology and hardness we have being studying the effect reactive gas flow, temperature, HiPIMS conditions and interface quality and density in 600 nm thin films varying superlattice periods. X-ray diffraction (XRD), Scanning electron microscopy (SEM), Transmission electron microscopy (TEM) and Hardnes nanoindentation is employed to characterize the synthesized films.With XRD we established distinct superlattices with extremely sharp interfaces and with SEM we have being able to capture the ideal morphology to maximize hardness and minimize the possible morphology error in the hardness measurements. TEM Analysis is also used to study with higher resolution interface characteristics. We find these carbides superlattices display higher hardness values for films synthesized with smooth interfaceswith value of 35 GPa vs 30 GPa at sharp interface, and optimized methane flow. The morphology of the film is affected by the carbon content and showed that at stoichiometric carbide the films are smooth without columnar structure, with an increased grain density which in turn increases the dislocation motion resistance. Further development of the synthesis processmight lead to new hardened carbide structures with unexplored hardness values.

The Future of Temperature Sensing
Room 320 - Session TS-WeA

The Future of Temperature Sensing III

Moderators: Dr. Olga Kozlova, LNE-CNAM, **Dr. Nikolai Klimov**, National Institute of Standards and Technology

2:15pm **TS-WeA-1 Enabling New Measurement Capabilities with Fiber-Optic Thermometry**, ***Stephan Krenek***, *René Eisermann,* Physikalisch-Technische Bundesanstalt (PTB), Germany*; Guillaume Failleau,* Laboratoire National de métrologie et d'Essais (LNE), France*; Xin Lu,* Bundesanstalt für Materialforschung und -prüfung (BAM), Germany*; Peter Thomas,* Norwegian Research Centre AS (NORCE), Norway*; Henrik Kjeldsen,* Danish Technological Institute (DTI), Denmark **INVITED**

Accurate temperature measurement and control are fundamental to advancements in industry and the energy sector. Transitioning to a clean industry is essential for ensuring future competitiveness. This transition necessitates not only the reduction of carbon emissions but also the assurance of reliable and affordable clean energy. Accurate thermometry is an enabling technology that facilitates the optimization of energy safety, storage, and transmission. It also contributes to the enhancement of industrial efficiency. Fiber optic thermometry has emerged as a promising solution for applications where conventional electrical temperature sensors are impractical. This technology offers unique advantages, including immunity to electromagnetic interference and the ability to make spatially distributed measurements over long distances. However, the lack of metrological characterization, and thus SI traceability, currently hinders its widespread adoption. As with all sensors, fiber optic sensors exhibit cross-sensitivities and aging effects that must be investigated, quantified, and minimized to ensure low uncertainty temperature measurements.

Over the past three years, the European project INFOTherm has begun to unlock the full potential of fiber optic thermometry by addressing current limitations and implementing calibration methods and infrastructure. A key aspect of this project was demonstrating fiber optic thermometry in real-world scenarios. Industrial case studies examined the ability of fiber optic thermometry to optimize energy infrastructure and improve the efficiency of processes in high-temperature industrial environments.

Case studies have been performed in thermal energy storage in molten salt tanks, geothermal systems, submarine cable monitoring, high-voltage

component diagnostics, and silicone and glass production. These successful case studies were made possible by improving fiber optic thermometry throughout the project, particularly by enabling the traceable calibration and reducing measurement uncertainties, while extending the operational temperature range.

This presentation will provide a comprehensive overview of the INFOTherm project, with a focus on the practical implementation of fiber optics in the energy and industrial sectors. Recent progress will be highlighted. This includes improved calibration techniques for distributed sensing methods and advancements in fiber optic sensors for high temperatures.

2:45pm **TS-WeA-3 Distributed Fiber-Optic Thermometry for High-Fidelity Temperature Metrology in Harsh and Thermally Heterogeneous Environments**, *KOUSTAV DEY, Grant Whitham,* ***Laura Bartlett****, Rony Kumer Saha, Farhan Mumtaz, Ronald J. O'Malley, Jeffrey D. Smith, Rex E. Gerald II, Jie Huang,* Missouri S&T

Recent advances in distributed optical fiber sensing are enabling transformative approaches for high-resolution temperature metrology in harsh manufacturing environments. In this work, we developed a scalable, high-resolution distributed thermometry platform based on Rayleigh backscattering (RBS)-enabled optical frequency domain reflectometry (OFDR) for real-time spatial thermal mapping during the aluminum casting process. The system utilzed silica optical fibers (UHNA1, Thorlabs) interrogated with a high-speed OFDR platform, enabling high-density thermal metrology with a resolution of approximately 0.65 mm (~1538 points m^{-1}) and acquisition rates up to 62 Hz. The sensing approach was successfully integrated into elevated-temperature casting environments, including the casting of AA356 aluminum in 3D-printed investment shells. Distributed thermal data were acquired throughout the full casting cycle, including shell preheating, molten metal pouring, and subsequent solidification at temperatures approaching 700 °C, showing trends consistent with thermocouple measurements. The platform effectively captured localized thermal gradients, transient heat-transfer phenomena, and the spatio-temporal evolution of temperature during solidification, while the optical fiber remained intact after molten metal pouring and was reusable for subsequent measurements, demonstrating the robustness of the sensing platform in harsh casting environments. Unlike conventional thermocouple-based systems, the distributed fiber-optic approach provided near-continuous thermal measurements along the length of a single optical fiber, significantly improving spatial sensing capability while remaining minimally invasive. The results demonstrate the strong potential of RBS-enabled distributed fiber-optic sensors as robust thermometry platforms for metal casting and other advanced manufacturing applications operating in extreme environments. This work further establishes a foundation for intelligent process monitoring, real-time thermal diagnostics, and digital twin-enabled manufacturing systems, while highlighting the broader applicability of distributed fiber-optic thermometry for next-generation harsh-environment sensing technologies.

3:00pm **TS-WeA-4 Toward SI-Traceable Photonic Thermometry using Dual-Comb Spectroscopy**, ***Peter Chang****, Nathan Brooks, Tsung-Han Wu,* Chi3 Optics

Precise measurements of temperature are an important requirement in many fields, with functions ranging from process control in manufacturing, to disease treatment in medicine, to military applications. Whereas the Standard Platinum Resistance Thermometer (SPRT) is a robust and simple method to measure temperature to uncertainties less than 10mK, their sensitivity to mechanical shock and need for routine calibration has motivated research to establish platforms based on photonic thermometry [1]. A photonic thermometer is composed of an element highly sensitive to temperature (a photonic thermistor), and a means to reference the device to a primary standard. For example, a prominent platform is the silicon photonic thermometer (SPoT), which uses the narrow resonance of a photonic crystal cavity that can be calibrated against the thermal Brownian motion of its nanomechanical resonator [2]. Here, we propose a platform based on dual-comb spectroscopy (DCS), where the absolute frequency axis retrieved in DCS is used to provide a primary standard. In particular, by leveraging developments in low SWaP and compact fully self-referenced frequency combs, we aim to employ a high resolution 50MHz dual-comb spectrometer covering 30nm of optical bandwidth in the C-band. This spectrometer can be paired with a fiber Bragg grating [3] or a NIST standard reference gas-cell [4] to resolve temperature-dependent frequency shifts below 100MHz with direct SI traceability. Its high resolution targets the 10 mK sensitivity range, while SI traceability can be provided either in the RF by locking the repetition rate to a reference oscillator, or in the optical domain by locking a comb line to an optical standard. Together, these capabilities point toward a compact and fieldable thermometry platform relevant to precision metrology in demanding environments.

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3:15pm **TS-WeA-5 A Practical Approach to Johnson Noise Thermometry**, *Robert Crabtree,* Isothermal technology Ltd, UK*;* ***Carl Baines****,* Isothermal Technology Ltd, UK

Johnson Noise Thermometry (JNT) offers a primary, electrically traceable approach to temperature measurement.

Achieved by directly linking the Johnson noise voltage across a resistive probe to temperature as defined by the Johnson-Nyquist equation. Presented is aconcise overview of JNT from its theory, through prior arts to modern techniques, and outlining real-world applications. Topics include noise signal acquisition and processing, andpractical challenges of implementation across laboratory and industrial environments. Recent advances in JNT development to realise a practical Johnson noise thermometer will also be examined, with a discussion of its evolving role within the broader landscape of precision thermometry.

3:30pm **TS-WeA-6 Validated Dissemination: What Makes a Primary-Standard Bridge Trustworthy in a Post-Redefinition Traceability Chain**, ***Abhishek Sengupta****,* WIKA Group, UK

Since the 2019 kelvin redefinition, thermodynamic temperature can be realized directly through methods anchored to the Boltzmann constant. Realization, however, is not dissemination - and dissemination determines whether a primary realization becomes a deployable, qualified measurement in the field. A calibrated kelvin still reaches accredited laboratories and industrial processes through standard platinum resistance thermometers and the ratio bridges that read them.

This contribution is from the manufacturer of one such instrument: the WIKA CTR9000, an AC resistance ratio bridge built on the ASL technology deployed at most national metrology institutes for ITS-90 realization and dissemination. One reason it occupies that role at parts-per-billion scale is architectural. Top-tier bridges derive accuracy from transformer-based ratio determination set by integer winding counts that cannot drift. The CTR9000 implements this in AC - continuously alternating excitation, inductive voltage divider ratio determination, quadrature balancing - where thermal EMFs sit at DC and never enter the measurement bandwidth, so each reading is a continuous measurement rather than a composite of two opposite-polarity readings combined by symmetry.

What gives the 20 parts-per-billion specification its standing is the framework of independent validations behind it: zero and unity checks, complement measurements by swapping resistors and evaluating the reciprocal, ratio test units against a calculable network, resistance bridge calibrators against a combinatorial standard, and long-term stabilization during manufacture. Each catches an error the others would miss, each works by physical manipulation of real ratios, independent of internal references. This carries the instrument from factory specification to qualified field deployment.

Drawing on a current cooperation with PTB on the CTR9000, the talk frames the AC bridge as the interface between primary realization and accredited dissemination. Of the methods enabled by the redefined kelvin, Johnson noise thermometry sits closest: a quantum voltage noise source provides the reference against which a sense resistor's thermal noise is compared, and the resistance contributes directly to realized temperature. As photonic, optomechanical, and noise-based primary thermometers move from laboratory demonstration toward deployable, qualified systems, each will face the question the bridge has answered over decades: not how

accurate it can be in principle, but what architecture and framework will make the trust transferable.

4:15pm **TS-WeA-9 Fiber Optic Phosphor-Based Temperature Sensors: Can It Replace Industrial Platinum Resistance Thermometers (IPRTs)?***, Noah J.J. Johnson,* ***Michael Goldstein****,* Accelovant Technologies Corporation, Canada

IPRTs are the industrial standard for highly accurate, reliable and repeatable temperature measurement in the range of -200°C to 650°C. Despite their rugged construction, IPRTs do suffer from drift due to mechanical shock and vibration necessitating costly routine recalibration. Fiber optic phosphor-based temperature sensors can potentially achieve drift free performance that require no recalibration over time. These sensors are also unaffected by electromagnetic fields, RF, MRI, and microwave radiation making them attractive for medical and high-voltage environments. The all optical sensing tip eliminates sparking and electrical hazards making them suitable for oil, gas, and mining industries. In this talk, we will present our successful effort towards commercializing fiber optic phosphor-based temperature sensors that outperform the tolerance specification of commercial IPRTs. Temperature measurement range (-200°C to 650°C), drift (<0.05°C for 1000 hours at 450°C) and repeatability (within ±0.01°C) measurements show they can potentially match current industrial performance standards. The presentation will highlight the technology and its overall suitability as an easily scalable, cost effective replacement of IPRTs in various industrial applications.

4:30pm **TS-WeA-10 Industry Panel Discussion - Scaling Up Temperature Innovation: Challenges, Opportunities, and Global Adoption -- Panelists: Isotech, WIKA, Fluke, Chi3 Optics, U.S. Air Force**

Panelists: Isotech, WIKA, Fluke, Chi3 Optics, U.S. Air Force

This industry panel brings together leaders from Isotech, WIKA, Fluke, Chi3 Optics, and the U.S. Air Force to examine how next–generation temperature–sensing technologies can move from laboratory innovation to broad industrial deployment. Panelists will discuss commercialization challenges, key roadblocks, and practical strategies to accelerate worldwide adoption of advanced temperature–metrology solutions.

Vacuum Technology
Room 321 - Session VT+FUS-WeA

Vacuum Technology Fusion

Moderators: Freek Molkenboer, TNO Science and Industry, the Netherlands, **Dr. Alan van Drie**, TAE Technologies

4:15pm **VT+FUS-WeA-9 The "Wall" in Fusion Reactors***, David Ruzic,* University of Illinois at Urbana-Champaign **INVITED**

Due to the recent invention of flexible high-field super-conducting magnets which can sustain fields up to 20 Tesla, commercial magnetic fusion energy may soon be a reality.These fields will contain a thermonuclear plasma that could have equivalent heat loads to the surface of the sun – some 60 MW/m^2.Nothing can withstand that power load, so much effort has gone into designing systems that will "only" experience on the order of 10 MW/m^2.That wall material is not allowed to contaminate the plasma or the fusion reaction will stop.This issue of the plasma-facing-component is one of the most serious engineering challenges.However, there are more challenges.A fusion device must make more tritium than it uses, and that includes tritium permeation.A breeder blanket will surround the plasma which will contain lithium.Neutrons from the D-T reaction will hit lithium and make more T.That tritium needs to be recovered and contained.Finally the structure of the fusion device must be able to withstand enormous transient loads from magnetic excursions and not fall apart due to transmutations and atomic displacements from the copious neutron flux.And, by the way, the whole system has to e vacuum tight.This talk will explain all of these challenges and describe the leading solutions and largest uncertainties.

4:45pm **VT+FUS-WeA-11 Overview, Construction Status, and Engineering Challenges of the Vacuum Systems for the Material Plasma Exposure eXperiment (MPEX)***, Jonathan Perry, Aftab Hussain, Adam Aaron, Ted Biewer,* ORNL

The Material Plasma Exposure eXperiment (MPEX) is under construction at Oak Ridge National Laboratory. MPEX will be a first-of-its-kind steady-state linear plasma device that will enable neutron-irradiated materials to be exposed to fusion reactor-relevant divertor plasma conditions for the study of plasma-material interaction. This facility will be capable of generating high heat fluxes and high ion fluences to test fusion divertor prototypic plasma-facing materials at steady-state for up to 10^6 seconds with in-situ diagnostics and magnetic fields up to 2.5 T. This presentation will provide an overview and construction status of the MPEX vacuum systems that promote efficient heating of the plasma, create an environment for prototypic divertor plasma conditions, enable in-situ diagnostics, and maintain vacuum during transportation and post-exposure diagnostic examination of the tested material. Due to the operating environment and performance requirements of MPEX, many engineering challenges came up during the design, fabrication, and assembly phases of the MPEX vacuum systems. This presentation will also discuss the lessons learned and implemented, as well as the knowledge leveraged from the ITER project and other facilities around the world, to develop, manufacture, and assemble the vacuum systems for MPEX. Unique cleaning and assembly techniques to ensure cleanliness is maintained throughout the assembly and installation process will also be discussed in this presentation.

This work was supported by the Oak Ridge National Laboratory managed by UT-Battelle, LLC for the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.

5:00pm **VT+FUS-WeA-12 Miniaturized, Fully Shielded High-Voltage Vacuum Feedthroughs from 50 kV to 300 kV***, Moein Borghei,* Avalanche Energy

High-voltage vacuum feedthroughs rated above 100 kV are rarely available as commercial off-the-shelf products, and those at 100 kV or below are often oversized and unshielded, i.e., have exposed electrodes at high voltage. These gaps limit researchers and engineers building fusion machines, electron guns, X-ray sources, ion beam systems, and other high-voltage vacuum platforms, who must either tolerate poor component fit or resort to lengthy custom procurement cycles.

To meet the diverse high-voltage needs of Orbitron fusion machines [1], we developed a suite of four fully shielded, CF-flanged feedthroughs. These models -the Thresher, Bigeye, Mako, and Hammerhead- span a wide voltage range from 50 kV to 300 kV. All designs utilize low-outgassing ceramic insulators, such as aluminum oxide and MACOR. The ceramic component is hermetically sealed to standard stainless steel conflat flanges, with leak rates lower than 1×10^{-9} atm·cc/s of He. The feedthroughs are fully shielded, eliminating exposure of high-voltage surfaces on the outside, thus enhancing integration within compact systems and operator safety.

The primary design objective was to minimize the footprint while ensuring reliable, steady-state operation. Mako and Hammerhead are within 15 cm and 20 cm flange sizes, respectively, both half the volume of the designs provided in the literature for the voltage class [2]. Similarly, Bigeye transmits 100 kV through a 7 cm flange compared to the 15 cm flange of the COTS feedthrough. Thresher does the same for 50 kV in a 3.4cm instead of 7 cm.

In this talk, we present experimental results and design methodology for insulator geometry, electrode designs, and electric-field stress mitigation that simultaneously enable achieving the rated voltage while maintaining hermetic seal integrity. We also present measured performance metrics across these feedthroughs, including dark current, bakeout impact, role of contaminants, and the conditioning process.

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2D Materials

Room 304 - Session 2D-ThM

2D Materials Devices and Applications

Moderators: Dr. Kai Xiao, Oak Ridge Natinal Laboratory, **Huamin Li**, University at Buffalo

8:00am **2D-ThM-1 Morphology and Adhesion of Carbon Nanowalls Grown via Microwave Surface Wave Plasma on Various Substrates**, ***Parker Hays,*** *Dhruval Patel, Dren Qerimi,* University of Illinois at Urbana-Champaign*; Michael Stowell,* Lyten*; David Ruzic,* University of Illinois at Urbana-Champaign

Carbon nanowalls (CNWs) have a wide range of applications in energy storage, sensing, and other technologies due to their high surface area, electrical conductivity, and mechanical strength. However, their deposition remains challenging, particularly on substrates such as aluminum where adhesion is poor, limiting their integration into practical devices.

In this work, a microwave surface wave plasma (MSWP) is used to deposit CNWs on aluminum, copper, and silicon substrates. Growth is performed via plasma-enhanced chemical vapor deposition (PECVD), using methane and hydrogen as precursor gases and argon to enhance plasma ionization. The high-density microwave plasma promotes methane dissociation into reactive carbon species, while hydrogen radicals preferentially etch amorphous or sp^3-bonded carbon. A heated sample stage is employed to promote surface mobility and favor growth pathways associated with nanowall formation.

CNWs are grown while varying experimental parameters, including gas composition, pressure, and substrate temperature. Resulting CNW morphology is characterized using scanning electron microscopy (SEM) and Raman spectroscopy, while adhesion is evaluated via triboindentation. Aluminum is expected to exhibit significantly lower adhesion compared to copper and silicon, motivating future efforts to incorporate adhesive interlayers for improved film stability. These results provide insight into substrate-dependent growth mechanisms and inform strategies for improving CNW adhesion in device-relevant systems.

8:15am **2D-ThM-2 Orientation-Independent Strong TERS Response in Anisotropic ReS_2 on Gold**, ***Andrey Krayev,*** HORIBA Instruments Incorporated*; Pavel Valencia-Acuna, Oliva Primera-Pedrozo, Chih-Feng Wang,* PNNL

Rhenium disulfide (ReS_2) crystallizes in a distorted 1T‘ lattice with triclinic symmetry arising from Re–Re dimerization, which produces in-plane anisotropic properties and a dense set of Raman-active modes with mixed atomic displacements. Prior conventional Raman microscopy studies in this material showed strong dependence of absolute and relative intensities of some Raman bands on the mutual orientation of the optical electric field and the in-plane crystalline axii. In presented study we show strongly enhanced (at least 10 times over the far field background) tip enahnced Raman scattering (TERS) response from 1-4 L ReS_2 on gold which not only enables high spatial resolution in the TERS maps, but also remains to great extent indifferent to the in-plane orientation of the ReS_2 crystals. We attribute this orientation indifference to the fact that in the gap mode TERS configuration optical electric field is normal to the crystal plane. Additionally, we demonstrate in our TERS spectra presence of low frequency bands the spectral position of which correlates with the local crystal layer number and matches very well previously published conventional Raman data which allows a straightforward nanospectroscopic assessment of the layer number even in sub-micron sized crystals.

8:30am **2D-ThM-3 Optical properties of 2D chiral perovskite thin films (R-MPA)2PbI4 and (R-BrPEA)2Pb2I4 from near infrared to Ultraviolet**, ***Suresh Chaulagain,*** The University of Toledo, USA*; Tingting Zhu, Zhaoning Song, Nikolas J. Podraza,* The University of Toledo

Two-dimensional (2D) chiral perovskites have drawn significant attention due to promising optoelectronic properties like tunable bandgap, high absorption coefficients, robust quantum confinement effects, circular dichroism, and prolonged environmental stability. 2D chiral perovskites are anticipated to exhibit the benefits of both lead halide-based perovskites and chiral materials. These attributes of 2D chiral perovskites make them suitable for light-emitting diodes, photovoltaics, photonic lasers, and circularly polarized light detection. Despite a wide range of potential applications, limited studies have been conducted on the optical properties of 2D chiral perovskites. In this work, we studied the optical properties of $(R\text{-}MPA)_2PbI_4$ and $(R\text{-}BrPEA)_2Pb_2I_4$ perovskite thin films on soda lime glass (SLG), single crystal (100) oriented $SrTiO_3$, and in a stack suitable for electrical characterization using spectroscopic ellipsometry to extract and compare their complex dielectric function spectra, band-to-band critical point transitions, and bandgap energies.Optical response of 2D chiral perovskite $(R\text{-}MPA)_2PbI_4$ and $(R\text{-}BrPEA)_2Pb_2I_4$ thin films have been extracted in the form of complex dielectric function ($e = e_1 + ie_2$) spectra and compared over the photon energy range from 0.73 to 5.89 eV. For the $(R\text{-}MPA_2PbI_4$ thin film, seven direct critical points are identified at 2.462, 2.541, 2.782, 2.83, 3.44, 4.12, and 5.69 eV, with their dimensionalities from critical point analysis. For the $(R\text{-}BrPEA)_2Pb_2I_4$ thin film, seven critical points are determined at 2.49, 2.638, 2.690. 3.15, 3.79, 4.17, and 5.86 eV with their dimensionalities from critical point analysis. The direct bandgaps for $(R\text{-}MPA)_2PbI_4$ and $(R\text{-}BrPEA)_2Pb_2I_4$ thin films are determined from Tauc plots to be 2.4323 ± 0.0003 and 2.453 ± 0.001 eV, respectively.

Acknowledgement

Public Affairs release approval #_____.

8:45am **2D-ThM-4 Molecular Dynamics Simulation of Plasma-Surface Interactions for Transition Metal Dichalcogenides**, ***Jaehong Kwon,*** Princeton University, Republic of Korea*; Jeremy Mettler, Vincent Donnelly,* University of Houston*; David Graves,* Princeton University

Transition metal dichalcogenide (TMD) semiconductors such as WS_2 are enabling a variety of new 2D devices that serve as complementary building blocks for alleviating challenges in silicon integrated circuits (ICs), owing to their atomically thin geometry, layer-tunable bandgap, and dangling-bond-free interfaces [1]. Because the electronic structure of TMDs is strongly thickness-dependent [2], device performance hinges on atomic-precision control of layer count. Plasma atomic layer etching (ALE), in which alternating O_2 and BCl_3 plasma steps thin the film one monolayer at a time, is a candidate process. To understand the atomistic mechanism of the O_2 modification step, we combine experiment and molecular dynamics (MD) simulation. In the experiments, WS_2 samples are exposed to a 20% O_2/Ar inductively coupled plasma, and the resulting surface chemistry is characterized by in-vacuum X-ray photoelectron spectroscopy (XPS).

To create an MD potential tailored to plasma–surface interactions on WS_2, we fine-tune the Universal Models for Atoms (UMA), a graph neural network (GNN)-based foundation machine-learning interatomic potential (MLIP) recently released by Meta FAIR [3]. Although GNN-based MLIPs incur higher computational cost than other MLIP architectures, they often deliver higher accuracy and accommodate additional element types without modification [4]. After fine-tuning, UMA reaches near-DFT accuracy on the W–S–O system (energy MAE ~5 meV/atom, force MAE ~80 meV/Å). Simulating 15 eV O_2^+ exposure of WS_2 at cumulative doses up to ~20×10^{15} cm^{-2}, we observe layer-selective modification: the topmost layer takes up chemisorbed oxygen, while physisorbed molecular O_2 and sulfur-containing species (in the form of SO_x) accumulate between the layers, and the layer immediately beneath shows only minor modification. The simulated dose-dependent oxygen uptake reproduces the trend measured experimentally by XPS. These results provide an atomistic baseline for the self-limiting selectivity needed in WS_2 plasma ALE and a template for applying GNN-based foundation MLIPs to other plasma–surface interaction problems.

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9:00am **2D-ThM-5 Operando SEM Study of WS_2 Growth**, ***Shaoliang Guan,*** *Stephan Hofmann, Jinfeng Yang, Hao Yu,* University of Cambridge, UK

Salt enhanced chemical vapor deposition of WS_2 and related 2D materials is widespread, and while many mechanisms including vapor-liquid-solid (VLS) mediated growth have been suggested, gaining a more detailed understanding remains challenging. We employ operando scanning electron microscopy to resolve the entire process of salt-assisted CVD of WS_2, focusing on a model system of individual, small (<100 μm), sapphire supported sodium tungstate (Na_2WO_4) salt particles. We reveal support interactions that lead a salt particle to develop a lateral halo interface, driven by surface eutectic melting above 630 °C. This halo dictates the salt

wetting as well as Na and W transport, and thus upon gaseous sulfur precursor exposure dominates the spatiotemporal WS_2 nucleation and mono- and multilayer domain expansion kinetics, all of which we can directly track by secondary electron (SE) contrast with a conventional InLens SE detector. Unlike for a conventional VLS mechanism, large (>20 μm) monolayer WS2 formation does not involve the salt droplet directly attached to the growth facets, rather the salt droplet drives WS_2 layer growth in the contiguous halo interface region with a continuous supply of W. We compare this to SiO_2 and NaOH treated sapphire where corrosive surface roughening dictates the salt wetting, and critically discuss our findings in the context of the connected wider literature.

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9:15am **2D-ThM-6 *in-situ* Characterization of Thermal Atomic Layer Deposition Process for Extrinsic P-Type MoS_2 Thin Films***, Sungjoon Kim, Jeffrey Elam,* Argonne National Laboratory

Computational energy consumption is increasing exponentially, making energy-efficient microelectronics and computing an urgent need. Three-dimensional integrated circuits (3D ICs) and neuromorphic computing promise to revolutionize information technology by drastically reducing the energy consumption of computers, and two-dimensional (2D) semiconductors like molybdenum disulfide (MoS_2) can enable such technologies. However, the development of complementary p-type MoS_2 is needed to fully leverage the benefits of 2D semiconductors. Moreover, thermal processes for thin film deposition are preferred over plasma-based techniques in high aspect ratio applications such as vertical gate-all-around transistors and 3D NAND.Here, we demonstrate the uniform and controlled deposition of extrinsically doped p-type MoS_2 using thermal atomic layer deposition (ALD). By varying the dopant cycle ratio, the final MoS_2's resistivity and charge carrier concentration can be precisely tuned. The resulting p-type MoS_2 was characterized using techniques including *in-situ* spectroscopic ellipsometry, *in-situ* FTIR, Raman spectroscopy, X-ray photoelectron spectroscopy, and Hall measurements. This work offers a pathway to deposit p-type 2D materials with tailored material properties.

9:30am **2D-ThM-7 Nanostructured TiS_2@TiO_2 Nanotube Arrays Fabricated by Magnetron Sputtering for Efficient Energy Storage***, Raman Devi,* IIC, Indian institute of technology Roorkee, India*; Ramesh Chandra,* Indian institute of technology Roorkee, India

The development of advanced electrode materials with high surface area, excellent electrical conductivity, and superior electrochemical stability is essential for next-generation energy storage applications. In the present work, anodized TiO_2 nanotube arrays are proposed as a binder-free electrode platform for enhanced energy storage performance. Titanium foil will be anodized to fabricate highly ordered TiO_2 nanotubes with large active surface area and efficient ion transport pathways. Subsequently, a TiS_2 thin film will be deposited over the nanotubular architecture using magnetron sputtering to improve the electrical conductivity and electrochemical activity of the electrode. The hybrid TiO_2 nanotube/TiS_2 structure is expected to combine the structural stability of TiO_2 with the high conductivity and pseudocapacitive behaviours of TiS_2, thereby enhancing charge transfer kinetics and electrolyte accessibility. The synthesized electrodes will be characterized using X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM), and electrochemical techniques including cyclic voltammetry (CV), galvanostatic charge–discharge (GCD), and electrochemical impedance spectroscopy (EIS). The proposed hierarchical nanostructured electrode is anticipated to exhibit improved specific capacitance, rate capability, and cyclic stability, making it a promising candidate for high-performance supercapacitor applications and future energy storage technologies

Keywords: Anodization, TiO_2 nanotube arrays, Magnetron sputtering, Binder-free electrode, Energy Storage

9:45am **2D-ThM-8 Low-Temperature Deposition and Annealing of NbXW1-XSY Thin Films for Photolithography-Compatible Processing***, Gia Rivers,* University of Michigan, Ann Arbor*; Rebecca A. Dawley,* University of Michigan*; Anil Adhikari, Steven J. Koester,* Notre Dame University*; Ageeth Bol,* University of Michigan, Ann Arbor

Two-dimensional transition metal dichalcogenides (2D-TMDs) are promising class of layered materials for next-generation metal-oxide semiconductor field effect transistors (MOSFETs). Tungsten diselenide (WSe_2) is one 2D p-type semiconductor that has generated interest as a channel material for scaled MOSFETs. However, device performance is limited by high contact resistance at the metal/semiconductor interface. Prior work has shown that a plasma-enhanced atomic layer (PEALD) deposited $Nb_xW_{1-x}S_y$ film grown at 300°C can serve as a doped contact interlayer and reduce contact resistance.[1,2] However, the elevated deposition temperature complicates integration with photoresist-based lithographic processing. Here, we report a supercycle PEALD process for $Nb_xW_{1-x}S_y$ deposition at 120°C to improve compatibility with certain photolithography fabrication flows. Initial $Nb_xW_{1-x}S_y$ thin films of a ~10nm thickness were deposited onto SiO_2/Si substrates and characterized using Raman spectroscopy, X-ray photoelectron spectroscopy (XPS, and four-point-probe measurements. Raman and XPS indicate that the as-deposited films are amorphous and sulfur rich, with S/(W+Nb) ≈ 3.5, and exhibit a high sheet resistance of $4.63x10^9$ μΩ*cm. To recover material quality after depositing at low temperatures, we investigate post-deposition annealing at 450°C and 900°C. After optimization of annealing conditions, XPS shows that the films approach more ideal stoichiometry with S/(W+Nb) ≈ 1.9, while Raman indicates improved crystallinity with the emergence of the characteristic A_{1g} and E^1_{2g} modes. Additionally, there is a large reduction in the sheet resistance to $4.88x10^3$ μΩ*cm after 450°C annealing and $3.04x10^3$ μΩ*cm after 900°C annealing. Finally, deposition on PMMA-patterned samples is used to assess process compatibility with resist-patterned device structures, demonstrating the viability of integrating low-temperature PEALD $Nb_xW_{1-x}S_y$ contact interlayers into lithography-based device workflows.

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11:00am **2D-ThM-13 Hierarchical Heterostructure of 2D Nicob@Co_3O_4 for Energy Saving Hydrogen Generation***, Krishna Modi, Anand Joshi,* Micro-Nano Research & Development Center, Parul University, India

The development of efficient and low-cost two-dimensional electrocatalysts for hydrogen generation is crucial for clean energy technologies.Herein, the rational engineering of two-dimensional Co_3O_4 and NiCoB heterostructure is studied for the energy-saving hydrogen production coupled with the methanol oxidation reaction. Initially, cobalt oxide (Co_3O_4) nanoflowers are deposited on Ni foam using a facile hydrothermal synthesis approach. Subsequently, NiCoB nanosheets are homogeneously deposited onto Co_3O_4 through a dip-coating-assisted chemical reduction strategy, resulting in the formation of a hierarchical nano-heterostructure. A fabricated nano-heterostructure was characterized using various characterization techniques, such as SEM, elemental mapping, and XPS. The SEM image suggests that the successful growth of NiCoB nanosheets on Co_3O_4 nanoflowers offers hierarchical heterostructure formation. Furthermore, XPS analysis suggests the presence of Ni 2p, Co 2p, B 1s, and O 1s elements. Electrochemical study demonstrates that the as-fabricated Co_3O_4@NiCoB nano-heterostructure exhibits excellent HER and OER performance, achieving an overpotential of 0.247 V vs RHE and 1.52 V vs RHE, respectively, at 100 mA/cm^2. Furthermore, introducing methanol into the electrochemical reaction has resulted in an overpotential of 1.33V at a current density of 100 mA/cm^2. Furthermore, the two-electrode NiCoB/Co_3O_4||NiCoB/Co_3O_4 cell provides a cell voltage of 2.03V for water electrolysis and 1.74 V for methanol-based electrolysis at a current density of 100 mA/cm^2, showing a significant reduction in energy consumption for the hydrogen generation. Additionally, NiCoB/Co_3O_4||NiCoB/Co_3O_4 provides the stability of 80 hrs at a higher current density of 100 mA/cm^2 in the methanol electrolysis configuration, and the formation of value-added formate species is confirmed from the NMR analysis. Overall, this study represents an important development of highly active, stable, and highly conductive metal oxide-metal boride-based nanocomposites for energy-saving hydrogen generation.

11:15am **2D-ThM-14 Hybrid Pd@Graphene Oxide–Magnetite Nanozyme Materials: Design, Properties, and Theranostic Potential***, Davide Patti, Giulia Lacanea, Giuseppe Attinasi, Luisa D'Urso, Giuseppe Forte,* University of Catania, Italy*; Irina Naletova,* National Council of Research, Italy*; **Cristina Satriano**,* University of Catania, Italy

Hybrid nanozyme materials that combine catalytic and functional properties are becoming increasingly interesting for advanced theranostic

applications. In this study, we present the design, synthesis and characterisation of a novel material consisting of palladium–graphene oxide–magnetite (Pd@GO–Fe_3O_4). Palladium nanoparticles were immobilised on graphene oxide sheets decorated with nanomagnetite to yield multifunctional hybrid architectures with combined catalytic, magnetic and biointerfacial properties. The physicochemical characteristics were systematically investigated using UV–visible, XPS, Raman and FTIR spectroscopies, as well as dynamic light scattering, zeta potential measurements, atomic force microscopy and electron microscopy. Nanozyme activity was evaluated through catalytic and light-assisted redox reactions, which revealed the pivotal role of interfacial interactions and Pd dispersion in catalytic performance. Magnetic responsiveness enabled efficient manipulation and recovery, while GO provided structural stability and enhanced surface functionality. Biointerface interactions were assessed in cancer cell models via cytotoxicity and intracellular ROS generation, revealing dose- and structure-dependent responses. Under light irradiation, the hybrid nanozymes exhibited photothermal and photocatalytic activity, demonstrating multimodal functionality. Overall, Pd@GO–Fe_3O_4 nanozyme hybrids represent a versatile nanocatalyst platform with tunable catalytic efficiency and theranostic potential.

11:30am **2D-ThM-15 Taguchi-Based Analysis of Wear Performance in SLA Printed Boron Nitride Composites**, ***Swathi Bale***, Government Engineering College, Hassan, Karnataka, India

This work uses the Taguchi technique to optimize wear behaviour in hexagonal boron nitride-reinforced stereolithography (SLA) composites. Cylindrical wear samples based on the ASTM G99 standard were created utilizing an Anycubic SLA printer and photosensitive resin reinforced with hexagonal boron nitride (h-BN) particles at different weight percentages (0, 0.5, 1.0, and 1.5 wt%). The following process characteristics were taken into account: Material composition (Mc), Build angle (Ba), Post-curing time (Pc), and Lift speed (Ls). Wear experiments were carried out using a pin-on-disc apparatus with a constant load of 10 N, sliding speed of 200 rpm, and sliding distance of 502.72 m/s. Scanning Electron Microscopy and Energy-Dispersive X-ray Spectroscopy (EDAX) were used to assess h-BN particle dispersion for the developed samples. The signal-to-noise (S/N) ratio and analysis of variance (ANOVA) were used to identify the best process parameters and their relative contributions to wear rate. The findings showed that material composition had the greatest impact on wear rate (49.724%), followed by lift speed (27.075%), post-curing time (16.934%), and build angle (6.266%). The morphology of the worn surface was studied by SEM analysis. The ideal combination of parameters for producing the lowest wear rate was found to be 1.5 wt% BN, 90° construction angle, 30 minutes post-curing period, and 15 mm/min lift speed. The outcomes of this work show that the Taguchi technique has the ability to optimize the wear behaviour of h-BN reinforced SLA composites, which can be useful in a variety of applications that need improved tribological features.

11:45am **2D-ThM-16 Advanced Nanostructured Graphene Devices for Real-Time Environmental and Agricultural Sensing**, ***RAPTI GHOSH***, University of Chicago, India

Sustainable agriculture requires continuous monitoring of nutrients and air quality to improve crop growth, reduce fertilizer waste, and increase resource efficiency. However, conventional nutrient analysis methods, such as ICP-MS, ion chromatography, and colorimetric assays, are expensive, laboratory-based, and unsuitable for real-time monitoring. Commercial CO_2 and O_2 sensors also face limitations because they are bulky, costly, and sensitive to humidity. To address these challenges, we propose an integrated platform of advanced printable devices and nanostructured materials for sensing and photonic applications. The system combines plant-derived graphene thin-film transistors (FETs) with curvature-engineered nanostructures for real-time monitoring of macronutrients and greenhouse gases in hydroponic and aeroponic systems. The sensor platform uses eco-friendly graphene ink synthesized from plant-derived carbon materials. The devices are fabricated using scalable inkjet or aerosol-jet printing to produce flexible and low-cost FET sensor arrays. The graphene channels are functionalized with selective receptors, such as ferritin for phosphate sensing and amine-containing molecules for CO_2 detection. These functional layers enable selective sensing through charge-transfer interactions at the transistor surface. In addition, curvature-engineered 2D heterostructures improve surface reactivity and electronic properties, enabling ultrasensitive detection of contaminants. This work integrates advanced materials, nanoelectronics, and intelligent sensing into a single multifunctional platform. The proposed system provides a scalable and sustainable approach for autonomous environmental monitoring, precision nutrient mapping, and next-generation smart agriculture technologies.

12:00pm **2D-ThM-17 Xenon Trapping in Two-Dimensional Silicate Nanocages under Air-Containing Gas Environments**, ***Laiba Bilal***, XenCage Technologies

Previous studies demonstrated that plasma-assisted ionization enables xenon trapping within two-dimensional silicate nanocages supported on metal powders. These investigations established the feasibility of noble gas confinement in scalable nanocage materials under controlled xenon environments. An important remaining question is whether xenon trapping can be maintained in the presence of atmospheric species introduced through air-containing gas mixtures.

In this work, we investigate xenon trapping in silicate nanocage powders exposed to xenon-air gas mixtures under near-ambient-pressure conditions. Silicate nanocages supported on transition metal powders were exposed to plasma-activated xenon in the presence of air and subsequently characterized using ambient-pressure and ultra-high-vacuum X-ray photoelectron spectroscopy. The experiments were designed to evaluate the influence of air-containing gas environments on xenon trapping and retention within the nanocage structure.

Preliminary results reveal clear Xe photoemission features following exposure and evacuation, indicating successful xenon trapping despite the presence of atmospheric gas components. These observations suggest that the confinement mechanism remains active in mixed-gas environments and that competing species do not completely suppress noble gas trapping under the investigated conditions. Ongoing analysis is focused on quantifying trapping behavior and evaluating the influence of gas composition on noble gas retention.

This work extends previous studies of noble gas trapping in two-dimensional silicate nanocages and provides new insight into trapping behavior under mixed-gas conditions. The results support future investigations of xenon and krypton capture, retention, and recovery in nanocage-based materials relevant to isotope production, nuclear technologies, and environmental applications.

Actinides and Rare Earths
Room 320 - Session AC-ThM

Actinides and Rare Earths Early Career

Moderators: Dr. MIles Beaux, LANL, **Dr. Krzysztof Gofryk**, Idaho National Laboratory, **Prof. Itzhak Halevy**, Ben Gurion Uni. Be'er Sheva, **Prof. Dr. Gertrud Zwicknagl**, Technical University Brauschweig

11:00am **AC-ThM-13 Scanning Tunneling Spectroscopy Reveals Extreme Stoichiometric Sensitivity in Actinide Oxides**, ***Benjamin Heiner***, *Miles Beaux,* Los Alamos National Laboratory

With the recent availability of single crystals, we have characterized the surface of Np2O5 using scanning tunneling spectroscopy (STS) at cryogenic temperatures. In addition to the band gap, two electronic features were observed on the surface: finite electron density in the previously observed band gap and a semimetallic suppression of the density of states at the Fermi Energy. These were unexpected and unpredicted, but using a proven theoretical model, we attribute these behaviors to areas of the crystal surface with variable oxygen vacancies. The model predicts that as oxygen vacancies are added to the calculation, the neptunium 5f orbital density fills in the band gap of pure Np2O5 until the crystal eventually becomes semimetallic. This work contextualizes the characterization of plutonium substoichiometric sesquioxide by STS, which contradicts calculation of plutonium oxides to be semiconductors. That the band gap of Np2O5 collapses into semimetallic behavior leads us to hypothesize that stoichiometric plutonium oxides would also have band gaps, but the electronic structure of actinide oxides are sensitive to even slight deviations to atomic ratios.

LA-UR-26-23359

11:15am **AC-ThM-14 Structural and Magnetism of Lanthanide- and Actinide-based Pyrochlores**, ***Binod Rai***, *Gia Thinh Tran,* Savannah River National Lab

Pyrochlore oxides are of significant interest because of their structural flexibility, radiation tolerance, and complex magnetic behavior arising from geometric frustration. In lanthanide- and actinide-based pyrochlores, the corner-sharing tetrahedral network promotes competing magnetic interactions that can lead to unconventional magnetic ground states and

emergent quantum phenomena. These materials are also promising candidates for nuclear waste immobilization due to their ability to accommodate radionuclides while maintaining structural stability.

In this work, we investigate the structural, magnetic, and thermodynamic properties of the solid-solution series $(Tb_{1-x}Er_x)_2Ti_2O_7$. The end-member compounds exhibit contrasting magnetic behaviors: $Tb2Ti_2O_7$ remains magnetically disordered at very low temperatures despite strong antiferromagnetic interactions, whereas $Er2Ti_2O_7$displays antiferromagnetic ordering. By systematically varying the Tb/Er ratio, we examine how competing anisotropies and exchange interactions influence the evolution of magnetic frustration and phase behavior. Structural characterization is correlated with magnetic susceptibility and heat-capacity measurements to establish composition-dependent trends. In addition, recent results on actinide-based pyrochlores will be presented, highlighting their structural stability and magnetic properties relevant to strongly correlated 5f-electron systems and nuclear materials applications.

11:30am **AC-ThM-15 Role of Surface Oxidation in the Interdiffusion Behavior of Uranium-Niobium Diffusion Couples**, ***Michelle Greenough***, *Joseph Boro, Adrian Gonzales, W. Preston Cole, Debra Rosas, Erik Oerter, Scott Donald, Tien Roehling, Tae Wook Heo,* Lawrence Livermore National Laboratory

Understanding uranium oxidation behavior under controlled environmental conditions is important for predicting the stability and long-term performance of uranium-based materials. In this study, oxidized pieces of uranium were then incorporated into uranium-niobium diffusion couples to serve as a system for evaluating the impact of oxide chemistry and thickness on uranium-niobium diffusion. Both the oxidized specimens and U-Nb diffusion couples were characterized using Auger electron spectroscopy (AES), X-ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM), and electron probe microanalysis (EPMA). These complementary techniques allowed for correlation between oxide characteristics and the nature of the formed diffusion couple. Oxide chemistry and thickness were demonstrated to influence the resulting diffusion material after testing several different relative humidities.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 and was supported by the LLNL-LDRD Program under Project No. 25-ERD-005.

11:45am **AC-ThM-16 Laboratory-Based X-Ray Absorption Spectroscopy of Actinide Materials**, *David Shuh, Alexander Ditter,* Lawrence Berkeley National Laboratory (LBNL)*;* ***Haisley Windsor***, Lawrence Berkeley Lab, University of California, Berkeley

Synchrotron radiation spectroscopy of actinide materials has led to marked improvement in the fundamental understanding of their *f*-electron chemistry and physics. Beamlines and endstations with unique spatial resolution, energy resolution, and intensity characteristics have made it possible to determine the chemical and physical properties of a range of actinide materials. The recent development of tunable laboratory-based x-ray instruments with sufficient performance, albeit not fully to the level of synchrotron radiation facility beamlines/endstations, are beginning to provide a reasonable alternative for x-ray measurements of actinide materials. The first results from the LBNL Sigray QuantumLeap x-ray absorption spectroscopy (XAS) spectrometer will be presented.

At the same time as interest and capabilities are growing in laboratory-based actinide XAS, there has been already been great activity in the tender x-ray region for high-resolution studies of actinide materials. As synchrotron radiation light source upgrades get underway at the Advanced Light Source (ALS-U) and at the National Synchrotron Light Source II (NSLS IIU), it is worthwhile to assess and present the possible impact of new, fully-optimized tender x-ray beamline/endstation capabilities on the field of actinide science conducted in energy region with respect to current capabilities.

12:00pm **AC-ThM-17 Scanning Tunneling Spectroscopy of Pu Compound Crystals**, ***Miles Beaux***, *Benjamin Heiner,* Los Alamos National Laboratory*; Andrew Yost,* Scienta Omicron*; William DeBenedetti, Filip Ronning, Eric Bauer, David Arellano, Derek Prada, Paul Tobash,* Los Alamos National Laboratory

Scanning tunneling spectroscopy (STS) has been performed on a variety of Pu compound crystals including PuB_4, $PuCoGa_5$, and $PuIn_3$, with the results revealing distinct characteristics of semiconductive, semimetallic, and metallic, respectively. Specifically, the STS measurement showed the PuB_4 to have a band gap of approximately 0.042 eV, $PuCoGa_5$ to have no band gap with an electron density of zero at (and only at) the Fermi energy (E_F), and $PuIn_3$ to have no band gap with electron density at E_F. STS measurements were performed at temperatures ranging from 25 Kelvin (above the supercritical transition temperature of $PuCoGa_5$) to room temperature. In addition to the STS results, structural scanning tunneling microscopy (STM) images were successfully obtained for the $PuIn_3$ and $PuCoGa_5$ surfaces. STM images of the $PuIn_3$ surface revealed step edges of approximate multiples of 0.8 nm consistent with a 111-surface orientation. STM images of the $PuCoGa_5$ revealed two distinct Moiré patterns consistent with different faces of the crystal structure.

AI/ML/Autonomous Experimentation for Thin Films Processing
Room 317 - Session AIML1-ThM

Linking AI/ML Tools with Diagnostics and Film Growth: PLD/CVD/ALD

Moderators: Prof. Renato Camata, University of Alabama at Birmingham, **Dr. Gregory Doerk**, Brookhaven National Laboratory

8:00am **AIML1-ThM-1 AI-Driven Synthesis by Pulsed Laser Deposition: Autonomous Experimentation and Human-AI Collaboration**, ***Sumner B. Harris***, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory **INVITED**

Thin-film synthesis with pulsed laser deposition (PLD) presents a vast design space of chemistries, structures, and non-equilibrium processing pathways that is challenging to navigate when targeting specific film properties. By combining automated synthesis platforms equipped with multimodal in situ diagnostics and a range of AI methods, we can generate testable hypotheses, autonomously explore large parameter spaces, uncover non-trivial correlations between diagnostics and film properties, and control the growth trajectory in real time. In this talk, I will discuss human–AI collaborative autonomous synthesis, which employs an LLM as a co-scientist to help generate testable hypotheses for oxide remote epitaxy and assists with additional LLM-based data analysis between batches of fully autonomous PLD experiments. I will further discuss how this example sets the stage for Agentic AI-driven synthesis and characterization platforms, incorporating cross-modal knowledge to make decisions and analyze results.This work was supported by the Center for Nanophase Materials Sciences (CNMS), which is a US Department of Energy, Office of Science User Facility at Oak Ridge National Laboratory. PLD synthesis was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division

8:30am **AIML1-ThM-3 Physics-Informed Gaussian Process Active Learning for Modeling of PLD Plume Dynamics**, ***Zahra Nasiri***, *Dorien Carpenter, Jacob H Paiste,* University of Alabama at Birmingham*; Sumner B Harris,* Center for Nanophase Materials Sciences, Oak Ridge National Laboratory*; Renato P Camata,* University of Alabama at Birmingham

In pulsed laser deposition (PLD), accurate models of plume particle flux and kinetic energy as functions of laser fluence and spot area are essential for autonomous thin film growth optimization. It is well established that Gaussian Process (GP) active learning can construct high-fidelity representations of these functions from a small number of strategically selected experiments. Physics-inspired structured mean functions have been identified as a promising direction for improving model performance and sample efficiency. Here, we present a fully developed physics-informed GP framework that embeds this physical structure directly into the surrogate modeling process.

We replace the conventional zero-mean GP prior with physically motivated baselines derived from an isentropic expansion model. For kinetic energy, the structured mean expresses the kinetic energy of ablated species in terms of a stagnation temperature at the beginning of expansion and the terminal Mach number of the plume. The terminal Mach number is derived from the Knudsen number for each combination of fluence and spot area through a known analytical relation involving the heat capacity ratio. The stagnation temperature is modeled through a secondary GP trained on fluid dynamics simulation data. For particle flux, the structured mean captures the scaling with the initial vapor density and the terminal Mach number, where the initial thermodynamic state is determined through the laser-target interaction. The primary GP learns only residuals from these baselines, reducing model complexity and improving sample efficiency.

Performance is evaluated via root mean square error (RMSE) and compared against zero-mean GPs and random sampling. Results from 100

independent runs confirm that embedding isentropic expansion physics dramatically reduces model error, with RMSE dropping from approximately 3.5% to 0.1%. We carry out experimental validation through real-time ion probe measurements of KrF excimer laser ablation of copper in vacuum. We will discuss how to interpret the time-dependent Mach number extracted from the surrogate model and its use to predict the angular distribution of the PLD plume, which is critical for film uniformity and thickness control. Finally, we generalize our approach to complex compound materials, with the iron-based superconductor FeSe as an initial target where stoichiometry control presents additional modeling challenges.

8:45am **AIML1-ThM-4 Multi-Objective Bayesian Optimization for Aligning Carbon Nanotube Growth Simulations with In-Situ SEM Observations**, *Ramakrishna Surya, Brendan Young, Brendan Alvey, James Keller, Matthias Young,* ***Matthew Maschmann,*** University of Missouri-Columbia

Carbon nanotube (CNT) forests exhibit exceptional potential for lightweight conductors, interconnects, thermal interfaces, and multifunctional materials, yet their effective properties remain far below those of individual CNTs because forest-scale behavior is governed by stochastic growth, CNT–CNT interactions, delamination, density loss, and evolving microscale morphology. This work presents an experiment-informed computational framework for matching numerical simulations of CNT forest growth with in-situ environmental SEM observations and simultaneous electrical measurements. CNT forests are synthesized across pre-patterned electrodes, enabling real-time imaging of morphological evolution while measuring conductance during growth. Image analysis and machine-learning-based feature tracking are used to extract CNT density and growth kinematics from SEM image sequences, providing quantitative structural targets for model calibration.

A three-dimensional finite element model captures CNT growth, mechanical interactions, van der Waals contact formation, delamination, and electrical network evolution. Because key model parameters, including growth-rate variability, CNT–CNT contact resistance, intrinsic CNT resistance, critical delamination stress, and initial CNT areal density, are difficult to measure directly, we use a multi-objective Bayesian optimization to efficiently calibrate the simulation. Gaussian process surrogate models guide active learning toward parameter combinations that minimize both density error and conductance error relative to experiment. This approach identifies Pareto-optimal parameter sets using fewer than 50 simulations from a search space exceeding 50,000 combinations. The resulting calibrated simulations reproduce experimentally observed density decay and conductance evolution, capturing the coupled effects of CNT junction formation, network degradation, and delamination. This work establishes a pathway for calibrating digital twins with experimental observations by combining in-situ measurement, physics-based simulation, and multi-objective active learning to infer latent model parameters and improve predictive fidelity.

9:00am **AIML1-ThM-5 QCMPy: Open-Source Python Codebase for in-Situ QCM Kinetics Monitoring**, ***Eden Goodwin***, *Maram Bakiro, Victoria Velez, Derek Reid, Seán Barry,* Carleton University, Canada

It is well known that not all chemical systems are equally prepared for modelling with Artificial Intelligence (AI). Well documented chemical systems with predictable structures and invariable synthesis have yielded phenomenal modelling results, as is best exemplified by the Nobel protein modelling AI software AlphaFold.[1] Small molecule systems are more difficult to model as they have inconsistent documentation, more dimensions of structural diversity, and significant variability in synthetic approach. Structural modifications can introduce substantial changes to the synthetic procedure, new decomposition pathways, intermolecular interactions, or even unpredicted functionality at the surface. These factors make iteration on and testing of models challenging. As such a different approach may yield better results: extraction of critical information from under-analyzed data.

A prime target for this data collection is an under utilized, robust, affordable, in-situ metrology: Quartz Crystal Microbalance (QCM). QCMs are used within Atomic Layer Processing (ALP) to measure in-situ the growth, etch, and modification of surfaces as they are exposed to highly reactive precursors. The relative mass gain due to each step of a sequential ALPs can provide valuable chemical insights, especially when coupled with other in-situ techniques. Careful kinetics analysis of sequential adsorptions of N-Heterocyclic Carbenes on surfaces revealed a previously unreported phenomenon: Atomic Layer Restructuring.[2] A reduction in the maximal coverage of the physiosorbed component revealed a significant reduction in the number of available surface sites and consequently surface roughness.

To translate kinetics modelling to a broader audience we have developed an open-source tool "*QCMPy*" that (1) separates a QCM trace of into cycle by cycle traces for each precursor then (2) aligns cycle traces using pulse detection algorithms and finally (3) conducts comprehensive cycle by cycle adsorption modelling. To demonstrate QCMpy we probe the growth kinetics of trimethyl aluminum using three different co-reactants: Water, Fumaric Acid and Salicylic acid. Analysis of the modeled parameters (ka, θmax) over each individual Molecular Layer Deposition cycle reveal pulsing drift and variability in our ALD-reactor, predict the transition from interfacial to bulk growth (Figure 1), predict the ideal growth per cycle from sub-saturative recipes and quantify the chemisorption/physisorption ratio of TMA and all co-reactants.

References

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2- Goodwin, E. et al. *ACS Nano* **2025**, *19* (16), 15617–15626.

9:15am **AIML1-ThM-6 Accelerating Peald Process Development with Explainable Machine Learning**, ***Hamidur Rahman***, University of Michigan, Ann Arbor*; Ian Campbell,* IMEC USA*; Paula Arellano-Vasquez, Joshua Kammeraad, Paul Zimmerman, Ageeth Bol,* University of Michigan, Ann Arbor

Plasma-enhanced atomic layer deposition (PEALD) has emerged as a promising route to synthesize emerging 2D materials, yet rationalizing its highly nonlinear, multi-parameter process space remains an open challenge. Machine Learning (ML) promises to address this challenge, but requires consensus on which models, validation schemes, and feature sets are appropriate for the relatively high-noise, small data sets that are typically generated in PEALD studies. We address this issue by a systematic, end-to-end methodology study to optimize the crystallinity and surface morphology of PEALD MoS_2. Building on a critical survey of prior approaches, we systematically evaluate ML practices on our own controlled experimental data set, collected through experiments designed to optimize material properties, to clarify which ML models reliably translate to the small-sample, high-noise regime characteristic of PEALD.

A PEALD process to synthesize MoS_2 is developed using metal $Mo(N^tBu)_2(NMe_2)_2$ precursor and combinations of Ar/H_2 plasmas and a tert-butyl disulfide co-reactant. Various ALD parameters, such as process pressure, plasma power, gas composition, etc., were systematically varied to guide the film growth towards more crystalline and minimal out-of-plane growth using Atomic Force Microscopy (AFM). The data were subsequently modeled using eight algorithms encompassing linear regressors, k-nearest neighbors, random forest variants, and gradient boosting methods. A comparative evaluation of these models is conducted to explore the relationships inherent in PEALD process parameters and forecast material properties. Incorporating Raman Spectroscopy features as auxiliary inputs was also explored, highlighting the potential of multimodal data in low-data ALD studies. Model interpretability techniques were applied to examine the contributions of individual steps in the PEALD cycle to material properties, providing physically meaningful insights that complement human interpretation of the underlying chemistry. The trained models drive inverse recipe design, yielding candidate process windows for target film properties. We further explore in-situ spectroscopic ellipsometry as a real-time surrogate for ex-situ characterization, paving the way toward closed-loop control. Finally, we outline a roadmap for a transferable PEALD digital twin, where MoS_2-trained models can be adapted via transfer learning to analogous precursor systems, laying the foundation for autonomous, ML-guided PEALD.

9:30am **AIML1-ThM-7 Non-Negative Matrix Factorization for in Situ Gas Analysis During Atomic Layer Deposition**, ***Andreas Werbrouck***, *Aditya Chalishazar, Dirk Poelman, Philippe F. Smet, Jolien Dendooven, Christophe Detavernier,* Ghent University, Belgium

In situ characterization of atomic layer deposition (ALD) processes enables the study of reaction mechanisms, kinetics, and industrial process control. An established way to monitor gas species in a reactor is quadrupole mass spectrometry (QMS). In past work, we have shown that time-resolved, full-range mass spectrometry data with very good sensitivity can be collected provided that steady-state reaction conditions are maintained. Another method for gas-phase characterization is capturing the optical emission from a cold cathode discharge (optical emission spectroscopy or OES). OES could quickly detect and characterize gas-phase constituents under non-steady-state conditions. Both methods yield dense, time-resolved series of

spectra, showing multiple correlated and potentially overlapping peaks. Therefore, we adopt non-negative matrix factorization (NMF), a machine learning technique, as a holistic way to analyze the obtained datasets. NMF is able to identify fingerprints of gas phase elements, and their time evolution. We evaluated the use of NMF for QMS and OES analysis by studying the trimethylaluminum (TMA)-H_2O and diethylzinc (DEZ)-H_2O ALD chemistries.

In the case of OES, we demonstrate that a naive analysis method of tracking channel intensities corresponding to specific emission lines is not sufficient to identify and separate reaction products. Using NMF, we were able to identify spectra and time signatures from precursor fragments and reaction products, confirming the established reaction mechanism between TMA and H_2O yielding CH_4. The NMF analysis also suggests that the discharge generates spurious H signals that can give rise to wrong interpretation of the H emission lines.

For QMS under steady state conditions, NMF easily and cleanly separates precursors and reaction products. Interpretation of mass spectra is easier, compared to OES, and the clean spectra and time traces NMF yields allow for faster identification of novel reaction products. This way, by using NMF on OES and QMS data, we reveal autocatalytic alkene formation during the DEZ-H_2O process, in addition to the generation of ethane.

With this work, we aim to draw attention to a relatively simple machine learning method that can be straightforwardly adopted by experimentalists. While in situ experiments are capable of yielding (very) large datasets, NMF helps to draw a complete picture of the gas phase during ALD processes.

9:45am **AIML1-ThM-8 Machine Learning Assisted Multiscale Simulation of Metal Deposition**, ***Michael Nolan,*** Tyndall Institute, Ireland; *Karl Ronnby, Samuel Delgado,* Tyndall National Institute, University College Cork, Ireland

The deposition of metals onto a multitude of substrates and the resulting interfaces are critical elements of many technologies, e.g. semiconductor devices, catalysts, sensors, etc. Atomistic simulations provide a powerful tool to select between different metal-substrate combinations for target technologies. Semiconductor devices using 2D materials require good quality interfaces between metal contacts and the 2D channel, back end of line interconnects require smooth conducting metal films that are immune to metal diffusion and catalysts using support metals benefit from metal islands with high density of active sites. In this contribution we present atomistic multiscale simulations of metal deposition and morphology evolution that use machine learning potentials to accelerate simulations and reach time and length scales that are out of reach with density functional theory (DFT). We use DFT to explore how the modification of TaN can promote a change in morphology of deposited copper from islands to lateral growth, computing activation barriers for critical metal migration processes using neural network ML potentials, which reduces the time for barrier calculation to a few minutes. With these barriers we employ kinetic Monte Carlo simulations to predict key film properties including roughness, covered surface area and density of defects. A similar approach is employed for Ru, which is of high interest for metal interconnects. Cu-Ru alloys are of interest and we present genetic algorithm studies of global minimum energies structures with an alloy ML potential and apply this to atom migrations. Finally, we explore Ru-TMD interfaces and dynamics to understand formation of Ohmic contacts found experimentally.

AI/ML/Autonomous Experimentation for Thin Films Processing

Room 317 - Session AIML2-ThM

AI/ML Tools in Molecular Beam Epitaxy & Flash Session

Moderators: Dr. Michael Nolan, Tyndall National Institute, University College Cork, **Ms. Campbell Sweet**, University of Missouri

11:00am **AIML2-ThM-13 AI/ML Techniques for Molecular Beam Epitaxy**, ***Stephanie Law,*** Pennsylvania State University **INVITED**

MBE synthesis offers precise control over film thickness, composition, and crystallinity by tuning a range of growth parameters. While this tunability enables tailored synthesis, it also introduces significant complexity, resulting in multidimensional growth spaces. Identifying optimal growth parameters within these complex spaces typically involves trial-and-error experimentation, in which growers use a combination of intuition and grid search methods to guide the choice of growth parameters. An alternative way to navigate complex growth spaces is through the use of Bayesian Optimization (BO) or AI-driven hypothesis generation, which can explore parameter space more efficiently and find global optimal growth parameters. By leveraging probabilistic models such as Gaussian Process Regression (GPR), BO can statistically select the most informative experiments, balancing exploration of new growth parameter spaces with exploitation of known good parameters. AI-guided hypothesis generation can be used to read the extant literature and generate experimental campaigns. In this work, we apply BO to efficiently explore the growth space for In_2Se_3 thin films on Al_2O_3 substrates using MBE. By integrating prior experimental data and employing GPR, we employed a data-driven synthesis campaign that significantly reduced the number of required experiments. Leveraging BO resulted in an increase in the fraction of γ-In_2Se_3 from ~50% to >90% in fewer than 10 samples. To further understand the influence of individual growth parameters on model predictions, we used SHapley Additive exPlanations (SHAP), w hich indicated that the indium flux is the most important parameter in predicting the film polymorph fraction, pointing toward defects as a method of stabilizing the polymorph. We also employed AI-guided experimental design to explore growth parameter space for In(Ga)Sb quantum dots. This approach led us to a clear understanding of how QD morphology and density depends on growth parameters, and how QD photoluminescence is correlated with both. These findings highlight the potential of data-driven optimization in complex materials synthesis and further solidify the growing body of evidence supporting the use of ML for efficient thin film experimental design.

11:30am **AIML2-ThM-15 Human-in-the-loop Agentic Design of Experiments for Molecular Beam Epitaxy Synthesis of In(Ga)Sb Self-Assembled Quantum Dots in an InAs Matrix**, ***Molly McDonough,*** Pennsylvania State University; *Priyanka Petluru, Aaron Muhowski,* Sandia National Laboratories; *Wesley Reinhart, Stephanie Law,* Pennsylvania State University

In(Ga)Sb self-assembled quantum dots (QDs) are a class of III-V nanostructures that have been studied primarily due to their broken-gap band alignment and emission wavelengths in the mid-wave (MWIR) and long-wave infrared (LWIR). The MWIR and LWIR regimes are crucial to many different technological areas including biosensing, trace gas analysis, environmental monitoring, and defense. However, options for compact, high efficiency emitters in this wavelength range are nascent. InSb and In(Ga)Sb self-assembled quantum dots (SAQDs) in an InAs matrix are a unique option for this wavelength regime due to their tunable emission wavelength by tailoring the lateral size and height of the SAQDs. Previous work on InSb SAQDs has yielded strong photoluminescence (PL) emission in the 3μm - 5μm range. For In(Ga)Sb SAQDs on InAs, emission out to 8μm has been successfully demonstrated.

Our work builds on latent knowledge by modeling the relationship between growth parameters, SAQD morphology and properties, and PL emission wavelength to create designer MWIR and LWIR emitters. We implement a human-in-the-loop agentic design of experiments process via tool-using large-language models to suggest growth conditions for maximal information gain per trial. The parameters explored here include how V/III beam equivalent pressure ratios, growth rate, deposition thickness, Ostwald ripening time, composition, and the use of bismuth surfactant influence our nanostructure morphology and emission characteristics. By this method, we achieve PL emission from In(Ga)Sb nanostructures in the 5μm to 7μm range. We observe the formation of In(Ga)Sb quantum dashes, which contrasts with existing studies on In(Ga)Sb quantum dots. The results presented here provide in-depth mapping of the synthesis-structure-property relationships in this system and more broadly demonstrate an effective and practical deployment of agentic hypothesis generation for synthesis exploration and device development.

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Advanced Microelectronic Materials and Devices Mini-Symposium
Room 318 - Session AM+EM+TF-ThM

Ferroelectric Thin Films

Moderators: Prof. Dr. John F. Conley, Jr., Oregon State University, **Dr. Daniel Pennachio**, Naval Research Laboratory

8:00am **AM+EM+TF-ThM-1 Processing and Properties of Ferroelectric Wurtzite Thin Films**, ***Jon-Paul Maria***, Penn State University **INVITED**

Ferroelectricity in wurtzite-based crystals was observed in 2019 and immediately introduced exciting opportunities to explore and discover new structure-property relationships in novel formulation spaces. These observations lead one to speculate that ferroelectricity might be found much more broadly, even “everywhere”, by introducing the appropriate disorder in a variety of hosts.

The presentation will begin with a brief history of ferroelectricity with specific attention to the last 10 years where this important property was discovered in new oxide and nitride crystals. The remaining content will focus on the structure-process-property relationships in the B-substituted AlN and Mg-substituted ZnO wurtzite systems. Materials can be prepared between 100 °C and 350 °C with very little difference in electrical properties. In the best cases, capacitors can be prepared down to 10 nm thickness while still exhibiting ferroelectric switching. Below 25 nm, however, leakage current becomes problematic during low frequency hysteresis measurements. Challenges to thickness scaling will be discussed with attention to the origins of property dependencies on structure , defects, and microstructure with film thickness. The presentation will also include examples where proximity effects in layered ZnO/$Zn_{1-x}Mg_xO$, AlN/$Al_{1-x}B_xN$, and $Zn_{1-x}Mg_xO$/AlN heterostructures can induce switching in pure ZnO and AlN layers, with opportunities for reducing net coercive voltage values.

8:30am **AM+EM+TF-ThM-3 Interfacial Control and Property Enhancement Through Proximity Ferroelectricity**, ***Ian Mercer***, *William Prudnick, Saeed Almishal, Pochun Hsieh, Stanislav Udovenko, Darren Pagan, Venkatraman Gopalan, Jon-Paul Maria,* Penn State University

Ferroelectric layers can induce switching in neighboring polar non-ferroelectric layers, this phenomenon is referred to as proximity ferroelectricity. Prior studies have only focused on bi- and trilayer geometries, leaving room to further study on interface effects. Here, we explore interfacial and surface contributions more broadly, including, for example, the density effects in AlN/$Al_{1-x}B_xN$ and AlN/$Al_{1-x}Sc_xN$ superlattices grown using reactive magnetron sputtering. In addition, we examine compositionally graded structures that smear the same chemical contrast into an interface-less continuum. To complement this understanding, we also compare materials whose surfaces are plasma modified to create a partnering interface that can also influence switching. Thin film morphology and structural quality is probed using atomic force microscopy (AFM) and x-ray diffraction (XRD), revealing smooth films with RMS roughness below 1 nm in all cases. For superlattices, distinct satellite peaks indicating sharp, periodic interfaces are present. Deep UV photoluminescence (PL) measurements surprisingly reveal evolution with increasing interface density. By examining coercive field, current transport, and switching kinetics, we find that the internal interfaces act as barriers to both domain propagation and leakage transport. We also find grading $Al_{1-x}Sc_xN$ from x = 0.38 to x = 0 through the film thickness produces a substantial increase in coercive field, with some structures exhibiting strong insensitivity to Sc composition. These results establish interface, compositional grading, and surface processing – well-established opportunities in III-nitride alloys – as new degrees of freedom in wurtzite ferroelectric materials, demonstrating that engineered surfaces and gradients can strongly modify bulk switching behavior beyond conventional composition control. This transition towards interface engineering allows finer control over coercive field, domain structure, and leakage current barriers, ultimately enabling surfaces to enhance navigation through property space.

8:45am **AM+EM+TF-ThM-4 Unveiling the Hidden Role of Interfacial Layer in Ta/HZO Ferroelectric Tunnel Junctions Band-Profile and Tunneling-Electroresistance Engineering**, ***Sanghyun Lee***, University of Kentucky*; Kent Price,* Morehead State University*; M. David Henry, Samantha Jaszewski,* Sandia National Laboratories, USA*; Alexander Blevins,* University of Kentucky, United States Minor Outlying Islands (the)

Ferroelectric tunnel junctions (FTJs) are promising two-terminal devices for neuromorphic computing, providing non-volatile, analog-tunable conductance via polarization-controlled tunneling. Their compact metal–ferroelectric–metal structure, low programming energy, and compatibility with CMOS processes make them suitable as synaptic elements for computing-in-memory. Hafnium oxide-based systems, such as $Hf_{0.5}Zr_{0.5}O_2$ (HZO), are especially notable for maintaining robust ferroelectricity at thicknesses below 10 nm, which supports scalable crossbar arrays for high-density neuromorphic computing.

The electrical performance of metal/HZO/metal FTJs is significantly influenced by interfacial chemistry; however, previous research efforts have consistently assumed an ideal, abrupt metal/HZO interface. In particular, Ta/HZO or Ti/HZO devices tend to form the unavoidable sub-stoichiometric TaO_x or TiOx layer due to tantalum's oxygen-scavenging properties. To bridge this research gap, we have investigated the interface layer and their material and device characteristics to unveil key physical mechanism. Utilizing in-house MATLAB modeling suites with Sentaurus TCAD simulators, the impact of this interlayer on band profile, tunneling pathways, and the resulting tunneling electroresistance (TER) is quantitatively assessed.

After fabricating and validating Ta/HZO (6 nm)/TaN devices, we characterized FTJs and developed a graded TaO_x interlayer device model with thicknesses from 0.3 to 1.5 nm and various permittivity values. Our model incorporates realistic oxygen vacancy concentrations (10^{19}–10^{21} cm^{-3}) and trap levels 0.5–1.2 eV below the HZO conduction band, which agrees well with experimental data. By integrating ferroelectric polarization, band bending, vacancy charge balance, the simulations represent the complete electrostatic and defect-mediated conduction mechanism at the Ta/HZO interface.

Our preliminary results uncover distinct regimes in which TaO_x either enhances or degrades FTJ performance. Thin, moderately defective layers (approximately 0.5 to 0.8 nm, oxygen vacancies around 10^{19} cm^{-3}) create a beneficial asymmetric barrier that increases TER by a factor of 3 to 6 compared to an ideal Ta contact, while maintaining read current. In contrast, thicker or highly oxygen-deficient TaO_x layers function as parasitic resistive elements, reducing low-resistance state current by more than an order of magnitude and generating significant internal bias fields. Simulated internal bias fields and coercive voltage shifts align with experimentally observed imprint trends, supporting the validity of the model.

9:00am **AM+EM+TF-ThM-5 Processing Window and Property Enhancement via Tellurium Co-Doping in Sputtered Ferroelectric $Zn_{1-x}(Mg, Te)_xO$ Thin Films**, ***William Prudnick***, *Ian Mercer,* Pennsylvania State University*; Ece Günay,* Carnegie Mellon University*; Po Chun Hsieh, Saeed Almishal,* Pennsylvania State University*; Elizabeth Dickey,* Carnegie Mellon University*; Venkatraman Gopalan, Jon-Paul Maria,* Pennsylvania State University

Wurtzite ferroelectric materials show promise for application in non-volatile random-access memory (RAM). $Zn_{1-x}Mg_xO$ (ZMO), a wurtzite material first reported to be ferroelectric in 2021, shows significantly higher polarization retentions than perovskite ferroelectrics, similar to $Al_{1-x}Sc_xN$ and $Al_{1-x}B_xN$ but with markedly lower coercive fields compared to other wurtzite ferroelectrics (~2-3 MV/cm vs. ~4-6 MV/cm). However, leakage current, imprint, and intolerance for elevated growth temperatures remain persistent hinderances. Herein, we report tellurium incorporation within ZMO via reactive RF co-sputtering. $Zn_{1-x}(Mg, Te)_xO$ (ZMTO) films maintain consistently low coercive fields (~2.4 MV/cm) even at elevated growth temperatures (up to 350° C with no diminishment in ferroelectric properties) while simultaneously decreasing imprint. X-ray diffraction (XRD) data indicate highly c-oriented films with improved out-of-plane crystallinity. Omega rocking curves show reduction in mosaicity compared to previously reported values (< 2° FWHM vs. ~4° FWHM). X-ray reflectometry (XRR) data demonstrate low rms roughness values consistently below 1.5 nm. Transmission electron microscopy (TEM) data indicate columnar growth and planar defects such as stacking faults consistent with previous reports. Selected-area electron diffraction (SAED) supports wurtzite phase uniformity. X-ray photoelectron spectroscopy (XPS) indicate tellurium is in the +4 oxidation state. Fourier transform infrared (FTIR) and Raman spectroscopies show tellurium with a 4-coordinate geometry indicative of Zn-site occupancy. We highlight photoluminescence spectroscopy (PL) data and expound upon dopant and temperature dependence of the defect landscape. We emphasize the underlying defect chemistry and doping strategies to overcome challenges in synthesis as they relate to material properties and structure enhancements.

9:15am **AM+EM+TF-ThM-6 Structurally Compatible Al-doped ZnO Bottom Electrode for Wurtzite Ferroelectric Mg-substituted ZnO Thin Films**, ***Sharon Yang***, The Pennsylvania State University; *Ece Gunnay,* Carnegie Mellon University; *William Prudnick,* The Pennsylvania State University; *Elizabeth Dickey,* Carnegie Mellon University; *Jon-Paul Maria,* The Pennsylvania State University

Epitaxial wurtzite heterostructures are prepared to eliminate, to the extent possible, structure defects and microstructure that may, in principle, interfere with or limit their ferroelectric properties and performance. In so doing, we attempt to achieve and understand the true intrinsic response. To do so, we begin with epitaxial c-axis oriented Al-doped ZnO (AZO) bottom electrodes grown on (0006)-Al_2O_3 via dual-cathode reactive RF magnetron co-sputtering. X-ray diffraction (XRD) indicates a single-phase c-axis oriented growth with x-ray omega and two-theta peak widths, electrical resistivity, and surface roughness values that all decrease with increasing substrate temperature and aluminum cathode power. The optimal AZO thin films exhibit an omega FWHM of 0.04° and surface roughness of 900 pm RMS, and a peak Hall mobility of 47 $cm^2/V{\cdot}s$, a Hall carrier density of 1.3E20 cm^{-3}, a minimum Hall resistivity of 1E-4 Ω·cm, and a STEM-EDS confirmed a composition of 1.7 at.% Al and uniform thickness of 43 nm. Infrared spectroscopic ellipsometry as function of Al content demonstrates tunable epsilon-near-zero behavior where the zero-permittivity wavelength ranged between 1970 and 3170 wavenumbers for 4.1E19 cm^{-3} and 1.3E20 cm^{-3} carrier concentrations respectively. Subsequently, $Zn_{0{\cdot}78}Mg_{0{\cdot}22}O$ (ZMO) films were deposited at room temperature, XRD indicating a strong c-axis growth of ZMO on AZO with FWHM of 0.86°. High-resolution TEM and STEM-EDS analysis revealed chemically abrupt ZMO/AZO interfaces. The heterostructure displays robust ferroelectric switching with a remanent polarization exceeding 88 $\mu C{\cdot}cm^{-2}$ and a coercive field below 2.8 $MV{\cdot}cm^{-1}$. Compared to previously reported ZMO films grown on non-epitaxial Pt bottom electrodes, these epitaxial oxide heterostructures exhibit comparable ferroelectric switching behavior while providing substantially improved structural compatibility and crystallographic coherence throughout the stack. These stacks are additionally attractive because they remain transparent throughout the visible spectral range, and these findings establish epitaxial AZO as a viable, highly compatible oxide bottom electrode platform for high-performance wurtzite ferroelectric thin films.

9:30am **AM+EM+TF-ThM-7 Stabilization of Antipolar Pbca Phase in Hafnium Zirconium Oxide via Aluminum Substitution**, ***Yong Kyu Choi***, University of Virginia, USA; *MinChul Kang,* Ames National Laboratory; *Tinase Ale,, Nicolas Lam, Andrea Watson, Kory Burns, Stephen McDonnell, Lin Zhou, Jon Ihlefeld,* University of Virginia, USA

Hafnium zirconium oxide (HZO) shows significant potential for non-volatile memory applications due to its ferroelectric properties. However, practical limitations such as insufficient endurance remain a significant challenging prior to commercialization. One promising approach to overcome this limitation is the implementation of antiferroelectric (AFE) behavior in HZO-based materials. Previous studies have demonstrated that cation substitution in HZO can induce AFE-like behavior within certain substitution concentration ranges. In Zr-rich HZO systems, this AFE response has commonly been attributed to the tetragonal phase. However, recent reports indicate that the observed AFE behavior may instead originate from the antipolar orthorhombic (*Pbca*) phase. This presentation discusses how varying an aluminum substitution concentration influences the phase stability and electrical properties of HZO thin films. Grazing-incidence X-ray diffraction, Fourier transform infrared spectroscopy, and scanning transmission electron microscopy are employed to investigate the structural transformation and AFE behavior of Al-substituted HZO capacitors. The results demonstrate that low aluminum substitution concentrations, such as 8:1 and 6:1 Al:HZO ratios, exhibit AFE behavior associated with stabilization of the antipolar orthorhombic *Pbca* phase.

11:00am **AM+EM+TF-ThM-13 Ferroelectricity in Atomic Layer Annealed Nitride-Based Thin Films**, ***Andrew Meng***, *Dominic Dalba, Dilan Gamachchi, Indeewari Karunarathne, Bipin Bhattarai,* University of Missouri-Columbia; *Xiaoman Zhang,* University of North Alabama; *Wangwang Xu,* Louisiana State University; *Somayeh Saadat Niavol,* University of Missouri-Columbia; *Dongmei Cao, W.J. Meng,* Louisiana State University **INVITED**

Wurtzite AlN-based materials exhibit strong ferroelectric behavior and offer potential for a wide memory window due to their high coercive field, making them promising candidates for non-volatile memory applications. Most studies on wurtzite AlN-based ferroelectrics focus on reactive sputtered thin films, which can suffer from deleterious effects of point defects caused by ion bombardment. Atomic Layer Deposition (ALD) can lead to films with fewer electronic defects at significantly lower growth temperatures. However, the crystallinity can be low even in plasma assisted processes. Nitrogen incorporation in ALD films also remains challenging. We demonstrate the growth of nanocrystalline wurtzite AlN thin films deposited by a three-step atomic layer annealing (ALA) process at 350°C consisting of trimethylaluminum and hydrazine precursor pulses and a nitrogen plasma annealing step. Interestingly, these films are ferroelectric without intentional extrinsic alloying, which we attribute to very high dielectric strength in excess of 10 MV cm^{-1}. The films exhibit a remanent polarization of ~ 35 μC cm^{-2}, and piezoresponse force microscopy experiments show phase and amplitude changes after DC poling consistent with ferroelectricity. We also demonstrate growth of AlBN using an ALA process. The ALA growth process for wurtzite AlN-based ferroelectric materials is potentially compatible with processing for silicon electronics and holds promise for next-generation semiconductor devices.

11:30am **AM+EM+TF-ThM-15 Ferroelectric and Rf Electrical Properties of Peald Scaln Thin Films**, ***Virginia Wheeler***, *Vikrant Gokhale, Margo Staruch,* US Naval Research Laboratory; *Jaime Hart,* Nova Research Inc; *Jonathan Chin, Peter Litwin,* NRC, US Naval Research Laboratory; *Neeraj Nepal,* US Naval Research Laboratory; *Gilbert Rayner, Jr, Noel O'Toole,* Kurt J. Lesker Company; *Nicholas Strnad,* Army Research Laboratory

Scandium aluminum nitride (ScAlN) has emerged as a transformative material for advanced microelectronics, driven by its exceptional piezoelectric response and robust ferroelectric properties. While traditional deposition methods, such as magnetron sputtering and molecular beam epitaxy (MBE), have enabled its initial integration, these line-of-sight techniques inherently lack the conformality required for next-generation, three-dimensional device architectures. Plasma-enhanced atomic layer deposition (PEALD) addresses this critical manufacturing bottleneck by providing self-limiting, atomic-scale control over film thickness and composition, enabling the uniform coating of complex, high-aspect-ratio structures. These benefits make PEALD ScAlN appealing for advancements in RF filters, where sub-nanometer thickness uniformity directly dictates acoustic performance and high-frequency bandwidth, and high-density 3D non-volatile memory (NVM) architectures requiring high-quality ultrathin layers. Consequently, the development of PEALD processes for ScAlN represents a critical pathway toward achieving next-generation, scaled, high-performance communication and at the edge computing technologies.

Using the PEALD process developed by Rayner et. al [1], 20-60nm ScAlN films were deposited on 50nm NbN/sapphire and Pt/SiO_2/Si templates with both 18% and 30% Sc. XRD and TEM confirm that all films are texture, polycrystalline in nature with roughness directly related to increasing Sc concentration and thickness. The 18% films exhibit low leakage, very flat permittivity (ε_r ~12-14) from 20 Hz to 3GHz, and low dielectric loss. However, increasing the Sc content results in more leaky films with strong dispersive permittivity and high loss, remarkably similar to MBE ScAlN/NbN films with 32% Sc.

Additionally, the 18% ScAlN/NbN film is confirmed to be ferroelectric, with measurements at the highest electric field achieved showing a remanent polarization value of 80 $\mu C/cm^2$. The coercive field, E_C, is approximately 5.5 MV/cm at room temperature and 50 kHz, comparable to previous reports of this composition. Although the measured polarization is below anticipated values, this is attributed to instrument limitations that precluded the application of higher electric fields, resulting in a minor loop with full saturation anticipated at increased field strengths. In-depth analysis of ferroelectric properties as a function of Sc content and substrate will be presented.

[1] Rayner et al, *JVSTA* 43, 020401 (2025).

11:45am **AM+EM+TF-ThM-16 Atomic-Scale Structure and Domain Mapping in Hafnia-Based Ferroelectrics**, ***Ece Gunay***, Carnegie Mellon University; *Sebastian Calderon,* Carnegie Mellon University, USA; *Rintaro Maki, Yuichi Shimakawa,* Kyoto University, Japan; *Daisuke Kan,* Osaka University, Japan; *Elizabeth Dickey,* Carnegie Mellon University, USA

Growing-memory architectures in logic circuits offer a promising pathway to reduce the energy cost associated with dense computing. These emerging device concepts require the integration of scalable, CMOS-compatible ferroelectric materials. Hafnium oxide, widely used as a gate dielectric, is inherently CMOS-compatible, and its ferroelectricity can be activated through cation alloying (e.g. Si, Zr, La, Y, etc.), which stabilizes a metastable orthorhombic phase and introduces new functionalities.

Because ferroelectric domains evolve and interact under applied bias, understanding their atomic-scale structure is critical for guiding device design. In this work, we investigated $Hf_{0.93}Y_{0.07}O_2$ freestanding membranes with in-plane polarization, enabling direct, real-space mapping of

ferroelectric domains. Y-alloyed membranes were fabricated on (100) $SrTiO_3$ using a $La_{0.67}Sr_{0.33}MnO_3$ buffer layer, which was selectively etched to produce freestanding membranes for atomic-scale characterization.

Aberration-corrected scanning transmission electron microscopy (STEM) with annular dark-field (ADF) imaging was used to resolve cation positions, revealing ferroelectric domains oriented along the [001], [010], and [100] directions of the orthorhombic phase, forming 90° domain walls. Differential phase contrast (DPC) imaging enabled direct imaging of the oxygen sublattice. Vector pair correlation function analysis was used to map structure and domains across more than ten regions.

The results revealed that tetragonal-like inclusions are consistently observed near grain boundaries and domain walls. These inclusions are only a few unit cells thick and preserve overall lattice parameters while exhibiting local in-plane distortions. Additionally, lattice defects are frequently observed near 90° domain walls, likely accommodating strain arising from domain misorientation.

Overall, this study provides atomic-scale insight into the structural heterogeneity and domain behavior of hafnia-based ferroelectrics, offering guidance for optimizing their functional properties in next-generation electronic devices.

This material was based upon work supported by the Center for 3D Ferroelectric Microelectronics Manufacturing (3DFeM2), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences Energy Frontier Research Centers program under Award Number DE-SC0021118.

12:00pm **AM+EM+TF-ThM-17 Correlating Biaxial Stress to Metastable Phases in $Hf_{0.5}Zr_{0.5}O_2$ on Substrates with Different Coefficients of Thermal Expansion**, ***Nooreen Qureshi,*** University of Virginia, USA*; Luke Johnson,* Purdue University, USA*; Jordan Hachtel,* Oak Ridge National Laboratory, USA*; Jon Ihlefeld, Kory Burns,* University of Virginia, USA

Zirconium-substituted HfO_2 (HZO) has emerged as a leading candidate for next-generation ferroelectric memory and logic devices due to its Complementary Metal-Oxide-Semiconductor (CMOS) compatibility, scalability, and demonstrated ferroelectricity at thicknesses approaching 1 nm. Among the competing factors governing the ferroelectric phase stability in HZO including dopant density, oxygen vacancy concentration, electrode capping, and grain size; mechanical biaxial stress remains comparatively underexplored yet critically influential.

In this work, HZO thin films were deposited by Atomic Layer Deposition (ALD) on substrates with systematically varied coefficients of thermal expansion (CTE) to controllably tune the biaxial strain state. Macroscopic characterization via X-Ray Diffraction (XRD) and Infrared Spectroscopy (IR) reveal strain-dependent peak shifts that directly reflect the biaxial stress imposed by the substrate. Electrical measurements demonstrate a clear strain-dependent phase transition; films on low-CTE substrates exhibit ferroelectric polarization-voltage responses, while high-CTE substrates drive an antiferroelectric-like response, implicating strain as a tunable lever for phase stabilization.

To connect macroscopic behavior to local structural heterogeneities, scanning nanodiffraction 4D-STEM (Scanning Transmission Electron Microscopy) was employed to map lattice strain at the nanoscale. The correlation between local strain fields and bulk electrical response provides mechanistic insight into how nanoscale inhomogeneities propagate to device-level performance. This multi-scale characterization framework offers a comprehensive approach for engineering phase stability in fluorite-structure ferroelectrics.

Atomic Scale Processing Mini-Symposium
Room 316 - Session AP+EL+MS+PS+TF-ThM

Advancing Spectroscopic Ellipsometry and Other in-Situ Techniques to Enable Atomic Scale Processing

Moderators: Prof. Dr. Marcel Junige, University of Colorado at Boulder, **Dr. Adrie Mackus**, Eindhoven University, Netherlands

8:00am **AP+EL+MS+PS+TF-ThM-1 Atomic Processes in Surface-Limited ALD Growth Studied by Real-Time Spectroscopic Ellipsometry**, ***Eva Schubert,*** *Ufuk Kilic, Yousra Traouli, Mathias Schubert,* University of Nebraska - Lincoln **INVITED**

We employ in-situ spectroscopic ellipsometry (SE) to investigate the growth dynamics of ultrathin transition metal oxide films (ZnO, WO_3, TiO_2, and Ga_2O_3) during plasma-enhanced atomic layer deposition (PE-ALD). To analyze the dynamic optical response, we introduce a dual-box regression model in which the first box represents surface roughness using an effective medium approximation (EMA), while the second box captures cyclic variations in subsurface layer thickness associated with molecular rearrangements occurring during each ALD cycle. This approach provides a time-resolved and quantitative description of both surface roughness evolution and subsurface film growth dynamics, enabling accurate characterization of layer-by-layer deposition processes.

Accurate extraction of film thickness, density, and roughness at elevated substrate temperatures requires precise knowledge of the temperature-dependent dielectric function (TDF), which can differ substantially from room-temperature values. In this work, the TDFs of the transition metal oxides were determined through multi-sample analysis using optical data obtained from films of varying thicknesses measured at different stages of the growth process. The incorporation of experimentally verified dielectric functions enables the dual-box model to reliably describe the evolving optical response during high-temperature deposition, allowing detailed monitoring of sub-monolayer coverage, interface formation, and roughness evolution throughout the ALD process.

Post-deposition structural and chemical characterization using scanning electron microscopy (SEM), atomic force microscopy (AFM), X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS) corroborates the in-situ optical measurements and provides complementary insight into film crystallinity, morphology, and composition.

The capability of in-situ ellipsometry as a powerful tool for investigating growth dynamics will also be demonstrated for multilayer fabrication, ultra-precise thickness control, and monitoring of phase transitions in materials synthesized using physical and chemical vapor deposition techniques.

8:30am **AP+EL+MS+PS+TF-ThM-3 Tracking Critical Points: In Situ Ellipsometry for Rapid Assessment of Atomic Layer Processes on III-V Interfaces**, ***John Murphy,*** *Glenn Jernigan, Michael Johnson, David Boris, Scott Walton, Jill Nolde,* U.S. Naval Research Laboratory

Plasma-enhanced atomic layer processing (PE-ALD, ALE) on semiconductor interfaces, especially III-V semiconductor interfaces, requires precise control of plasma–surface interactions to achieve oxide-free interfaces and low-defect dielectric interfaces. Conventional post-process characterization (XPS, AFM, CV profiling) is time-consuming and inefficient for navigating large, nonlinear plasma process parameter spaces. In this work, we demonstrate an *in situ* spectroscopic ellipsometry (SE) methodology that provides a real-time, model-light assessment of III-V surface quality by tracking high-energy critical-point amplitudes directly from the pseudodielectric function, without constructing full multilayer optical models. Notably, critical points in the 4–5 eV range have photon penetration depths of ≈10 nm in III-V semiconductors, making them highly sensitive to near-surface chemistry.

This methodology is illustrated on InAs (100) surfaces during remote Ar/H2 plasma treatments, aimed at reducing native oxides. In the case of InAs (100) surfaces the E_0' critical point (≈4.4 eV) is used as the primary surface-quality metric during plasma treatments. While second-derivative analysis of the directly measured pseudodielectric function provides temperature dependent energy positions for critical points and the magnitude of which are calibrated using chemically clean reference surfaces.

Variations in the normalized E_0' amplitude are monitored as function of various substrate temperatures (100–300 °C), plasma powers (100–500 W), and H_2 flow fractions (1.25–6.25%) to capture the interplay between oxide removal, metallic species formation, and plasma-induced disorder with greater sensitivity and immediacy than conventional XPS metrics. These variations can be used to rapidly define practical processing windows and enable efficient down-selection within large plasma parameter spaces. The results highlight a generally useful strategy for integrating in situ critical-point tracking into atomic layer processing of III-V materials and suggest straightforward extensions to other compound semiconductor and dielectric growth environments.

8:45am **AP+EL+MS+PS+TF-ThM-4 Intelligent Sustainable ALD Research Platform Integrating On-Demand Precursor Delivery with *in situ* Imaging Ellipsometry**, ***Takeshi Momose,*** *Hiroshi Nishizato,* Kumamoto University, Japan*; Yugo Nakaya,* HORIBA STEC, Co., Ltd. / Kumamoto University, Japan*; Kanta Ishida, Shota Oda, Kinichi Nasu,* Kumamoto University, Japan*; Lianhua Jin,* University of Yamanashi, Japan*; Hiroshi Okajima,* Kumamoto University, Japan

The development of efficient and sustainable processes in atomic layer deposition (ALD) is becoming increasingly important for the fabrication of

next-generation three-dimensional (3D) semiconductor devices. However, conventional run/vent precursor delivery systems are inherently inefficient, with precursor dosing durations reported to be only 1-10% of the total cycle time, resulting in over 90% of the precursor being discarded without contributing to film growth. Furthermore, the development of the ALD process, especially the conformality of high-aspect-ratio (HAR) features, typically relies on time-consuming offline characterizations. In this study, we developed an integrated intelligent ALD research platform that combines on-demand precursor delivery with *in situ* imaging ellipsometry for real-time conformality analysis.

The platform integrates two key technologies. First, to achieve stable and precise on-demand precursor delivery, we developed an in-house piezoelectric-valve system. By applying a machine learning (ML) and control engineering approach, we achieved feedforward valve control, thereby successfully compensating for the inherent hysteresis and nonlinear flow responses of the valve. This allowed the achievement of ideal step-wise gas pulses with a settling time of only 60 ms, compared with 2 s in the uncontrolled condition. This precise control significantly enhances the precursor utilization efficiency while maintaining rapid pulse operation. Second, an in-house lateral high-aspect-ratio (LHAR, AR = 300) test structure combined with imaging ellipsometry was employed to quantitatively monitor the temporal evolution of the precursor penetration depth (PD) during ALD. Sample imaging was enabled by installing an Offner optical system on our custom-built ellipsometer, which allowed us to determine the PD formed in a groove on the Si substrate. As this is currently in an offline setting, we plan to install it in an ALD chamber with on-demand precursor delivery for real-time PD monitoring.

The integration of these technologies enables the instantaneous evaluation of the effect of precise changes in the precursor dose and pulse duration on conformality within HAR features. Initial experiments using trimethylaluminum (TMA) demonstrated that PD evolution in LHAR structures could be tracked. The proposed platform concept leads to a foundation for data-driven, low-waste, and rapidly adaptive ALD process development, contributing to reduced precursor consumption, shorter development cycles, and more sustainable atomic-scale manufacturing.

9:00am **AP+EL+MS+PS+TF-ThM-5 Real-Time Insights into Plasma-Based Atomic-Scale Processing via Ellipsometry**, ***Gottlieb Oehrlein***, University of Maryland College Park **INVITED**

Single-wavelength ellipsometry (SWE) has been employed as an attractive diagnostic technique for real-time, non-invasive monitoring of thin-film evolution during semiconductor processing. Characterized by high temporal resolution and sub-angstrom sensitivity, SWE allows for the precise detection of surface modifications without disrupting the plasma environment. These aspects, combined with relative ease of integration into complex process chambers, make SWE a premier tool for tracking atomic-scale processing. Because of its rapid sampling capabilities, SWE is an invaluable tool for probing the primary kinetics of plasma-surface interactions. We will discuss several case studies where ellipsometric monitoring provides critical insights into complex surface mechanisms, including the achievement of high material etching selectivity for dielectric materials, semiconductors and metals, atomic layer etching (ALE), and the dynamics of electron-beam enhanced remote plasma processing.

While ellipsometry excels at tracking processes including endpoints across diverse materials, optical data alone cannot resolve complex surface chemistry. This talk emphasizes the methodological importance of coupling ellipsometric data with chemical analysis, e.g. X-ray Photoelectron Spectroscopy (XPS) or other materials characterization techniques, to construct robust, chemically informative surface models. Integrating these complementary diagnostics bridges the gap between optical observations and fundamental chemical mechanisms.

Acknowledgements

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9:30am **AP+EL+MS+PS+TF-ThM-7 Spectroscopic Ellipsometry for Screening Chemical and Microstructural Properties of MoS_2 Thin Films Grown by Plasma Enhanced ALD**, ***Douglas Heine***, University of Michigan, Ann Arbor; *Paula Arellano,* University of Michigan; *Ageeth Bol,* University of Michigan, Ann Arbor

The two-dimensional layered semiconductor MoS_2 has attracted significant interest for applications in next-generation electronics, photonics and electrocatalysis due to its favorable electronic and optical properties. Plasma-enhanced atomic layer deposition (PEALD) provides a scalable route for the growth of MoS_2 thin films, offering excellent thickness control, conformality, and relatively low deposition temperatures, which are advantageous for integration into device architectures. However, PEALD grown MoS_2 films often exhibit complex microstructures, consisting of small and misaligned grains. Such structural disorder can adversely affect device performance due to the strong optical and electronic anisotropy of MoS_2[(1)].
In this presentation, we report the development of a model that rapidly estimates electronic and microstructural properties of PEALD-grown MoS_2 thin films from ellipsometry data. The influence of misaligned, out-of-plane oriented grains (“fins”) is described using a Bruggeman effective medium approach for intrinsically anisotropic inclusions[(2)], while local structural disorder is incorporated through modest variations in the intrinsic optical constants. The model is applied to a broad set of films grown under different deposition conditions, and the extracted parameters are correlated with independently measured film properties, including composition, crystallinity and roughness. By enabling rapid insight into the film microstructure and electronic properties, this ellipsometry-based analysis facilitates the development of PEALD processes that yield higher quality MoS_2 films.

(1) Toolbox of Advanced Atomic Layer Deposition Processes for Tailoring Large-Area MoS2 Thin Films at 150 °C. M. Mattinen et al. ACS Applied Materials & Interfaces, 2023 15 (29), 35565-35579.
(2) Bruggeman formalism versus “Bruggeman formalism”: particulate composite materials comprising oriented ellipsoidal particles. T. G. Mackay and A. Lakhtakia. Journal of Nanophotonics, 2012 6 (1), 069501-069501.

9:45am **AP+EL+MS+PS+TF-ThM-8 Monitoring Electron Beam-Assisted Atomic Layer Etching via Real-Time Ellipsometry and in-Situ XPS: Insights on the Early Stages**, ***Vennela Vuruputuri***, Department of Physics, and Institute for Research in Electronics and Applied Physics, University of Maryland; *Robert Bruce,* IBM TJ Watson Research Center; *Nathan Marchack,* IBM TJ Watson Center; *Marinus Hopstaken,* IBM TJ Watson Research Center; *Gottlieb Oehrlein,* Department of Material Science and Engineering, and Institute for Research in Electronics and Applied Physics, University of Maryland

Electron beam assisted etching of plasma functionalized materials has emerged as a novel approach to processing damage sensitive materials. This method employs synergistic interactions between low energy electrons and reactive neutral species to enable material removal while mitigating ion bombardment induced damage and achieving higher atomic precision. While this seems to be a promising approach, the influence of electron irradiation on surface chemistry, defect formation and bond scission are not well understood. Clarifying these mechanisms is essential to establishing electron beam-assisted atomic layer etching (EB-ALE) as a viable method for nanoscale fabrication. In this work, we investigate the EB-ALE of chlorinated single crystal silicon (c-Si) surfaces prepared using a remote plasma source with Ar/Cl_2 gas mixtures. The study examines the dependence of surface coverage, material modification and etching behavior on key parameters, including neutral exposure, and flood gun parameters like electron energy and dose delivery. ALE relies on self-limiting surface reactions, and one key question is if the EB-ALE process can maintain a constant etch depth per cycle as surface roughness, defect or byproduct accumulation evolve. The surface evolution is monitored in real time using in-situ ellipsometry, and it is further characterized using X-ray photoelectron spectroscopy (XPS) and atomic force microscopy (AFM) to analyze changes in chemical composition and surface roughness respectively. Together, these measurements will provide a framework to better understand the mechanisms governing EB-ALE and ensure predictive control over low-damage atomic scale processing.

Acknowledgements

This material is based upon work supported by the National Science Foundation under the award number NSF CMMI – 2350338.

11:00am **AP+EL+MS+PS+TF-ThM-13 Building Intelligence Through in Situ Techniques for Atomic Layer Processes**, ***Parag Banerjee***, University of Central Florida **INVITED**

Note: This abstract was initially for TF, but I request that the talk be moved to Gary W Rubloff (GWR) Symposium as it is much more topically relevant.

Atomic layer processing, which consists of atomic layer deposition (ALD) and atomic layer etching (ALE), provides the ultimate processing toolbox for dimensional and compositional control of thin films. In this talk, I will first provide a historical perspective of how specifically, *in situ* techniques implemented for atomic layer processes have impacted our understanding

of surface physical and chemical mechanisms that impart atomic layer processes their singular deposition and/or etching characteristics. For example, early work using *in situ* techniques such as, quadrupole mass spectrometry (QMS), Fourier transform infrared spectroscopy (FTIR) and quartz crystal microbalance (QCM) laid the foundation for understanding of the popular ALD chemistries of Al_2O_3 and ZnO. Next, I will showcase the use of *in situ* QMS and spectroscopic ellipsometry (SE) to rapidly screen new precursor molecules and deposit materials for a myriad of applications ranging from lasing fibers to passivation contacts for solar cells. The use of tandem *in situ* techniques will be highlighted which allows for unambiguous determination of both chemical and physical aspects of growth mechanisms during atomic layer processes. Last, due to the massive amounts of data obtained during *in situ* monitoring of processes, machine learning (ML) algorithms can now be successfully used to interpret process performance against process parameters, determining end points and establishing process – property causality. In summary, this presentation highlights the evolution of atomic layer diagnostics from foundational surface chemistry to modern, AI-driven process optimization.

11:30am **AP+EL+MS+PS+TF-ThM-15 Real Time Spectroscopic Ellipsometry and Passivation Studies of Ultra-Thin a-Si:H Films for C-Si / a-Si:H Heterojunction Solar Cells**, ***Venkanna Kanneboina***, *Prabin Dulal, Bishal Bishal Shrestha, Madan K. Mainali, Balaji Ramanujam, Ambalanath Shan, Nikolas J. Podraza,* University of Toledo

High passivation quality and excellent electronic properties of ultrathin hydrogenated amorphous silicon (a-Si:H) layers are essential to fabricate high efficiency crystalline silicon (c-Si) / a-Si:H heterojunction intrinsic thin layer (HIT) solar cells. The quality of the surface passivation of both undoped and doped a-Si:H layers deposited on c-Si are studied using minority carrier lifetime (τ_{eff}) measurements. Stacks of undoped a-Si:H / n-type c-Si / undoped a-Si:H, n-type a-Si:H / undoped a-Si:H / n-type c-Si / undoped a-Si:H / n-type a-Si:H, n-type a-Si:H / undoped a-Si:H / n-type c-Si / undoped a-Si:H / p-type a-Si:H are fabricated by radio frequency plasma enhanced chemical vapor deposition (RF-PECVD). Real time spectroscopic ellipsometry (RTSE) is performed to monitor growth during the deposition of the stacks to determine the structural and optical properties of the undoped and n- and p-type doped a-Si:H. To prevent epitaxial growth on the c-Si wafers, the first layer of undoped a-Si:H is deposited at relatively low temperature of 120°C without hydrogen dilution followed by a second layer of higher quality undoped a-Si:H with hydrogen dilution deposited at 160°C. The influence of additional hydrogen plasma treatment (HPT) on the passivation quality of a-Si:H layers on c-Si is studied by subjecting the undoped a-Si:H on both sides of the c-Si wafers to a hydrogen plasma. Passivation studies are performed on stacks of undoped a-Si:H deposited on both sides of c-Si, and then with an additional stack of doped a-Si:H. The symmetrically deposited bilayers of undoped a-Si:H effectively passivated the c-Si. The best τ_{eff} = 11.61 ms is obtained with HPT on undoped a-Si:H bilayers for 30 seconds at 200°C. The sample is exposed to atmosphere for about 30 min before it is loading into PECVD chamber and the measured τ_{eff} is 8.25 ms prior to deposition of the n-type a-Si:H. The τ_{eff} is recovered about 3 ms with doped n-type a-Si:H stack, whereas 1 ms is recovered with the n- and p-type a-Si:H stack. The passivation quality of single layer of ~6 nm undoped a-Si:H is also studied with variation of temperature from 120 – 200°C. In this case, the τ_{eff} decreased from 3.85 to 1.6 ms as the temperature increased from 120 – 200°C. High efficiency c-Si / a-Si:H HIT solar cells are fabricated using these optimized, high quality ultrathin a-Si:H layers.

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11:45am **AP+EL+MS+PS+TF-ThM-16 Quantifying Interface Formation in InP/Al_2O_3: ALD Films Probed by XPS and MIS C-V**, ***Fabiano Borges***, University of Campinas (Unicamp) and Federal Institute of Education, Science and Technology of São Paulo (IFSP), Brazil*; Cassio Almeida,* Semiconductor Laboratory (LabSem), Center for Telecommunication Studies (CETUC), Pontifical Catholic University of Rio de Janeiro (PUC-Rio), Brazil*; Ângela Albuquerque,* Brazilian Nanotechnology National Laboratory (LNNano, Brazilian Center for Research in Energy and Materials (CNPEM)), Brazil*; Gustavo Vieira,* Institute for Advanced Studies (IEAv), Department of Aerospace Science and Technology (DCTA), Brazilian Air Force, Brazil*; José Diniz,* University of Campinas (UNICAMP), Brazil

Abstract

Surface passivation of n-type InP was evaluated by X-ray Photoelectron Spectroscopy (XPS) depth-profile analysis after depositing an Al_2O_3 layer [1] with and without plasma treatments (oxidation (O2), nitriding (N2), oxidation followed by nitriding (O2N2), and nitriding followed by oxidation (N2O2)). To compare samples, we use the atomic fractions of Al2p, In3d, P2p, O1s, N1s, and C1s and two metrics [2]: top-film O/Al ratio at the first depth, with values near 1.5 indicating stoichiometric Al_2O_3; (ii) interface depth, the etch time where the sum of In+P≥20%.

The data show that O2 yields a stoichiometric surface (O/Al = 1.37) and the deepest interface (75s), consistent with a thicker interfacial oxide. N2 presents a very low O/Al (0.12) with detectable N and no interface onset within 120s, indicating a dense nitride/oxynitride barrier. N2O2 is intermediate (O/Al=1.42; interface 50s) with no residual N, suggesting oxidation of the nitride. The control sample shows oxidation (O/Al=0.51; interface 45s), while O2+sputtering produces the lowest O/Al (0.14) and the shallowest interface (35s), indicative of a less oxidized/less dense film.

Electrical C-V corroborates the chemical trends: the O2 sample exhibits a median flat-band voltage Vfb=0.00V (-0.30V for the control) and a donor density of the same order (2×10^{19} vs 1×10^{19} cm^{-3}), indicating a flatter band alignment without doping degradation. Altogether, O2 delivers the most stoichiometric Al_2O_3, a thicker/interfacial oxide and superior C-V metrics, pointing to improved passivation of InP compared with ALD on untreated surfaces; N2 forms a robust nitride that retards sputter breakthrough; and ALD delivers denser, more stoichiometric Al_2O_3 than sputtering.

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Acknowledgments

This research is supported financially by IFSP, FINEP, CNPq and UNICAMP. This research used facilities of the Brazilian Nanotechnology National Laboratory (LNNano), part of the Brazilian Centre for Research in Energy and Materials (CNPEM), a private non-profit organization under the supervision of the Brazilian Ministry for Science, Technology, and Innovations (MCTI). The Spectroscopy and Scattering staff is acknowledged for the assistance during the experiment 20220304. The InP substrate weresupplied by LabSem of PUC-Rio. The author thanks the support of the Instituto de Estudos Avançados of the Brazilian Air Force.

Applied Surface Science
Room 321 - Session AS-ThM

Complex Data Analysis For Applied Surface Science

Moderators: Dr. Jonathan Counsell, Kratos Analytical Inc, **Dr. Jeffrey Terry**, Illinois Institute of Technology

11:00am **AS-ThM-13 Data-Driven Analysis Using Explainable AI (XAI) for Surface Analysis Data, Including Mass Images**, ***Satoka Aoyagi***, Seikei University, Japan **INVITED**

Sophisticated analysis methods, such as secondary ion mass spectrometry, provide rich information about a sample, from which we could generally extract and interpret only a part of it. The effective application of machine learning methods to such data is useful for extracting hidden yet important information with which to characterize the sample. Although there are a variety of methods to analyze complex datasets, the methods that also provide the information on the analysis processes are crucial for analyzing scientific data. This presentation focuses on such methods, known as explainable AI (XAI). Unsupervised learning methods, such as principal component analysis (PCA), non-negative matrix factorization (NMF) and autoencoder (AE), are useful for understanding the outline of the data and sample that are analyzed. Supervised learning methods are powerful for further analysis, such as exploring related factors of a particular material or characteristic in a sample. Combining unsupervised and supervised learning methods provides detailed information on related variables, such as groups of mass peaks from the same material, and on the relationships between particular sample conditions and chemical structures. The application of unsupervised learning methods, such as PCA, NMF and AE, and supervised learning methods, such as artificial neural network (ANN)-based methods [1-3] and Random Forest [4], to organic complex sample datasets is introduced. Moreover, ANN-based systems are useful in dealing with datasets including non-linear factors such as matrix effects, which cause peak intensity changes regardless of the concentration of a target material. The weights of ANN systems indicate which variables are important for the purpose of the analysis, suggesting whether an ANN system outputs

answers depending on the appropriate variables. For example, quantitative analysis including interface evaluation of multilayers in depth profiles often requires correction methods. ANN is generally powerful for the ANN-based system developed for secondary ion mass spectrometry (SIMS) data of three-component systems, which is introduced here.

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11:30am **AS-ThM-15 Data-Driven Automation for X-Ray Photoelectron Spectroscopy (XPS)*, David Valley,*** *James Johns, Jiayue Lin, Jennifer Mann, Kateryna Artyushkova,* Physical Electronics

We are presenting a set of data-driven tools aimed at simplifying XPS analysis while using data-driven decision making processes to maintain flexibility for advanced use. The approach uses both machine learning and analytical models to automate key steps in both sample setup and data acquisition.

In XPS analysis, typically samples are small, or cut to a smaller size to accommodate the instrument. As a result, multiple samples will fit on a sample holder (platen) and in a high throughput instrument, multiple sample holders can be put in the instrument at once, resulting in potentially 100s of samples in the instrument at any given time.XPS users have identified pain points of the repetitive, tedious work of creating analysis points on each sample mounted on the platen. To address this necessary, but time-consuming step usually performed by the user, we have developed three machine learning models to automatically detect the platen type, platen-photo alignment, and the sample locations on the platen. These are used to automatically qualify the platen upon introduction to the instrument and populate potential analysis positions.

A second set of tools is to use statistical methods to optimize the basic analysis routines that are the starting point for XPS analysis. XPS analysis requires the acquisition of a wide energy range survey spectrum to identify the elements on the surface of the sample, followed by narrow scans that focus on the elements of interest to get higher signal-to-noise for quantification purposes and/or reveal the chemical state of a particular element. We introduce a data-based optimization routine to determine the time balance to get the best data quality for the region acquisitions scans based on a measurement of the survey scan. From the signal-to-noise of the equal time-based survey acquisition we extrapolate the expected error in the atomic percent quantification and choose optimum routines. The optimum is not a unitary choice and there is a pareto optimal front of possible acquisitions states. Based on user input we create an objective function which fits the user's desire for the acquisition result.

11:45am **AS-ThM-16 Computational Assessment of Environment-Dependent Mineral Surface Transformations*, Jennifer Bjorklund,*** *Sara Mason,* Center for Functional Nanomaterials, BNL

Understanding how mineral surfaces evolve and react under environmentally-relevant conditions is crucial to predicting interfacial processes governing resource recovery, nutrient cycling, and aqueous geochemistry. Minerals like pyrite (FeS_2) and struvite ($NH_4MgPO_4 \cdot 6H_2O$) are environmentally and technologically important systems whose surface chemistry is sensitive to aqueous conditions, with reactivity ultimately controlled by termination, hydration, protonation state, and local atomic configuration. Here, using an approach that combines Density Functional Theory (DFT) calculations with atomistic thermodynamics, we characterize surface stability, transformation pathways, and their impact on reactivity under relevant chemical conditions.

For pyrite, we explicitly compare hydroxylation and protonation of exposed surface sites to determine stable interfacial configurations as a function of aqueous conditions (pH, temperature, pressure). We further assess possible modes and energetics of arsenic (As) incorporation into near-surface and surface sites, identifying preferred structural motifs and their influence on local electronic structure. Building on these structural models, we evaluate gold (Au) adsorption energetics to understand how environmentally induced surface transformations and dopant incorporation modify interfacial binding and reactivity relevant to gold deposition and ore formation processes.

For struvite, we investigate pH-dependent stability of multiple surface terminations derived from the underlying bulk composition, explicitly sampling variations in protonation and hydration states. By constructing thermodynamic comparisons of these stable configurations, we identify dominant surface structures under varying aqueous conditions and quantify how protonation and hydration influence stability and reactivity. These results provide molecular-level insight into the transformations of struvite surfaces under realistic environmental conditions associated with nutrient release.

Together, these insights highlight how aqueous conditions drive surface transformations in mineral systems and how these transformations control downstream interfacial reactivity. By linking surface stability, protonation/hydration, dopant incorporation, and adsorption energetics, this work provides a unified framework for understanding environmentally-relevant responsible mineral interfaces at the atomic scale.

12:00pm **AS-ThM-17 Surface and Subsurface Chemistry of IrOx Electrocatalysts: A Multi–Technique Approach Integrating ToF–SIMS, XPS, and Multivariate Analysis*, Lonneke van Eijk,*** Colorado School of Mines, USA*; Genevieve Stelmacovich,* LAM Research*; Michael Walker,* Colorado School of Mines, USA*; Rebecca Hamlyn,* Lawrence Berkeley Lab, USA*; Zhao Li, Xiaoping Wang,* Argonne National Laboratory, USA*; Ethan Crumlin,* Lawrence Berkeley Lab, USA*; Alexey Serov,* Oak Ridge National Laboratory, USA*; Deborah Myers,* Argonne National Laboratory, USA*; Svitlana Pylypenko,* Colorado School of Mines, USA

Understanding the surface and subsurface chemistry of IrO_x electrocatalysts is essential for advancing performance of Proton Exchange Membrane Water Electrolyzers (PEMWEs). Commercial IrO_x powders exhibit diverse physicochemical properties and the interplay between various properties and activity and stability is still under investigation. In this work, six commercial IrO_x catalysts were examined. Initial studies used a suite of characterization methods including bulk structural and compositional techniques such as XRD, PDF, SAXS/USAXS, and XAS, as well as surface sensitive structural and compositional methods BET surface area analysis and XPS. These measurements were combined with electrochemical properties, including electrical conductivity and electrochemical measurements in rotating disk electrode configuration to assess activity and stability. This work also includes analysis of the same set of samples with ToF–SIMS, to further access surface and near-surface chemical information, extending into the bulk through depth profiling, to corroborate and complement other methods. This is accomplished using a three–stage framework for interpreting IrO_x surface chemistry using PCA.

First, ToF–SIMS is examined independently to determine how fragment distributions, depth–dependent signals, evaluated in the context of matrix effects to understand how they correlate with IrO_x composition, oxygen environments, and defect-related chemistry. This step clarifies how ToF–SIMS can be reliably applied to complex oxide electrocatalysts and what chemical information it uniquely provides. Second, ToF–SIMS results are correlated with XPS to refine chemical-state assignments. ToF–SIMS fragment trends are used to validate or challenge XPS peak-fitting models, improving confidence in oxidation-state and oxygen-species interpretation. Finally, ToF–SIMS and XPS parameters are correlated to bulk compositional and structural parameters along with electrochemical metrics. PCA reveals cross–technique correlations that reveal how surface chemistry and subsurface structure relate to catalyst performance and robustness. By combining complementary vacuum–based methods with statistical analysis, this work demonstrates how multi–characterization strategies resolve ambiguities that cannot be addressed by any single technique. The resulting framework provides a generalizable approach for using ToF–SIMS and XPS together to interrogate complex oxide surfaces and highlights the power of integrated surface analysis for understanding structure–chemistry relationships in advanced electrocatalysts.

Advances in Battery Engineering, Interface Design, and Characterization Mini-Symposium
Room 319 - Session BT1+AS+CA+TF-ThM

Interface Engineering in Batteries

Moderators: Prof. Dr. Adriana Creatore, Eindhoven University of Technology, **Prof. Alexander Kozen**, University of Vermont

8:00am **BT1+AS+CA+TF-ThM-1 Plasma and Electrochemical Modification of Battery Cathode Surfaces to Enhance Voltage Stability and Thus Energy Density**, ***Paul Braun,*** University of Illinois Urbana-Champaign **INVITED**

The energy density of battery cathodes increases dramatically with increases in voltage. However, higher operating voltages, in particular above 4.3V leads to significant capacity degradation. Because the mechanism of capacity degradation is often a surface-initiated reaction, modification of the exposed surface of the cathode material is a promising approach to increase energy density without adding significant mass or volume to the battery. Two approaches we are investigating to increase the voltage stability of $LiCOO_2$, a common battery cathode material, include surface modification via a plasma process, and electrochemical deposition of a high voltage stable material. Both methods result in a thin layer of high voltage stable material on the surface of the active cathode material. The plasma modification forms a nanoscale layer of disordered rocksalt on the underlying layered $LiCoO_2$ while the electrochemical modification grows a layer of lithiated manganese oxide on the underlying $LiCoO_2$. In both cases, the cyclable energy density of the $LiCoO_2$ is increased significantly.

8:30am **BT1+AS+CA+TF-ThM-3 Interfacial Engineering of Battery Materials using Atomic Layer Deposition**, ***Neil Dasgupta,*** University of Michigan, Ann Arbor **INVITED**

Interfaces and interphases play a critical role in battery performance, both in current state-of-the-art Li-ion batteries (LIBs), as well as next generation battery technologies. Therefore, there are great efforts to understand, control, and improve the properties of battery interfaces and interphases. This quickly becomes a multi-dimensional optimization problem, where the required properties of interfaces span from performance (i.e. fast rate capability), stability (i.e. long calendar life) and compatibility with the adjacent chemical and material phases. To address these challenges, there has been increasing interest in the application of 'artificial interphase' layers, which are typically comprised of nanoscale thin-film coatings along electrode-electrolyte interfaces. From a manufacturing perspective, it is critical that these surface coatings be deposited in a conformal, reproducible, scalable, and low-cost manner.

Towards these goals, our research group has developed a range of surface coating layers for battery applications, both for LIBs with liquid electrolytes, as well as next-generation systems such as Li metal anodes and solid-state batteries. In this talk, I will summarize recent progress towards precise and tunable interfacial control in batteries with both liquid and solid electrolytes, using atomic layer deposition (ALD) as an enabling platform. I will describe the development of advanced ALD chemistries, beyond the binary oxide systems that are typically employed. In LIBs, I will describe how surface coatings can simultaneously enable low-temperature and fast charging of graphite anodes without Li plating. In solid-state battery systems, I will describe the stabilization of cathode/solid electrolyte interfaces, enabling high-voltage cycling above 4.5 V. Finally, I will describe our efforts towards scalable manufacturing of ALD-coated battery electrodes, through the development of atmospheric-pressure spatial ALD technologies.

9:00am **BT1+AS+CA+TF-ThM-5 Atomic Layer Deposition (ALD) Tuned Interfaces for High-Performance Lithium- and Manganese-Rich Cathodes**, ***Jahnavi Manikantan Sudharma,*** Argonne National Laboratory; *Jeffrey Elam,* Argonne National Laboratory, USA

The growing deployment of renewable energy and the rapid expansion of artificial intelligence and machine learning infrastructures place increasingly dynamic demands on modern electrical grids, requiring the need for high-performance, renewable energy-storage technologies. While nickel (Ni)-rich layered oxides remain the state-of-the-art materials for lithium-ion battery cathodes, their reliance on costly and supply-constrained Ni and cobalt (Co), motivates the development of alternative materials. Lithium- and manganese (Mn)-rich (LMR) cathodes offer a compelling solution due to their high energy density and reversible capacities enabled by anionic redox. However, oxygen loss associated with this redox process induces severe surface and interfacial degradation, including electrolyte decomposition, transition-metal migration, and Mn dissolution, which hinder long-term cycling stability of these cathodes. Suppressing Mn dissolution at the surface is still a key challenge. Advancing surface engineering, structural tuning, and electrolyte optimization is therefore critical to unlocking the full potential of LMR cathodes for next-generation energy-storage systems. Atomic layer deposition (ALD) being a self-limiting thin film growth method characterized by the sequential exposure of chemical species, offers a promising strategy to stabilize the interfaces by depositing tailored ultrathin, uniform and conformal coating layers on the surface and thereby mitigating the surface degradation of the cathode. Surface coatings applied through atomic layer deposition (ALD) offer a highly controlled route to stabilize these interfaces; however, the fundamental mechanisms governing how different ALD chemistries interact with LMR surfaces remain poorly understood. In this presentation, I will discuss our recent study combining in situ measurements of ALD chemistries, ex situ thin film characterization, and electrochemical testing of prototype batteries. By systematically investigating ALD coating chemistries including lithium phosphate (Li_3PO_4) and lithium borate ($LiBO_x$), we elucidated how ALD surface reactions govern coating composition, structure, and protective functionality and how this functionality affects cycling performance. These insights will inform rational interface-engineering strategies, enabling the practical deployment of high-energy, cobalt-lean Mn-rich cathodes for next-generation lithium-ion batteries.

9:15am **BT1+AS+CA+TF-ThM-6 Atomic Layer Deposition for Lithium Metal Anode Stability**, *Niels Hoogedoorn, Meike Pieters, Cristian van Helvoirt,* ***Mariadriana Creatore,*** Eindhoven University of Technology, Netherlands

High-performance lithium-ion batteries (LIBs) are hampered by phenomena such as dendrite growth, electrolyte decomposition and uncontrolled interface formation between electrode and electrolyte. This is especially the case of next-generation battery materials, such as Si-anodes, Li-metal anodes and solid-state electrolytes. To address these challenges, atomic layer deposition (ALD) offers a promising pathway by engineering ultrathin conformal interfacial layers with atomic-scale precision.

In this contribution we present our recent work on ALD processes on lithium metal anodes (LMAs). The studies include: Al_2O_3, LiPO, LiPON and LiF, all developed in a FlexAL ALD-reactor (Oxford instruments). The supercycle approach for the process development of LiPO is highlighted: a novel Li-precursor, Lider™, is combined with an oxygen plasma (O_2*) and trimethyl phosphate (TMPO). The films are free of carbon impurities, despite that, during the subcycle of Lider + O_2*, Li_2CO_3 is detected by XPS in combination with a vacuum transfer unit. We find that a chemical vapour transformation [1] occurs, where the subsequent exposure of Li_2CO_3 to TMPO, leads to the abstraction of carbonate from the film, towards C-free LiPO [2].

Additionally, we discuss the deposition of these ALD layers on LMAs and their effect on the critical current density (CCD) of the LMAs, tested in a Li | argyrodite | Li symmetric cell. A home- built vacuum transfer module is used to transport the LMAs between a glovebox and the ALD reactor, where the ALD layers are processed at 120 °C. The CCD is the maximum electrical current per unit area that the anode can withstand before reaching failure, typically caused by lithium dendrite induced shorting. Depending on the material, and layer thickness, the ALD layers improve the CCD by more than 40%. For example, in the case of 10 Al_2O_3 cycles, the maximum sustainable current density increases from 2.4 mA/cm^2 to 3.4 mA/cm^2, thereby demonstrating enhanced stability against dendrite shorting. These results illustrate how engineering ALD interface layers can improve the CCD of LMAs and mitigate challenges in LMA stability. Moreover, these studies propose CCD measurements as screening approach of ALD chemistry and processing conditions towards their implementation and testing in full LIB cells.

[1] M. Y. Young et al., *J. Phys. Chem. C*2019, *123,* 9,23783.

[2]M. J. Pieters et al., *J. Phys. Chem. C*2026, 130, 15, 5458.

9:30am **BT1+AS+CA+TF-ThM-7 Buffer Layer Oxidative Polymerization to Stabilize Li Metal Anodes for Lithium Ion Batteries**, ***Amit K. Datta,*** *Blaine D. Kelly, Dilan M. Gamachchi, Indeewari M. Karunarathne, Campbell A. Sweet, Andrew C. Meng, Matthias J. Young,* University of Missouri

Li metal anodes promise an order of magnitude higher energy density than conventional graphite anodes in Li ion batteries, however, the practical use of Li metal as an anode remains limited by several factors such as unstable interfacial reactions, continuous electrolyte decomposition, and dendritic Li growth, leading to rapid cell failure. Oxidative Molecular Layer deposition (oMLD) offers the ability to deliver thin film polymer coatings with electronic, ionic and chemical properties of interest for improving stability of Li metal anodes, but oMLD employs harsh oxidants that are not

compatible with Li metal substrates. In this work, we demonstrate an approach we term buffer layer oxidative polymerization (BLOP), to enable the delivery of oMLD coatings onto Li metal. We investigate three BLOP derived polymer coatings on Li metal: polyhydroquinone (pHQ), poly(2,5-dimercapto-1,3,4-thiadiazole) (pDMCT), and poly(p-phenylenediamine) (pPDA). These three coatings were selected as representative classes of coatings based on their electronic and ionic conductivity differences: pHQ exhibits both Li ion conductivity and electronic semiconductivity, pDMCT shows only Li ion conductivity and pPDA shows anionic conductivity and electronic semiconductivity. Galvanostatic charge-discharge measurements in Li-Li symmetric cells show differences in the stability enhancement among the different coatings, with a clear benefit for BLOP vs. oMLD and MLD. Electron microscopy on these coatings helps understand the crosslinking depth achieved from BLOP coatings generated by different organic monomers. Overall, this work demonstrates the oxidative synthesis of multiple polymeric thin films directly on Li metal without degrading the substrate and identifies that coatings with Li ion conductivity and electronic semiconductivity show improved Li metal stability over the alternatives.

9:45am **BT1+AS+CA+TF-ThM-8 Modulation of Anode-Free Sodium Battery Interfaces through Atomic Layer Deposition of NaF***, **Jonathan Thurston,** Aaron Melemed, Neil Dasgupta,* University of Michigan

Sodium-based batteries are a promising alternative to lithium-ion technologies due to the higher earth abundance and lower cost of sodium. Furthermore, when Na metal electrodes are used in an “anode-free” configuration, the theoretical energy density is competitive with that of lithium-ion systems. However, the effects of the current-collector surface chemistry on the subsequent Na plating/stripping and solid electrolyte interphase (SEI) composition remains limited.

In this study, we synthesize an “artificial SEI” of NaF using atomic layer deposition onto the surface of Cu current collectors (CCs). Thermal ALD of NaF is successfully demonstrated using sodium *tert*-butoxide and ammonium fluoride precursors. We investigate the impact of the NaF surface layers on the subsequent morphology of deposited sodium using electron microscopy. A multi-modal suite of near-edge X-ray absorption spectroscopy (NEXAFS), X-ray photoelectron spectroscopy (XPS), and infrared spectroscopy (IR) are used to characterize the composition and structure of the resulting SEI as a function of depth and battery cycling. Our results show that the NaF layer encourages more homogenous plating with controlled nucleation sites, while bare Cu CCs have more sporadic nucleation sites for Na metal and a more dendritic mossy plating morphology. Additionally, electrochemical impedance spectroscopy (EIS) and chemical state identification indicate that a more stable SEI is formed in the first few cycles for NaF-coated Cu CCs, while an evolving SEI is observed for uncoated Cu CCs. Our work demonstrates the importance of surface layers in anode-free battery current collectors, while investigating the dynamic nature of the SEI composition and structure throughout cycling.

Advances in Battery Engineering, Interface Design, and Characterization Mini-Symposium
Room 319 - Session BT2+AS+CA+TF-ThM

Advanced Battery Electrodes

Moderators: Prof. Alexander Kozen, University of Vermont, **Dr. Tanguy Terlier**, Rice University, **Dr. Andrew Westover**, Oak Ridge National Laboratory

11:00am **BT2+AS+CA+TF-ThM-13 Understanding the Electrically-Limited Reaction Kinetics and Dynamics for Conversion Electrode Iron Fluoride***, **Chuan-Fu Lin,*** Catholic University of America **INVITED**

To maintain efficient reaction kinetics in standard electrodes, fast and stable ionic and electronic conductive networks are required for long-term reversibility, and this poses the major challenges for conversion-type electrode materials. The phase separation reaction, CM + Li^+ + e^- -> M (reduced metal) + LiX (Li compounds), induced by the lithiation process deteriorates the structural integrity, which certainly destroys the original ionic and electronic pathways and reconstructs new ones. However, it is still unclear whether the transports of conversion electrode are benefited or hindered from the reconstruction of transport pathways due to phase separation, yet the dynamic evolution of electrical conductivity in these systems remains overlooked.

This work aims to investigate the electrically-limited reaction of conversion electrodes upon phase separation and recombination by studying the structural, electrical, and electrochemical properties of amorphous and crystalline iron (III) fluoride (FeF_x) thin films synthesized via sputtering deposition. Using a binder-free lateral device architecture and probing measurement, we dynamically mapped resistivity evolution during electrochemical cycling. While pristine crystalline films exhibit lower initial resistivity than amorphous films, deep lithiation triggers a dramatic drop in resistivity by over five orders of magnitude in both structural variants. Despite the massive volume fraction of the insulating LiF byproduct (1 : 4.17 for Fe : LiF ratio), the resistivity reduced to ~0.35 Ω·m, demonstrating a common conduction pathway formed by a metallic Fe network within the nanocomposite. Correlating this resistivity evolution with X-ray Photoelectron Spectroscopy (XPS) spectra reveals the electrically-controlled reaction dynamics of the thin-film conversion electrodes. Conversely, delithiation results in a resistivity increase of two orders of magnitude, driven by a rate-dependent electrochemical "trapping effect." Fast charging causes isolated Fe domains electronically stranded within the LiF matrix and driving irreversible capacity loss. These results elucidate the coupling between chemical quantifications, reaction dynamics, and electrical properties, providing understanding of the influence of the electrical conductivity for high-energy-density conversion cathodes.

11:30am **BT2+AS+CA+TF-ThM-15 Correlating Electrical Property Evolution and Reversibility in Sputtered ZnO Thin-Film Conversion Electrodes***, **Sukanya Goswami,** Chuan-Fu Lin,* The Catholic University of America

During conversion reaction in Lithium-ion batteries, electrical properties shift as reaction kinetics vary with phase separation, state of charge, and evolving conductivity. Understanding how these dynamic electrical transitions govern reaction control is essential for optimizing conversion electrodes. This study probes the evolution of ZnO conversion electrodes during cycling, examining the electron transport, reversibility and capacity retention. Because the literature on ZnO remains limited, it provides a simple benchmark for testing broader conversion-mechanism concepts and for comparing phase separation and recombination process across conversion materials in LiBs. **Sputter-deposited ZnO thin films** were cycled in a lithium-ion half-cell configuration and their electrical transport properties tracked ex-situ using **two-probe resistivity measurements** after each set of cycles.

The resistivity data reveal a clear and progressive deterioration in electronic transport over cycling. Starting from values on the order of **10^{-4} Ω.m** in the early cycles, resistivity increases by several orders of magnitude, reaching **1-7 Ω.m** by **cycle 30**. This monotonic rise reflects a gradual breakdown of the conductive percolation network as the conversion reaction proceeds. Persistent differences in resistivity during early cycling reveal an asymmetry between lithiation and delithiation, likely caused by sluggish reconversion kinetics of the phase-separated products. These electrical changes correlate directly with coulombic efficiency. When the electrode maintains sufficient conductivity, capacity retention is upto **95%**. Conversely, as resistivity rises sharply with progressive cycling, coulombic efficiency becomes irregular and drops. This correlation implicates degradation of electronic transport, driven by delamination caused by the volume expansion during phase transformation, as the primary mechanism governing capacity fades.

To understand the structural and chemical origins of these changes, cycled electrodes were characterized by **XRD, XPS, and SEM**. XRD tracked phase separation and recombination between ZnO, metallic Zn and Li_2O. XPS provided insight into surface chemical states and irreversible interfacial species, while SEM captured morphological degradation including delamination. Together, these results establish a direct link between electronic conductivity, conversion reaction reversibility and coulombic efficiency, offering a framework for mitigating kinetic limitations in ZnO based thin film cathodes.

11:45am **BT2+AS+CA+TF-ThM-16 Molecular Mapping Investigations of Prelithiation Alloy Formation via Thermal Evaporation on Silicon Based Electrodes***, **Gabriel Parker,** Amanda Musgrove, Gabriel Veith, Ivan Matyushov, Xiao-Ying Yu,* Oak Ridge National Laboratory, USA

Abstract: Silicon based composites have become increasingly popular as potential anodes for lithium-ion batteries due to their large storage capacity, relative abundance, and low cost. However, these anodes often see reduced initial columbic efficiency (ICE) due to disruptive volume expansion up to 300% and continuous unstable solid electrolyte interphase (SEI) layer formation. Prelithiation, the process of adding excess reservoir of Li to the electrode to compensate for irreversible SEI formation losses during their sample preparation, has proven to solve the issue of immediate capacity loss. Thermal evaporation is a prelithiation technique with limited studies on its effectiveness. In this study, time-of-flight

secondary ion mass spectrometry (ToF-SIMS) is used to investigate the benefits of prelithiation via thermal evaporation. ToF-SIMS provides chemical mapping and spatial information in 2D and 3D visualizing the deposition of lithium, identifying Li_xSi_y alloy and $Li_xSi_yO_z$ silicate formation, and the distribution of lithium passivation into the electrodes. Passivation under different atmospheric conditions, such as inert Argon (Ar) and Ar/carbon dioxide (CO_2), highlights the impact of the environment on the passivation effectiveness and formation of Li_xSi_y alloy and $Li_xSi_yO_z$ silicate. The ToF-SIMS molecular imaging and depth profiling results indicate that prelithiation via thermal evaporation effectively distributes lithium throughout the depth profile thickness of several hundred nanometers. It induces a greater degree of $Li_xSi_yO_z$ silicate formation over Li_xSi_y alloy. The results provided by the ToF-SIMS are corroborated by electrochemical measurement of the electrodes under inert Ar and Ar/CO_2 environments indicating that the Ar/CO_2 electrode retained a higher specific capacity over multiple cycles. Our ToF-SIMS characterization results show the effectiveness of thermal evaporation in producing a more stable electrode and an electrode with an effective lithium reserve that can preserve its capacity.

Keywords: Solid-state batteries, solid-electrolyte interface, ToF-SIMS, prelithiation, molecular imaging.

12:00pm **BT2+AS+CA+TF-ThM-17 Engineering Conformality of Lithium–Terephthalate Thin Films via Precursor Selection***, **Anish Philip**, Joakim Jestilä, Milad Madadi,* Aalto University, Finland*; Jussi Kinnunen,* Chipmetrics Ltd, Finland*; Antti Karttunen, Maarit Karppinen,* Aalto University, Finland

Lithium-terephthalate (Li-TP) is recognized as a highly promising anode material for lithium-ion batteries.[1] The advantages of atomic/molecular layer deposition (ALD/MLD) technique have enabled the realization of Li-TP thin films in a highly controllable manner needed for its use in thin-film microbattery configuration.[2] However not much attention has been paid to understand the importance of selecting an appropriate lithium precursor for controlling the thin film properties and conformality, even though Li-TP materials are highly desirable from the battery application point of view. Given their potential application in 3D thin-film microbatteries, understanding both conformality and thin-film coverage (penetration depth) are also crucial. In this research, we investigated the impact of different lithium precursors on the Li-TP thin film properties, conformality and penetration depth (PD). The lithium precursors evaluated were: lithium tert-butoxide (LiO^tBu), lithium bis(trimethylsilyl)amide (Li-HMDS) and lithium 2,2,6,6-tetramethyl-3,5-heptanedionate (Li-THD); for the first two precursors the ALD/MLD process was developed/optimized as they had not been previously employed for the Li-TP thin film growth. For conformality measurements, we utilized lateral high-aspect-ratio (LHAR) PillarHall[3] structures and a novel imaging ellipsometry technique that enables film thickness determination even at Ångström level. To support the experimental work, a detailed computational survey of the precursors was conducted. Through DFT optimizations combined with highly accurate DLPNO-CCSD(T) energy calculations the most prevalent oligomeric forms under typical ALD conditions were determined; the effective diameter (d_{eff}) and mean free path (MFP, λ) of the precursor's oligomeric form were found to play a major role in determining the conformality characteristics of the resultant Li-TP thin films (Figure 1). Among the three precursors investigated, Li-HMDS was found to result in Li-TP thin films with superior conformality characteristics. The current approach of using theoretical calculations to predict film conformality based on precursor molecular structure can significantly reduce the amount of experimental work required and streamline the screening process for precursors aimed at enhancing conformal coating.

References

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[2] M. Nisula, M. Karppinen, Nano Lett., **1**6, 1276–1281, 2016.

[3] A. Philip et.al., Small, **20**, 2402608, 2024.

Plasma Science and Technology
Room 315 - Session PS1-ThM
Advanced Ion and Reactant Control I

Moderators: Dr. Sebastian Engelmann, IBM T. J. Watson Research Center, **Prof. Dr. Christophe Vallee**, UAlbany

8:00am **PS1-ThM-1 Plasma Prize Talk: Drilling Really Tiny Holes in Glass: The Role of Ion Energy Control in Nano-Fabrication***, **Steven Shannon,*** North Carolina State University **INVITED**

You would be amazed at how reliant our high technology economy relies on a process that at first glance sounds very straight forward... drilling holes in glass. Of course, this description simplifies things. These holes are as small as several hundred atoms in diameter and are as much as 200 times deeper than they are wide, and they are one of the most critical components in advanced interconnect layers for logic devices and the backbone of advanced memory devices.

Plasma assisted etching is used to fabricate these tiny holes. By combining the non-equilibrium chemistries and directed energetic ions formed in plasma systems, highly anisotropic holes can be cut into dielectric layers. This talk will focus on one aspect of these processes, the energetic ions that strike the surface. The role of these ions in anisotropic etching of these features and efforts to control and measure the direction and energy of these ions to further extend the capabilities of these processes will be discussed. Mechanisms for approximating and measuring the energy of ions that drive these processes will be discussed. Finally, current and future research paths for further extending the capabilities of these critical ion driven processes will be presented.

8:30am **PS1-ThM-3 Time-Domain RF Matching and Ion Energy Control in Pulsed Bias Capacitively Coupled Plasmas***, **Yeon Geun Yook,*** University of Michigan*; Hyunjae Lee,* Samsung Electronics, Republic of Korea*; Mark J. Kushner,* University of Michigan

Pulsed-bias capacitively coupled plasmas (CCPs) are widely used in advanced semiconductor plasma etching processes to control ion energy, surface charging, and etch profiles. In practical RF systems, the voltage waveform produced by the generator is not necessarily delivered directly to the wafer electrode due to intervening impedances, including the match-box. Even when the impedance of the plasma reactor is well matched to the power supply though the match-box with continuous-wave (CW) excitation or late during the power-on phase of pulsing, a mismatch can occur during the power-on and power-off transitions. This mismatch is due to the finite transient response of the matching network, stored energy in circuit components, blocking-capacitor charge dynamics, and time-varying plasma impedance. These effects can distort the electrode voltage and self-bias waveform, thereby modifying the ion energy distribution delivered to the wafer.

In this work, the effects of time-domain RF matching transients on ion-energy control in pulsed-bias dual-frequency CCPs sustained in Ar/HF mixtures were computationally investigated using the Hybrid Plasma Equipment Model (HPEM). The bottom electrode is modeled with a π-type matching network and blocking capacitor through which the bias power is applied. First, the matching capacitors are tuned to minimize reflected power for long pulsed biases which have achieve a quasi-steady state. The effects of generator rise/fall times, pulse period, and blocking-capacitor value on plasma properties are analyzed, including time-dependent reflected power, network loss, stored energy, plasma absorbed power, and self-bias voltage.

The consequences of pulse power delivery on phase-resolved ion energy and angular distributions (IEADs) to the wafer during the rise, top-flat, fall, and off phases were investigated. Waveform compensation was explored as a possible strategy to mitigate matching-induced waveform distortion and improve ion-energy control. The plasma properties obtained from the HPEM were used as input to the Monte Carlo Feature Profile Model (MCFPM) to evaluate the impact of RF matching transients on etch profiles during cryogenic etching.

8:45am **PS1-ThM-4 Tailored Voltage Waveforms in Capacitively Coupled Plasmas: Effect of Voltage Transition Slope on Ion and Electron Dynamics in Argon Discharges***, **Syed Zulqarnain**, Basak Bagci,* North Carolina State University*; Harutyun Melikyan, Ebony Mays,* Micron Technology*; Steven Shannon, Amanda Lietz,* North Carolina State University

Capacitively coupled plasmas (CCPs) are extensively employed in selective and anisotropic etching of semiconductor materials and deposition of thin films. Tailored voltage waveforms offer a promising approach to

independently control ion energy and flux at the electrode surface, providing an additional degree of freedom for tuning the ion energy distribution function (IEDF). A square-shaped bias waveform is particularly attractive because its flat negative plateau maintains a near-constant sheath voltage, allowing ions to arrive at the substrate with narrow, well-defined energy. The negative phase must exceed the ion transit time across the sheath to ensure acceleration under a near-static potential, while the longer positive phase allows complete charge neutralization before the next pulse. This asymmetry makes the duty cycle a physically meaningful design parameter. At each polarity transition, the sheath boundary rapidly expands or collapses, transferring energy into electrons. The slew rate (dV/dt) sets the sheath expansion velocity, governing the intensity of this heating burst and the sheath potential during the transition. Ions crossing the sheath in this window experience a time-varying potential, shaping the tail of the IEDF. The slew rate is thus a fundamental control variable that simultaneously couples waveform shape to sheath dynamics, electron power absorption, and ion bombardment. In this study, a dual-frequency CCP discharge in pure argon at 10 mTorr is investigated using the Monte Carlo collisions-based particle-in-cell code, EDIPIC[1]. A 60 MHz sinusoidal waveform on the upper electrode sustains the discharge and controls plasma density, while a 400 kHz asymmetric square voltage waveform on the lower electrode controls ion bombardment. The waveform uses a short negative phase (~0.5 μs) sufficient for ion transit and a longer positive phase (~2.0 μs) for full charge neutralization before each pulse. As the transition slope varies from near-instantaneous to gradual, its influence on sheath dynamics, electron heating, and power deposition is explored through time-resolved analysis over a single low-frequency cycle. The simulated IEDFs are compared against experimentally obtained IEDFs via retarding field energy analyzer, alongside comparisons of plasma density and sheath width. This investigation elucidates the interplay among the dual-frequency drive, waveform transition dynamics, and plasma response, providing insight into how square-wave tailored waveforms can control plasma dynamics in low-pressure CCP discharges*, with extensions to O_2 admixtures.*

1.https://pcrf.princeton.edu/capabilities/modeling-tools-and-computer-codes/edipic-code/

9:00am **PS1-ThM-5 Studies of Rf-ICP Source with a High Voltage Nanosecond-Tailored Voltage Waveform Biased Substrate***, **Yerbolat Ussenov**, Yevgeny Raitses,* Princeton Plasma Physics Laboratory

High-voltage substrate pulsing is a promising technique for tailoring peak ion energies and narrowing ion energy distribution functions (IEDFs) in high-aspect-ratio (HAR) plasma etching [1,2]. By utilizing a non-sinusoidal asymmetric bias (100–600 kHz) characterized by short positive pulses (~hundreds of ns) and extended negative phases, surface charge neutralization can be achieved while maintaining precise control over ion bombardment. In this study, we investigate the impact of pulsed substrate biasing [3] on a cylindrical inductively coupled plasma (ICP) source. Time-averaged axial distributions of plasma parameters and electron energy distribution functions (EEDFs) were characterized via Langmuir probe diagnostics and compared against steady-state (pristine) plasma conditions. To capture the transient discharge physics, time-resolved dynamics were analyzed through instantaneous floating potential measurements at different substrate to probe distance. Furthermore, the spatio-temporal evolution of optical emissions near the substrate was evaluated using phase-resolved optical emission spectroscopy (PROES) equipped with an ICCD camera and light emission filter. Also, the Doppler shift laser induced fluorescence (LIF) implemented to test the possibility of time resolved IEDF measurements. Our preliminary results demonstrate that the pulsing significantly alters the local plasma properties near the substrate. The underlying physical drivers are discussed.

This work was conducted at the Princeton Collaborative Research Facility (PCRF), which is supported by the U.S. DOE under Contract No. DE-AC02-09CH11466. The authors are grateful to Prof. Vince Donnelly for sharing ICP design, and Eagle Harbor Technologies, Inc. for providing their pulser.

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9:15am **PS1-ThM-6 Experimental Investigation of Tailored Voltage Waveforms in Dual-Frequency Ar/O_2 Capacitively Coupled Plasmas***, **Basak Bagci**, Syed M. Zulqarnain, Amanda M. Lietz, Steven C. Shannon,* North Carolina State University

Tailored voltage waveforms in capacitively coupled plasmas (CCPs) provide a powerful approach for controlling ion energy distributions and electron heating in semiconductor plasma processing. In low-pressure CCP discharges, waveform asymmetry and transition dynamics strongly influence sheath evolution, plasma potential, and ion acceleration, making waveform tailoring particularly attractive for applications requiring independent control of ion energy and ion flux. While these effects have been extensively investigated in noble gas plasmas, significantly less attention has been given to electronegative gas mixtures relevant to semiconductor manufacturing.

In this work, experimental measurements are performed in a dual-frequency and single-frequency CCP reactor operating in argon/oxygen mixtures at pressures near 10 mTorr. A 60 MHz sinusoidal waveform applied to the upper electrode sustains the plasma, while a low-frequency asymmetric pulsed waveform applied to the lower electrode controls ion bombardment dynamics. The influence of oxygen admixture and waveform transition characteristics on plasma behavior is investigated using synchronized plasma diagnostics. Ion energy distribution functions (IEDFs) are measured using a retarding field energy analyzer (RFEA), while electron density is obtained using a hairpin resonance probe. Simultaneous voltage measurements are acquired using VI probes to correlate plasma response with applied waveform dynamics.

The addition of oxygen significantly modifies the discharge through electronegativity-driven changes in electron density, sheath structure, and ion transport. Variations in waveform transition slope and duty cycle alter sheath expansion dynamics and electron heating during polarity transitions, producing measurable changes in the IEDF shape, energy spread, and high-energy ion population. Comparisons between pure argon and Ar/O_2 mixtures reveal how electronegative chemistry couples with tailored voltage waveforms to influence plasma stability and ion bombardment characteristics.

These measurements provide experimental insight into waveform-controlled plasma dynamics in electronegative CCP discharges and contribute to the development of advanced plasma control strategies for semiconductor processing applications.

9:30am **PS1-ThM-7 Passive Antenna Control of Ion Energy in Inductively Coupled Plasmas: Mechanism Study via Antenna Design Variation***, **Minsu Choi**,* Department of Physics, Chungnam National University, Republic of Korea*; Chulhee Cho,* Institute of Quantum Systems (IQS), Chungnam National University, Republic of Korea*; Inho Seong, Wonnyoung Jeong, Byeongyeop Choi, Seonghyun Seo, Isak Lee,* Department of Physics, Chungnam National University, Republic of Korea*; Youngseok Lee,* TEK R&D center, Tokyo Electron Korea*; Shinjae You,* Department of Physics, Chungnam National University, Republic of Korea

Ion energy is a critical parameter in plasma etching processes, governing etch rate, selectivity, and profile control. Conventional ion energy control requires an additional RF bias power source, which increases system complexity and cost. Passive antenna technology has recently been proposed as a bias-free alternative for ion energy modulation in inductively coupled plasmas (ICP), where ion energy is tuned through changes in the plasma potential. However, the mechanism by which a passive antenna modifies the plasma potential remains poorly understood.

In this work, we elucidate this mechanism through a systematic comparison of three antenna configurations: a closed-loop antenna, an open-ended antenna, and an open-ended antenna with an anodized surface. These designs were chosen to selectively suppress the two candidate pathways for plasma potential control —conduction current to the antenna and voltage generation at the antenna terminals. Plasma parameters, including electron density, electron temperature, and plasma potential, were measured using a Langmuir probe. Our results reveal two key contributions to passive antenna–driven ion energy control: (1) the collection of plasma electrons by the passive antenna, and (2) the voltage that develops at the open end of the antenna. Both effects act in concert to elevate the plasma potential and thereby increase ion energy at the substrate.

9:45am **PS1-ThM-8 Effects of Ar/O2 Gas Mixture Ratios on Ion Energy Distribution Functions in a Dual-Frequency CCP**, ***Tanjina Akter***, *Syed Zulqarnain, David Kanfer, Basak Bagci, Duncan Trosan,* North Carolina State University*; Chenyao Huang, Mark J. Kushner,* University of Michigan*; Amanda Lietz, Steven Shannon,* North Carolina State University

The investigation of ion energy distribution functions (IEDFs) formed by a powered sheath above a cathode can help optimize etching processes during the micro and nano fabrication. Capacitively coupled plasmas (CCP) have been routinely used to fabricate these structures. The coupling of ion flux and ion energy in a single-frequency CCP configuration limits its application for large-scale production. Hence, an independent control of ion flux and mean energy is required, which can be obtained by a multiple-frequency RF power configuration. Dual-frequency CCP can provide decoupled ion flux and ion energy, where the high-frequency component of the discharge produces charged particles and sustains the plasma, and the low-frequency component accelerates the ions to the surface [1]. A dual-frequency CCP configuration, with 60 MHz for the high-frequency (HF) and 13.56 MHz for low-frequency (LF), has been used in this experiment to observe the IEDF by placing a Retarding Field Energy Analyzer (RFEA) on the LF electrode. Bimodal IEDFs were found by the RFEA for the pressure range of 1-50 mTorr, electron densities of 10^9-10^{11} cm^{-3}, the sheath potential of 50-100 V, and the sheath thickness of 0.5-0.1 cm in the dual-frequency CCP using argon and argon-oxygen gas mixtures. The variations of IEDFs, electron density, and sheath thickness with different argon–oxygen gas mixture ratios were examined under constant HF and LF power conditions. The independent control of density and sheath voltage using a dual frequency configuration was also used to study the role of gas mixing under identical density and voltage conditions that primarily dictate the IEDF to better understand the impact of molecular and electronegative effects on the evolution of IEDF's in these CCP reactors. A Particle-In-Cell (PIC) simulation has been performed to validate the experimental results.

This work is supported by the Department of Energy (DOE) grant DE-SC0024545.

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Plasma Science and Technology
Room 315 - Session PS2-ThM

Advanced Ion and Reactant Control II

Moderators: Dr. Suman Bhaumik, TEL Technology Center, America, LLC, **Dr. Mingmei Wang**, Lam Research Corporation

11:00am **PS2-ThM-13 Energy-Resolved Angular Distribution of Ions Impinging on Biased Electrode in Dual-Frequency Capacitively-Coupled Ar Plasma**, ***Hirotaka Toyoda***, Nagoya University, Japan **INVITED**

The ion angle distribution (IAD) on the biased electrode is one of the factors that determine the shape in high-aspect-ratio etching, and experimental insights into how the IAD varies with plasma parameters are extremely important as fundamental data for etching shape simulations. Therefore, we have developed a specially designed dual-frequency capacitively coupled plasma (CCP) source to measure the angular distribution of high-energy ions incident on the RF electrode. In this apparatus, particles are extracted from the plasma into a drift tube through a sampling orifice connected to the RF electrode, and after passing through the drift tube, they are detected by a microchannel plate (MCP) assembly with a fluorescent screen, offering angular resolution of less than 0.01 degrees. From Ar plasma experiment, it was revealed that the IAD consists of a intense Gaussian peak (angular width: <0.5°) and a weak tail component (angular width: >1°). The width of the main peak decreased with increasing LF power, indicating that sheath acceleration contributes to the narrowing of the angular width. To investigate the collision effect within the sheath in more detail, the pressure was varied while keeping the sheath thickness constant by controlling the plasma density. As a result, the width of the main peak deviated from the expected tendency at high pressure and high sheath voltage, suggesting that sheath collisions increase the angular width. To further investigate the behavior of ions within the sheath, energy-resolved IAD measurements were performed using the Time-of-Flight method. It is known that ions passing through an RF-oscillating sheath have an energy distribution from high to low energy, and similar results were obtained in our energy-resolved IAD measurements. Furthermore, the main peak width decreased with energy, and assuming that the width of the main peak is determined by the ion temperature and sheath acceleration energy, the ion temperature was found to be ~0.04 eV regardless of the ion energy. This indicates that the main peak is generated by high-energy collisionless-ions and low energy ions those experienced charge-exchange collisions without momentum transfer. The behavior of the tail component of the IAD was also investigated by varying pressure. With increasing pressure, a relative increase in the tail component was observed. Monte Carlo particle simulations within the sheath suggested that the tail component originates from small-angle scattering of background Ar neutral particles and Ar ions.

Acknowledgement

The author thanks K. Kurihara, H. Fukumizu and their colleagues from KIOXIA corporation for their support and discussion.

11:30am **PS2-ThM-15 Tailored Voltage Waveforms in Inductively Coupled Plasmas for Cryogenic Etching using Ar/HF Gas Mixtures**, ***Yifan Gui***, *Yeon Geun Yook, Chenyao Huang, Mark J. Kushner,* University of Michigan, Ann Arbor

In microfabrication, fabricating high aspect ratio (HAR) dielectric features has relied on capacitively coupled plasma (CCP) reactors using fluorocarbon chemistries. In these systems, process parameters are tuned to optimize the production of C_xF_y fragments and ion energy distributions with the end goal of balancing polymer deposition and chemical sputtering to maintain profile control and etch rate. Inductively coupled plasmas (ICPs) have not been extensively used for dielectric etching due to the difficulty in controlling the fragmentation of the fluorocarbon gases. Cryogenic plasma etching of dielectrics typically uses HF based chemistries which rely on water-HF condensation and physisorption rather than the thickness and composition of the fluorocarbon polymer passivation layer. Consequently, the need to optimize C_xF_y dissociation is eliminated, which then makes ICPs more attractive for cryogenic etching systems. Decoupling plasma generation by the source power and ion acceleration by the bias power is also less difficult using ICPs.

In this presentation we discuss results from a computational investigation of the use of voltage waveform tailoring (VWT), specifically a rectangular bias (RB) waveform, in ICPs for cryogenic etching of dielectrics. RB waveforms generate a more mono-energetic ion energy distribution to the substrate compared to sinusoidal biases. This investigation was performed using, the Hybrid Plasma Equipment Model (HPEM), a modular simulator designed for low-pressure plasma systems. This study focuses on the evolution of incident fluxes and energy angular distributions (EADs) for electrons and ions onto wafers for ICPs operating at pressures of tens of mTorr with Ar/HF feed gas. We will discuss the impact of an expanded operational space (plasma source type, power/voltage scaling, and waveform) on the resulting EADs and flux uniformity across the wafer.

Work supported by Lam Research, Samsung Electronics and Department of Energy Office of Fusion Energy Sciences.

11:45am **PS2-ThM-16 Mechanisms of Si, SiCl, SiCl2, and Cl radical production and their role in isolated sidewall taper formation in pulsed Ar + Cl2 plasmas**, ***V S Santosh K Kondeti***, Princeton University Plasma Physics Lab*; Leonid Dorf, Zihao Ding, Geuntak Lee, Sonam D. Sherpa, Takumi Yanagawa, Leonid Belau,* Applied Materials Inc.*; Yevgeny Raitses,* Princeton University Plasma Physics Lab

In chlorine-based plasma etching of silicon, sidewall taper in isolated features originates from the deposition of chemical by-products, which is governed by the generation and transport of reactive radicals. In this work, we investigate the mechanisms of Si, SiCl, $SiCl_2$, and Cl radical production and decay in a pulsed inductively coupled Ar + Cl_2 plasma with a pulsed bias voltage using time-resolved laser induced fluorescence diagnostics. The measurements show that SiCl radicals are produced predominantly in the gas phase through electron-impact dissociation of higher silicon chlorides ($SiCl_x$, x = 2–4), with $SiCl_2$ acting as a key precursor species. In contrast, $SiCl_2$ is generated primarily at the wafer surface and chamber walls through ion-assisted processes and desorption. The measured Si radical dynamics indicate that Si atoms are produced in the gas phase and sputtering of the wafer. Cl radicals are produced by the dissociation of the precursor Cl_2 gas during the plasma on-phase. $SiCl_2$ and Cl radicals increase in density in the afterglow after turning of all power suggesting that $SiCl_2$ is formed by this reaction SiCl + Cl_2 → $SiCl_2$ + Cl in the afterglow, before all species decay in density. The observed radical dynamics demonstrate that sidewall taper is governed by the buildup and decay of depositing species with a large

sticking coefficient such as Si/SiCl, which can be controlled through modulation of plasma pulsing parameters. These results provide a mechanistic framework corelating plasma-phase chemistry to feature profile evolution and offer pathways to minimize by-product deposition for improved anisotropic etching.

This work is supported by Applied Materials and a Cooperative Research and Development Agreement (CRADA) between the Princeton Plasma Physics Laboratory and Applied Materials through the U.S. Department of Energy (contract DE-AC02-09CH11466).

12:00pm **PS2-ThM-17 Control of Electron Angular Distributions onto Substrates Using Non-Sinusoidal Low Frequency Biases in Capacitively Coupled Plasmas***, **Max Kellermann-Stunt**, James Prager,* University of Michigan*; Josh Perry, Paul Melnik, Timothy Ziemba,* Eagle Harbor Technologies*; Mark J. Kushner,* University of Michigan

Independent control of ion and electron energy distributions onto plasma facing surfaces is an important challenge for high-aspect-ratio (HAR) semiconductor etching. In capacitively coupled plasmas (CCPs), ions are accelerated through the sheath toward the wafer with relatively narrow angular distributions, while electrons generally reach the wafer during limited portions of the radio frequency (RF) cycle and often have broader angular distributions. The difference between the ion energy angular distribution (IEAD) and electron energy angular distribution (EEAD) can contribute to asymmetric charging in HAR features, leading to notching, microtrenching and twisting. Non-sinusoidal bias waveforms are being developed to narrow, in in both energy and angle, IEADs delivered to the wafer. These voltage waveforms ideally have a short positive portion and longer, constant negative. portion. A desired consequence of this waveform is an electric-field reversal in and near the sheath that will accelerate electrons towards the wafer with narrow angular distribution and high energies.

In this work we have computationally investigated EEADs and IEADs onto biased substrates in a CCP using non-sinusoidal waveforms. The investigation was conducted using the Hybrid Plasma Equipment Model (HPEM). Comparisons are made to experimental measurements of ion and electron energy distributions onto the substrate using an RFEA (retarding field energy analyzer).The experimental system consists of a CCP powered on the top electrode at 60 MHz with the bottom pedestal electrode biased by the non-sinusoidal waveform at 400 kHz. Measurements and simulations were performed for pure argon and argon-molecular gas mixtures with pressures ranging from 3 mTorr – 20 mTorr. The HPEM code was modified to enable simulation of electron energy distributions using very low frequency biases.

This work was supported by Eagle Harbor Technologies and the US Department of Energy Office of Fusion Energy Science under Award Number DE-SC0024861.

Surface Science
Room 305 - Session SS-ThM
Reduced Dimensional Systems

Moderators: Dr. Rachael Farber, University of Kansas, **Prof. Nan Jiang**, University of Illinois - Chicago

8:00am **SS-ThM-1 Large Moiré Potential in a Weakly Interacting Organic/2D Material Heterostructure***, **Oliver Monti**,* University of Arizona **INVITED**

Layered materials provide an exceptional platform for manipulating electronic states and spin properties, with examples ranging from the emergence of strongly correlated phases to exciton condensates and the appearance of multiferroicity. Key to these advances in creating a sandbox for materials “synthesis” is the concept of proximitization of two materials. Conventionally, this is achieved by few-layer heterostructures of 2D materials to create moiré potentials by lattice mismatch and twist angle. The depth of this potential is often restricted to some tens of meV. Achieving deeper moiré potential would enable the control of correlated phenomena to significantly higher temperatures, expanding the utility of moiré heterostructures and potentially revealing new phenomena. In this presentation, I will discuss how this can be achieved in a hybrid organic/van der Waals layered material heterostructure, with the case of C_{60}/T_d-WTe_2. We employ angle-resolved photoemission spectroscopy and scanning tunneling microscopy to reveal that the interface forms a quasi-periodic moiré potential owing to a lattice mismatch between C_{60} and T_d-WTe_2. The C_{60} rotational orientation on the surface establishes a quasi-periodic superlattice locked to the moiré pattern, which in turn modulates the molecular bandgap. This manifests as a moiré potential with an unusually deep modulation depth of 130(20) meV.

This discovery reveals a new path for creating highly tunable moiré heterostructures that lend themselves for creating flatband systems that may enable the study of correlated physics at elevated temperatures. The wide space of available organic molecules in combination with the growing library of 2D materials makes this a promising new avenue to pursue, with the potential to afford larger wavelength moiré structures with fewer defects than conventional 2D/2D heterostructures fabricated by exfoliation and transfer can provide.

8:30am **SS-ThM-3 Epitaxial Moiré-Graphene for Resonance Excitonic Energy Transfer in Moiré -Graphene-TMDC Heterostructures***, **Abdullah Al-Mahboob**, Asish Kundu, Dario Stacchiola, Jerzy T. Sadowski,* Brookhaven National Laboratory

Two-dimensional (2D) quantum materials, specifically, Moiré-Graphene (MGr) and Van der Waals heterostructures (HSs) of quantum materials have attracted great interest because of their exotic quantum properties and having promises in novel optoelectronic and photonic applications. HSs made of stacking atomically thin layers of transition-metal dichalcogenides (TMDCs) allow us to manipulate the optical and spintronic properties. In TMDC HSs of monolayers having the resonance between dark excitonic states, recently, we observed unconventional energy transfer (ET) process massively enhancing photoluminescence (PL) and valley polarization (VP) [1]. In-order to elucidate underlying mechanism, we synthesized scalable epitaxial MGr (EMGR) in ultra-high vacuum system and fabricated HSs of WSe_2-hBN-EMGr in Ar-atmosphere. We employed in-situ, low-energy electron microscopy and X-ray photoemission electron microscopy (LEEM/XPEEM) for in-situ growth study and electronic/structural characterization of both EMGR and HSs, high-resolution ARPES for obtaining band-structure of EMGR and series of optical, microscopy and spectroscopy techniques for the study of the resonant excitonic exchange in HSs. The electronic band structure of EMGR revealed that the energy of optical transition between Moiré Dirac-cone to Van Hove Singularity states across M-point in EMGr has matching with resonance excitation energies in WSe_2. The observed optical data could be understood via vvacuum-fluctuation-mediated phonon-bypass mechanism suppressing non-radiative recombination of exciton and valley depolarization in Van der Waals HSs.

Research was carried out at the Center for Functional Nanomaterials and the National Synchrotron Light Source II at Brookhaven National Laboratory under Contract No. DE-SC0012704.

[1] Arka Karmakar, Abdullah Al-Mahboob, Natalia Zawadzka, Mateusz Raczyński, Weiguang Yang, Mehdi Arfaoui, Gayatri, Julia Kucharek, Jerzy T. Sadowski, Hyeon Suk Shin, Adam Babiński, Wojciech Pacuski, Tomasz Kazimierczuk, Maciej R Molas, Twisted MoSe2 Homobilayer Behaving as a Heterobilayer, Nano Lett. 24, 31, 9459–9467 (2024).

8:45am **SS-ThM-4 Can the Binding Energy of H_2O Admolecules on the Ice Ih(0001) Surface Exceed the Bulk Cohesive Energy?***, **Jörg Meyer**,* Leiden University, Netherlands

The adsorption of water molecules on ice surfaces is of significant importance in many respects, in particular for gaining a deeper understanding of ice crystal growth. There is a wide distribution in the binding energy of the admolecule on the ice Ih surface due to the proton disorder, and previous theoretical calculations have indicated that it can even exceed the cohesive energy of the crystal at certain sites [1]. While the accuracy of those calculations has been contested [2] and direct measurement of these binding energy remains elusive, such strong binding sites have been tentatively brought up to rationalize experimental observations [3].Here, we study the adsorption of a water molecule on the ice Ih(0001) surface using recently developed polarizable many-body interaction potential functions [4,5], which provide high accuracy for a number of ice properties. We show that sites with binding energy larger than the cohesive energy are found on surfaces with a wide range of proton ordering. Although the binding energy is dominated by electrostatics, it is also significantly influenced by dispersion interactions. Furthermore, we show how the local environment at the binding site affects the binding energy, and propose a descriptor that serves as a predictor of the binding energy at a given site.[1] E. R. Batista and H. Jónsson, Comp. Mater. Sci. 20, 325 (2001).[2] C. Thierfelder, A. Hermann, P. Schwerdtfeger, and W. G. Schmidt, Phys. Rev. B 74, 045422 (2006).[3] M. Mehlhorn and K. Morgenstern, Phys. Rev. Lett. 99, 246101 (2007).[4] E. Ö. Jónsson, S. Rasti, M. Galynska, J. Meyer, and H. Jónsson, J. Chem. Theory Comput. 18, 7528

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9:00am **SS-ThM-5 Templated Growth and Intercalation Pathways of Nickel Nanoclusters on Graphene/Ir(111)**, ***Shilpa Choyal,*** University of Illinois at Chicago*; Nan Jiang, Michael Trenary,* University of Illinois Chicago

Two-dimensional graphene moiré superlattices on transition-metal substrates provide periodic templates for organizing metal adatoms into size- and shape-controlled nanostructures with tailored catalytic and magnetic properties. Despite extensive studies of other transition metals, the growth and thermal evolution of nickel on graphene/Ir(111) have remained largely unexplored. Here, we report a comprehensive scanning tunneling microscopy (STM) investigation of Ni nanocluster nucleation, growth, and intercalation on the Gr/Ir(111) moiré superlattice under ultra-high vacuum.

At room temperature, Ni deposition produces well-defined triangular nanoclusters with edges aligned along the ⟨110⟩ direction of Ir(111), reflecting the templating effect of the moiré. Site-resolved STM analysis reveals strong selectivity: 77% of clusters nucleate at fcc regions, 23% at atop sites, and none at hcp sites — a preference attributed to local rehybridization of graphene toward sp^3-like bonding upon Ni adsorption. By comparing stepwise and continuous deposition, we identify two distinct growth regimes: continuous deposition produces uniform triangular islands with narrow size distributions, whereas stepwise growth yields broader, irregular morphologies governed by uphill diffusion, Ostwald ripening, and Ehrlich–Schwoebel barriers.

Annealing to ~900 K drives complete intercalation of Ni beneath graphene. STM reveals two distinct inverted moiré contrasts "round" and "clover-like" corresponding to site-selective Ni occupation within the supercell. The intercalated Ni grows pseudomorphically, adopting the Ir(111) in-plane lattice and preserving the original (10×10)/(9×9) moiré periodicity. The random spatial distribution of intercalated islands beneath an intact graphene monolayer, combined with Ni's strong C-binding affinity, supports an exchange-intercalation mechanism in which transient Ni–C bonding enables atom-by-atom penetration followed by graphene self-healing. Stepwise annealing up to 1500 K shows partial Ni desorption while the moiré remains intact.

These findings elucidate registry-controlled growth and demonstrate a viable route for fabricating low-roughness graphene-based heterostructures, with implications for spintronics, heterogeneous catalysis, and graphene-based device engineering.

9:15am **SS-ThM-6 Probing local structural variations in metal–organic framework thin films using nano-FTIR**, ***Tomoko Shimizu,*** *Yukihiro Matsumoto, Kento Takenaka,* Keio University, Japan*; Hiromasa Sato,* Institute for Molecular Science, Japan*; Yuto Fujita,* Keio University, Japan*; Toshiki Sugimoto,* Institute for Molecular Science, Japan

Precise control over coordination structures and orientation is crucial for integrating metal–organic framework (MOF) thin films into functional devices.Structural defects, such as missing metal ions or unbound functional groups leading to incomplete coordination, can markedly impact the pore architecture and alter material properties. Therefore, techniques capable of probing local bonding states and defect distributions are essential for understanding and ultimately controlling structural irregularities in MOF films.

In this study, we employed infrared scattering-type scanning near-field optical microscopy (IR s-SNOM), which combines atomic force microscopy (AFM) with nano-Fourier transform IR spectroscopy (nano-FTIR), to definitively characterize local coordination bonding in a representative MOF thin film, NAFS-1, fabricated at the air/liquid interface and transferred to Si substrates[1].

Variations in structural features and nano-FTIR spectra revealed inhomogeneities in coordination bonding and orientation. In NAFS-1 prepared by the conventional method, which incorporated a water-rinsing step after each film transfer cycle, peaks attributed to uncoordinated carboxyl groups (COOH) were found to be distributed throughout the film,indicating incomplete coordination. In contrast, certain sparse features, such as particle-like aggregates and large, elevated features, exhibited enhanced coordination, as evidenced by the increased intensity of the carboxylate (COO^-) vibrational peaks. Notably, while omitting the post-transfer water-rinsing step increased structural inhomogeneities at the nanoscale, macroscopic spectroscopies, such as the transmission-mode FTIR and UV-Vis absorption spectroscopy, suggested more effective coordination and expanded conjugation.

Our findings emphasize the necessity of integrating nanoscale imaging with spatially resolved spectroscopy to identify the local crystallinity and orientation of MOF thin films. This approach provides a crucial framework for evaluating and optimizing the structural integrity of this class of materials, preventing misinterpretation of macroscopic data that would otherwise obscure irregularities due to averaging effects.

[1] Matsumoto *et al*., Langmuir, Accepted.

9:30am **SS-ThM-7 Spatially Resolved Understanding of Electronic-Metal Support Interactions on Pristine and Defected Cu/TiO_2(110)**, ***Lindsey Penland,*** The University of Kansas*; Hirushan Arachchige, Nadith Dissanayake,* The University of Kansas, Sri Lanka*; Rachael Farber,* The University of Kansas

Oxide-supported metal nanoparticle catalysts are commonly used in heterogeneously catalyzed chemical transformations due to their high selectivity, efficiency, and stability. There is a unique interplay between the metal nanoparticles and oxide support which results in strong metal support interactions (MSI). These MSI lead to observed changes in catalytic activity. Electronic metal-support interactions (EMSI), a subcategory of MSI characterized by electronic perturbations attributed to charge transfer across a metal/support interface, have a direct influence on the physicochemical properties of oxide supported metal nanoparticles. There are, however, several coexisting factors that can influence the degree of EMSI in a system such as the identity, size, and morphology of the nanoparticles and the Lewis acidity and oxygen defect density of the oxide support. Consequently, the coexisting nature of these factors makes it difficult to distinguish their respective effect on EMSI. As such, there is a need to develop a thorough understanding of the material properties leading to EMSI in a controlled and isolated way. In this work, insight into how the electronic landscape of a Cu/TiO2(110) model catalyst evolves as a function of EMSI was obtained through the use of low-temperature scanning tunneling microscopy (LT-STM) and spectroscopy (STS). It was found that the local density of states (LDOS) of clean rutile TiO2(110) has subtle variations in the valance region depending on the exact surface reconstruction of the TiO2(110) substrate. STM characterization post sub-monolayer Cu deposition highlighted variations in Cu morphology induced by thermal aggregation. LDOS measurements taken atop, near, and away from Cu particles show that electronic perturbations occur not only at the immediate metal/support interface but also extend into the near-interfacial region surrounding the Cu particles. Distinct variations in the LDOS perturbation radius and intensity suggest the degree of EMSI is correlated to nanoparticle size and morphology. These findings not only highlight how the presence and morphology of metal nanoparticles have direct influence on the electronic structure of the support but also opens the door to determining how electronic heterogeneity may play a role in heterogeneously catalyzed transformations. Ongoing and future work is focused on expanding these findings to structurally heterogeneous surfaces to understand how the inherent electronic heterogeneity of defected TiO2(110) influences the EMSI between Cu and TiO2(110).

9:45am **SS-ThM-8 Engineering Surface Confinement and Isolated Active Sites for Selective C–C Cleavage in Polyolefin Upcycling**, ***Wenyu Huang,*** Iowa State University

Transforming polyolefin waste into uniform, high-value chemicals is a significant challenge in catalytic surface science. Most heterogeneous catalysts lack the necessary spatial control over polymer chain conformations, leading to statistical C–C bond scission and the formation of undesirable gases. This work demonstrates a catalyst design strategy that suppresses non-selective reactivity by integrating isolated transition-metal sites into structurally well-defined porous architectures. By manipulating the interplay between surface-active sites and nanoscale confinement, we create a catalytic environment capable of guiding long hydrocarbon chains through a processive mechanism. This design facilitates controlled adsorption and activation while utilizing geometric constraints to favor the production of liquid-range hydrocarbons over terminal scission products. We characterize the relationship between pore topology and catalytic selectivity, providing fundamental insights into how engineered surface environments can unlock new reactivity patterns. These findings offer a scalable framework for developing highly selective catalysts tailored for sustainable polymer upcycling and circular chemical manufacturing.

11:00am **SS-ThM-13 Structure and Electronic Properties of Two-Dimensional Iron-Based Oxides on Silver**, ***Lindsay R. Merte***, Malmö University, Sweden **INVITED**

Reduced dimensionality can stabilize oxide structures, coordination environments, and electronic states that differ substantially from those of bulk materials. Two-dimensional iron oxides grown on silver surfaces exemplify this, forming structures distinct from both bulk iron oxides and from strongly bound wetting layers observed on more reactive substrates such as platinum. In particular, a 2D-Fe_3O_4 phase forms with mixed Fe^{2+}/Fe^{3+} valence and both tetrahedral and octahedral coordination, analogous to bulk magnetite but composed exclusively of close-packed layers. Incorporation of cobalt or nickel is expected to modify the electronic structure and catalytic behavior of these oxides, making them attractive model systems for energy-conversion materials. Here we present structural and electronic characterization of pure and mixed Fe–Co and Fe–Ni two-dimensional oxide phases prepared by co-evaporation on Ag surfaces using STM, synchrotron XPS and NEXAFS, surface X-ray diffraction, and anomalous diffraction techniques. Complementary DFT calculations are used to explore the atomic structure and electronic properties of the observed phases. We further demonstrate anomalous surface X-ray diffraction measurements under ambient-pressure conditions, enabling element-selective structural characterization of these complex multicomponent 2D oxide phases during exposure to reactive environments.

11:30am **SS-ThM-15 A Multiscale Framework for Oxygen Adsorption, Surface Reconstruction, and Reactivity on Ag(111)**, ***Bright Daniel***, University of Tennessee Knoxville; *Braden Penuel,* University of Tennessee, Knoxville; *Carson Mize,* Leiden University, Netherlands; *Lonnie Crosby, Sharani Roy,* University of Tennessee Knoxville

Understanding oxygen behavior on Ag(111) is central to improving silver-based catalysts for ethylene epoxidation, yet capturing this behavior across realistic length and time scales remains a fundamental challenge. While density functional theory (DFT) provides atomic-level insight, its limited system size restricts direct exploration of coverage effects, subsurface oxygen formation, and surface reconstruction under catalytic conditions.

In this work, a multiscale framework was developed to bridge this gap by integrating DFT, lattice-gas modeling, and Monte Carlo (MC) simulations. First, DFT calculations were used to systematically study oxygen adsorption on Ag(111), including adsorption energetics, coverage-dependent surface saturation, subsurface oxygen formation, and pairwise interaction energies. The computed trends were consistent with experimental observations and prior theoretical studies, providing a reliable foundation for model development.

These DFT-derived interactions were then used to construct a lattice-gas model, enabling efficient exploration of large surface models beyond DFT-accessible scales. Monte Carlo simulations in both canonical (NVT) and grand canonical (μVT) ensembles were employed to probe oxygen adsorption behavior as a function of temperature and chemical potential. This approach captures coverage-dependent ordering, subsurface incorporation, and thermodynamic stability of oxygen populations. Building on this framework, the model was extended to investigate surface reconstruction by incorporating Ag–Ag and Ag–O interactions. Co-adsorption of oxygen and silver adatoms reveals emergent restructuring phenomena driven by oxygen coverage and local coordination environments, providing insight into dynamic surface evolution under reaction-relevant conditions. Finally, configurations derived from these studies were used to examine ethylene epoxidation pathways with and without chlorine promotion, linking surface structure directly to catalytic performance.

Overall, this work establishes a unified, physics-based framework that connects atomistic energetics to mesoscale surface behavior, offering a pathway to rationally design and control catalytic surfaces under realistic conditions.

11:45am **SS-ThM-16 Atomic-Scale Study of Boron Nanostructure Growth on Platinum**, ***Nozomi Shirato***, Argonne National Laboratory

Low-dimensional boron nanostructures have attracted significant attention due to their intricate structural polymorphism, unique electronic states, and catalytic relevance. Despite growing interest, the growth mechanisms governing boron nanostructure formation on metal substrates remain poorly understood. Here, we investigate the growth of boron on an Pt(111) single crystal surface, aiming to understand the complex interplay between surface geometry, boron-boron interactions, and boron-platinum binding that collectively drives polymorph selection and structural evolution. Low-temperature scanning tunneling microscopy (LT-STM) is employed to characterize the intricate surface structures at atomic resolution, revealing the detailed morphology of the resulting nanostructures. X-ray photoelectron spectroscopy (XPS) measurements provide insight into the chemical states of boron and its bonding conditions with the substrate. Combined, the techniques reveal structural and chemical states of boron growth on Pt(111) and lay the groundwork for tailoring boron nanostructures for catalytic applications.

12:00pm **SS-ThM-17 Differentiable Multivariate Curve Resolution for X-Ray Absorption Spectroscopy**, ***Changhae Kim***, *Jennifer Bjorklund, Brian Lee,* Brookhaven National Laboratory; *Esteban Fornero,* Instituto de Desarrollo Tecnológico para la Industria Química, Argentina; *Dario Stacchiola, Xiaohui Qu, Sara Mason,* Brookhaven National Laboratory

Time-resolved *in situ* X-ray absorption spectroscopy (XAS) is a premier technique for probing atomic structure and reaction dynamics. Deconvolving spectral sequences into invariant components and relative concentrations can draw direct connections between spectroscopic data and chemical kinetics. However, chemically meaningful deconvolution remains challenging. Multivariate curve resolution (MCR) is widely used for this purpose, but conventional implementations offer limited flexibility for incorporating prior knowledge. Here, we present a differentiable optimization framework inspired by machine learning fields that enables simultaneous regression of spectra and concentration profiles, with flexible, chemically informed constraints. We demonstrate this approach on XAS measurements of redox reactions at the $CuGaO_2$ (011) surface. The method can isolate small surface signals from the dominant bulk contributions and can distinguish catalytically active species by leveraging coupled multi-species kinetics, capabilities which are challenging to achieve with conventional approaches. In addition, preprocessing with a blind-spot denoising network can improve robustness. These results highlight the potential of differentiable MCR for analyzing complex, multi-dimensional spectroscopic data.

The Future of Temperature Sensing
Room 320 - Session TS-ThM

The Future of Temperature Sensing IV

Moderators: Dr. Nikolai Klimov, National Institute of Standards and Technology, **Dr. Sesha Challa**, NIST-Gaithersburg

8:00am **TS-ThM-1 Magnomechanical Noise Thermometry**, ***John Davis***, University of Alberta, Canada **INVITED**

Virtually every quantum technology needs to be operated at some level of low temperatures to generate and protect low energy quantum states.As a result, cryogenics has become a critical enabling tool in the race to develop quantum technologies.Yet little attention has been paid to the thermometry that allows us to quantify these low temperatures.As an example, most users of a dilution refrigerator simply take for granted that the resistive temperature sensor they use to measure millikelvin temperatures is accurate (and actually represents their experimental temperature).A such, we believe that a renewed focus must be put on primary temperatures sensors in the sub-kelvin regime to ensure that quantum technologies and their enabling cryogenics can be accurately measured and compared between laboratories.To this end, we are working on a type of mechanical noise thermometry using the techniques of cavity optomechanics.I will provide the background and context of this temperature sensor and where we are in its development.

8:30am **TS-ThM-3 Compact Blackbody Radiation Atomic Sensor (CoBRAS)**, *Eric Norrgard,* National Institute of Standards & Technology; ***William Newman***, National Institute of Standards and Technology

The NIST Fundamental Thermodynamics group is leveraging the physical properties of atoms to provide accurate metrology of radiative temperature. Atoms are quantum systems whose interactions with electromagnetic radiation have been characterized with exquisite precision and, in many cases, are amenable to ab initio calculation. Compact Blackbody Radiation Atomic Sensor (CoBRAS) uses fluorescence detection of optically excited atoms in vapor cells to determine temperature. A CoBRAS temperature measurement is fast, with statistical uncertainty as low as 0.1% in one second. We provide an update on the temperature precision, range, and sensitivity of the CoBRAS. We also describe a new fiberized CoBRAS sensor with a form factor similar to traditional four-wire resistance thermometers.

8:45am **TS-ThM-4 Electro-Optic Frequency Comb Doppler-Broadening Thermometry**, ***Sean Bresler,*** University of Maryland, College Park/National Institute of Standards and Technology (NIST)*; Erin Adkins,* National Institute for Science and Technology (NIST)*; Stephen Eckel,* National Institute of Standards and Technology (NIST)*; David Long,* National Institute for Science and Technology (NIST)*; Benjamin Reschovsky, Daniel Barker,* National Institute of Standards and Technology (NIST)

We demonstrate Doppler-broadening thermometry based on direct optical frequency comb spectroscopy of an 85Rb vapor with a chirped electro-optic frequency comb (EOFC). The direct EOFC Doppler-broadening thermometry measurements are accurate to within their approximately K statistical uncertainty. We experimentally compare direct EOFC spectroscopy with conventional Doppler spectroscopy using a single-frequency, step-scanned laser probe. Our results show that direct EOFC spectroscopy mitigates transit-induced optical pumping distortion of the atomic lineshape, which is the dominant systematic temperature shift in alkali atom Doppler-broadening thermometry. Optical Bloch equation simulations of conventional and direct EOFC Doppler spectroscopy confirm that EOFC spectroscopy can use higher optical power to reduce statistical noise without optical pumping distortion. Our results indicate that EOFC Doppler-broadening thermometry is a promising approach to realizing a primary thermometer with size and measurement rate sufficient for applications including pharmaceutical manufacturing and nuclear waste monitoring.

9:00am **TS-ThM-5 Towards Practical Integrated Primary Thermometry with Optomechanical and Photonic Techniques**, ***Olga Kozlova,*** LNE-Cnam, France **INVITED**

Temperature is one of the most commonly measured physical quantities and influences nearly every physical, chemical, and biological process. Photonic and quantum-based approaches have the potential to transform practical thermometry by enabling *in-situ* traceability without requiring sensor removal for recalibration. A further advantage of these optical methods is their compatibility with silicon photonics, allowing on-chip integration thus to have the potential to radically improve thermal management of semi-conductor devices.

In this presentation, I will give an overview of the progress of European Partnership in Metrology Joint Research Project: Photonic and Quantum Sensors for Practical Integrated Primary Thermometry (PhoQuS-T) [1]. This project aims to develop integrated optical practical primary thermometry from 4 K to 500 K to enable *in-situ* traceability for practical applications.To achieve this, we combine several techniques: photonic thermometry using ring resonators; optomechanical noise thermometry and quantum correlation thermometry with opto-mechanical resonators. In addition, key challenges such as robust packaging over a wide temperature range are being addressed, along with metrological validation of the developed sensors and the exploration of future application possibilities.

At the current stage of the project, recent progress in photonic thermometry and optical noise thermometry from 4 K to 300 K, using 1D- and 2D- optomechanical sensors, will be presented. The next steps toward self-calibration using quantum thermometry (quantum correlation techniques [2]) will also be discussed. An overview of advances in high-resolution photonic sensors based on ring resonators operating over an extended temperature range (80 K to 500 K) will be given, along with updates on the development of a novel active thermometry approach [3]. Progress in packaging techniques (including gluing, welding, and mechanical support) for the developed sensors will also be presented.

Finally, developments toward practical application of such photonic sensors (including temperature monitoring of photonic integrated chips for optical clocks and assigning temperature in quantum-based pressure measurements) will be discussed.

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[2] https://www.science.org/doi/10.1126/science.aag1407

[3] https://doi.org/10.1098/rsta.2024.0459

9:30am **TS-ThM-7 Two-Dimensional Silicon Optomechanical Crystals for Quantum-Referenced Temperature Sensing**, ***Daniel Ramos,*** CSIC, Spain*; María José Martin Hernandez,* CEM, Spain*; Irene Castro,* CSIC, Spain*; Iago Sanchez,* CEM, Spain

Accurate temperature sensing at the nanoscale remains a central challenge for emerging quantum, photonic and nanomechanical technologies, where local heating, weak thermal anchoring and limited calibration accuracy can strongly affect device performance. Optomechanical systems offer a route to temperature sensing based on the thermal occupation of mechanical modes, enabling local, contactless and potentially self-calibrated thermometry through the optical readout of mechanical motion.

Here we present the design and first experimental realization of a two-dimensional silicon optomechanical crystal engineered as a platform for temperature sensing across the transition from the classical thermal regime toward the quantum regime. The device integrates a telecom C-band optical cavity and a co-localized GHz radial-breathing mechanical mode within a two-dimensional phononic shield. This architecture combines strong optical–mechanical confinement with improved thermal anchoring to the substrate compared with conventional one-dimensional optomechanical cavities, reducing absorption-induced heating while preserving high displacement sensitivity.

The geometry was optimized using three-dimensional simulations and machine-learning-assisted parametric sweeps to achieve operation in the resolved-sideband regime, high optical and mechanical quality factors, and strong optomechanical coupling. These characteristics enable sensitive monitoring of the mechanical noise spectrum as a function of temperature and provide the basis for sideband-resolved thermometry at low phonon occupation. In this regime, the Stokes and anti-Stokes sidebands provide a direct route to absolute quantum thermometry, since their asymmetry is determined by the mean phonon population rather than by an external thermal calibration.

We discuss how this two-dimensional optomechanical platform can be used for temperature sensing from elevated temperatures down to cryogenic conditions, with particular emphasis on quantifying local optical heating, calibrating phonon occupation, and approaching the quantum ground state. By combining heterodyne sideband readout, optomechanical cooling and sideband-asymmetry thermometry, the device provides a route toward quantum-referenced nanoscale temperature sensing. These results position two-dimensional silicon optomechanical crystals as a promising integrated platform for future temperature sensors operating beyond conventional calibration limits.

9:45am **TS-ThM-8 Developing Thermal Magnetic Imaging for Advanced Semiconductor Packaging**, ***Frank Abel,*** *Thinh Bui, Mahadi Rajib,* National Institute of Standards and Technology (NIST)*; Brian Donovan,* United States Naval Academy*; Solomon Woods,* National Institute for Science and Technology (NIST)

As the number of transistors on a single chip has approached its physical limit, the architectural complexity of semiconductor packaging in the form of heterogeneous 3D integrated components has been developed to meet the demand for high performance computing. However, with increased complexity comes significant thermal management issues, which are a crucial factor in designing new high-density semiconductor packages. These challenges require new measurement techniques to quantify temperature and heat flow during operational conditions through opaque materials with greater than 1 mm of depth penetration. For the past 5 years, our team at NIST has been developing magnetic imaging instrumentation and magnetic nanoparticle thermometers for 3D temperature imaging. Here, we present our progress in designing temperature- and signal-sensitive magnetic nanoparticle tracers integrated into proxy semiconductor materials, including silicon substrates, thermal interface materials (TIMs), and underfills. Along with the demonstration of solid-state imaging of embedded tracers in silicon imaging phantoms.

Vacuum Technology
Room 321 - Session VT-ThM

Vacuum Technology Big Vacuum Systems and Accelerators

Moderators: Prof. Dr. Sefer Avdiaj, University of Prishtina, **Eleni Marshall**, STFC Daresbury Laboratory

8:00am **VT-ThM-1 Ultra-High Vacuum Systems for Next Generation Gravitational Wave Detectors**, ***Jordan Vanosky,*** LIGO Laboratory, California Institute of Technology **INVITED**

LIGO, the Laser Interferometer Gravitational-wave Observatory consists of two, 4-kilometer long, L-shaped interferometers, which operate under Ultra High Vacuum conditions in order to detect gravitational waves from cosmic sources. The next generation of gravitational wave detector, Cosmic Explorer, targets a 10x increase in sensitivity and will consist of two 40 kilometer long beamtubes, a potential 90 million liter UHV system. Cosmic Explorer will enable a greater survey of the universe for gravitational wave sources, but this scale brings unique challenges for fabrication and qualification of the ultra-high vacuum system. Improving on the methods

and techniques that built LIGO is essential in order for an 80-kilometer long vacuum system to be feasible. New materials, fabrication methods, installation procedures, and bakeout techniques must be considered in order to reduce costs and installation time.

8:30am **VT-ThM-3 New Method for Bake-Out of Large Vacuum Systems**, ***Freek Molkenboer***, *Corné Rijnsent, Thom Oosterveer, Han Velthuis, Herman Bekman, Andrey Ushakov, Dirk van Baarle,* TNO Science and Industry, the Netherlands

Thermal bake-out is a well-known and commonly used method for removing contaminants from the inner surface of a vacuum system. However, the economic and practical scalability of this method for very large systems or systems with a high thermal mass poses quite some challenges.

The Einstein Telescope will be the largest vacuum system on Earth and will require the removal of water and other contaminates after installation underground. The currently foreseen method is thermal bake-out using Joule heating of the beam tube. The beam-pipes have a diameter of 1 meter, and due to the layout of the Einstein Telescope, a total of over 120 kilometers of beam-pipe is needed.

TNO will investigate the technical feasibility of using plasma techniques to remove water and other contaminates from the inner surface of the beam tube. For this study, a dedicated setup has been designed and built to assess whether plasma assisted cleaning can achieve the low partial pressure requirements as are needed for the Einstein Telescope.

During the presentation, we will discuss the realization of the experimental setup, as well as the outcome of the first half year of experiments.

8:45am **VT-ThM-4 in-Situ Bakeout of Beam Line Assemblies Under Project Constraints: A Measurement-Driven Approach Validated on the LCLS-II He Installation Campaign**, ***Pierre Ribault***, *Giulia Lanza, TC Chen, Dale Gill, Dentell Reed, Robert Coy,* SLAC National Accelerator Laboratory

The LCLS-II High Energy upgrade installation at SLAC uses a specific bake procedure for its beam line assemblies (BLAs): in-situ heating at 50 °C for eight hours, with an additional in-situ heating step on the BLA ceramic. The reason is practical. We want to desorb more water during the in-situ pumping phase, so that the total pump-down time of the full line stays within the project budget. This abstract describes how the bake parameters were chosen, the measurements that supported them, and the fleet-scale validation we are running on the HE installation.

Water dominates the outgassing budget at room temperature on stainless steel and ceramic surfaces, and it sets the in-situ pump-down time. Heating the BLA accelerates water release from the metal surfaces. The ceramic is harder to bake through bulk heating because of the thermal coupling in the integrated assembly, so we added a dedicated heating step for it. Both steps were sized so that the per-BLA outgassing fits within the budget for the full line.

We measured the outgassing of representative HE BLAs before installation rather than relying on extrapolated values. These measurements were used to refine the predictive model and to set the duration and temperature of the in-situ ceramic heating step. The 24-hour per-BLA pumping target was derived from the assembly time and the post-bake pumping requirement, set against the line-level pump-down budget defined by the project.

About twenty-three identical BLAs will be installed and baked over the course of one year. Each is monitored continuously by a SLAC particle-free turbo cart, which provides residual gas analysis with networked acquisition and a common time base across stations. The campaign gives us a chance to compare nominally identical units baked under the same procedure, and to look at the spread between them.

The presentation will cover four points. The engineering reasoning behind the bake parameters and the ceramic heating step. The outgassing measurement campaign and how it fed into the model. The first comparisons between predicted and observed bake trajectories on the BLAs installed by the time of the symposium, including the disagreements. And what the fleet data tells us about the spread between BLAs that should, on paper, behave the same way.

We submit this work as a documented case of a project-driven bake procedure: how it was designed, what data supported the design choices, and how the campaign is being monitored. The intent is to share the approach and the dataset with the community.

9:00am **VT-ThM-5 ESS Vacuum System Commissioning for Beam on Target**, ***Marcelo Juni Ferreira***, European Spallation Source ERIC, Sweden*; Artur Gevorgyan, Laurence Page, Adrien Besson, Hilko Spoelstra,* European Spallation Source, Sweden

The European Spallation Source (ESS) is a multidisciplinary research infrastructure and neutron source facility based on a 2 GeV, 5 MW proton linear accelerator (LINAC). The facility uses superconducting radio-frequency (SRF) cavities assembled under particle-free conditions to accelerate the proton beam, which produces neutrons through spallation on a helium-cooled tungsten wheel. The facility can host up to 42 neutron instruments.

The ESS Vacuum Group is responsible for all technical vacuum systems across the Accelerator, Target, and Neutron Scattering Instruments (NSS).

This presentation will provide an overview of the installed vacuum systems for the commissioning phase of the proton accelerator and monolith target systems for Beam-On-Target in Q1 2027. It will cover the vacuum hardware, the EPICS-based vacuum control interface, and the system's early performance, including the first beam to the tuning beam dump. The presentation will also describe the Target monolith vacuum system and comment on the installation of neutron instruments.

9:15am **VT-ThM-6 Engineering and Validating Vacuum Systems for the Spallation Neutron Source Second Target Station**, ***Austin Chaires***, Oak Ridge National Laboratory

The Second Target Station (STS) project at the Spallation Neutron Source (SNS) requires specialized vacuum systems to support particle transfer, inert experiment environments and safety requirements. This work outlines the engineering responsibilities and validation methodologies used to design vacuum environments across the STS target and instrument systems. Various vacuum systems must fulfill diverse functional needs, including clearing proton and neutron flight paths, isolating the inert environments of instruments, managing hazardous hydrogen gas concentrations under National Fire Protection Association (NFPA) safety standards, and providing thermal insulation for liquid hydrogen target cooling. Additionally, vacuum is used to safely remove water from highly active, radioactive components destined for disposal. To mitigate radiation exposure and ensure system robustness, the engineering approach leverages twenty-five years of SNS operational lessons learned to integrate As Low As Reasonably Achievable (ALARA) principles, modular common pump stations, and redundant pumping pathways. Design validation is achieved through a multi-faceted analytical approach combining empirical formulas, vendor consultation, and software modeling via ANSYS APDL and VacTran. For novel configurations, multiple parallel analytical methods are cross validated to guarantee compliance. This comprehensive design and validation framework ensures system readiness as the STS target and instrument vacuum systems approach final design reviews this year in anticipation for the Department of Energy (DOE) project milestone critical decision (CD) 2/3 approval to proceed to procurement.

9:30am **VT-ThM-7 Gas Dynamic Modeling of an Upgraded Titanium Arc-Gettering Neutral Beam Pumping System**, ***Alan Van Drie***, TAE Technologies

Fusion Neutral Beam Injection (NBI) systems impose demanding vacuum pumping requirements due to the need to maintain gas pressures in the 2–3 mTorr range within the beam neutralizer section while simultaneously reducing downstream pressures to the 10^{-5} Torr range to minimize beam re-ionization losses and cold gas bleed into the main fusion vessel.

This work presents modeling and prototype testing of an upgraded multi-scale finned titanium arc-gettering pumping system developed in support of higher-voltage and longer-duration upgrades to the NORMU neutral beams. The objective of the pumping upgrade is to increase effective pumping speed and gas capacity within the restricted geometric envelope of the neutral beam vessel. Gas modeling across both transitional and molecular flow regimes was used to evaluate pressure and density distributions, gas transport, and pumping effectiveness within complex neutral beam geometries. The distributed finned geometry was developed to improve hydrogen isotope pumping performance while addressing engineering integration and conductance constraints associated with upgraded neutral beam architectures.

AI/ML/Autonomous Experimentation for Thin Films Processing

Room 317 - Session AIML1-ThA

AI/ML in Materials Characterization

Moderators: Mr. Lucas Kuehnel, University of Missouri, **Dr. Andreas Werbrouck**, Ghent University, Belgium

2:15pm **AIML1-ThA-1 Combining Optimization and Agentic Control in Automated Scanning Probe Microscopy**, ***Boris Slautin***, *Sheryl Sanchez, Jordan Marshall, Mahshid Ahmadi, Sergei Kalinin,* The University of Tennessee **INVITED**

Closed-loop optimization is increasingly used in automated microscopy for tasks ranging from experimental parameter tuning to mapping unknown structure–property relationships. The core idea is to guide the experiment by selecting the next most informative measurement location or parameter set while accounting for uncertainty, noise, and limited experimental budget. However, when the objective, decision space, and constraints must be defined in advance, the automation remains largely local to a specific task. This becomes limiting for hierarchical or evolving experiments that require coordinated measurement selection, quality control, parameter adjustment, mode switching, and refinement of the experimental question.

The emergence of agentic AI provides a complementary route for automated microscopy. Many experiments are not a single optimization loop, but a set of coupled steps involving data acquisition, image analysis, quality control, parameter adjustment, and physical interpretation. Closed-loop methods are powerful for well-defined local optimization or exploration tasks, but the connection between these steps often still requires expert judgment. Agentic systems can help provide this connecting layer by supporting experiment-level orchestration, propagating information between local loops, incorporating physical context, and dynamically planning the next experimental step. In this sense, agentic control should not replace classical optimization, but rather coordinate optimization modules, data-analysis routines, physical constraints, and microscope-control actions within a broader automated experiment.

In this work, we develop an agentic system for automated scanning probe microscopy (SPM), demonstrated on ferroelectrics using piezoresponse force microscopy as the example. The agent provides global orchestration of the experiment by connecting microscope control with image and spectroscopy analysis, incorporating physical context, and making higher-level decisions about the experimental trajectory. Classical optimization are integrated as local modules for tasks that can be formulated quantitatively, such as tuning measurement parameters or selecting informative measurement locations.

We deploy this approach in a real experimental setting, where the agent coordinates microscope actions, analysis routines, and local optimization loops during PFM measurements. Although demonstrated for ferroelectric PFM, the same architecture can be extended to broader automated experimental problems, including thin-film processing, synthesis–characterization loops, and structure–property mapping.

2:45pm **AIML1-ThA-3 Multi-Agent System for Optical Microscopy of 2D Materials Characterization**, ***Haozhe "Harry" Wang***, Duke University

Optical microscopy remains an indispensable tool for the rapid characterization of two-dimensional materials, yet conventional workflows depend heavily on trained operators to navigate samples, identify regions of interest, and interpret complex image features — creating a persistent bottleneck in experimental throughput. Here, we present a multi-agent system built on foundation models that fully automates the optical microscopy pipeline for 2D material characterization, from stage navigation to image acquisition to quantitative analysis.

Our architecture decomposes the microscopy workflow into specialized, cooperating agents: a navigation agent that performs intelligent search over the substrate, a perception agent that segments and classifies material features in real time, and an analysis agent that extracts quantitative descriptors such as layer number, domain morphology, and spatial coverage. These agents communicate through a structured orchestration layer, enabling adaptive decision-making — for example, dynamically adjusting scan density in response to local material heterogeneity or prioritizing high-value regions for higher-magnification imaging. Built on the ATOMIC (Autonomous Technology for Optical Microscopy and Intelligent Classification) framework, the system leverages large vision models to achieve zero-shot generalization across material systems and substrate types without task-specific fine-tuning.

We demonstrate the system on chemical vapor deposition-grown 2D semiconductors, where it achieves classification accuracy exceeding 99% while autonomously generating statistically representative maps of growth outcomes across centimeter-scale substrates. By eliminating manual intervention and enabling continuous, unsupervised operation, the multi-agent architecture transforms optical microscopy from a serial, operator-dependent technique into a scalable, intelligent characterization platform — laying the groundwork for closed-loop integration with upstream synthesis and downstream property measurements in autonomous materials laboratories.

3:00pm **AIML1-ThA-4 A Reference Architecture for Complex Scientific Chatbots Based on ChASE, an AI Assistant for SIMS**, ***Jordan Barrette***, *Jerry Hunter, Prateek Maheshwari,* Beamline Incorporated

Secondary Ion Mass Spectrometry analysis planning requires synthesizing multiple knowledge sources: textbook physics governing sputter rate, ion yields, depth resolution, and matrix effects; institutional memory encoded in years of past setups; and analyst judgment about instrument state and sample characteristics. We present ChASE (Chat-bot Augmented for SIMS Expertise), a chatbot-style AI assistant for SIMS laboratories that integrates theoretical, historical, literature, and tribal knowledge into a unified decision-support tool. Rather than treating the underlying language model as an oracle trained to know everything a priori, we instruct it as a research expert—one that synthesizes information from many sources, much as a lab scientist draws on tribal knowledge, reference literature, recent work, and customer expectations.

The presentation outlines the architecture of ChASE, composed of three primary components: technical “skills,” tribal knowledge, and a reference literature corpus. Using this architecture, we demonstrate automated setup guidance that consults and reconciles historical setups, theoretical predictions, laboratory best practices, and published experimental methods. Building on the suggested setup guidance, we demonstrate automated scheduling across the current job queue. The setup-related predictions produced—sputter rate, required depth, estimated tuning overhead—roll up into time estimates that are compared against similar historical runs to produce expected and worst-case total analysis times, giving lab managers a preliminary schedule with built-in margin.

Central to this research-expert approach is the skill framework, which mirrors the way an experienced analyst decomposes a complex problem into prerequisite questions before synthesizing an answer. Skills are applied recursively: complex tasks decompose into collections of prerequisite subtasks that themselves constitute skills. For instance, a “SIMS Setup Predictor” skill leverages “Primary Ion Predictor,” “Mass Resolution Predictor,” and “Depth Resolution Predictor” as constituent skills. Each is a sophisticated model on its own, built on the same reference architecture—hence the recursive nature—supporting prediction models for ion yield, mass interference, and cascade mixing, respectively. We compare the architecture’s response accuracy for complex scientific tasks with a standalone language model and more common adaptation approaches such as pre-training, fine-tuning, prompt engineering, and retrieval-augmented generation. Finally, we discuss strengths and limitations of the approach, within the context of the ultimate goal—an AI framework that can be expanded beyond SIMS.

3:15pm **AIML1-ThA-5 Leveraging Automated Characterization and Machine Learning to Optimize Defects for Quantum Sensing**, ***Dane deQuilettes***, Princeton University

Spins in solid-state materials, molecules, and other chemical systems have the potential to impact the fields of quantum sensing, communication, simulation, and computing. In particular, color centers in diamond, such as negatively charged nitrogen vacancy (NV−) and silicon vacancy centers (SiV−), are emerging as quantum platforms poised for transition to commercial devices. A key enabler stems from the semiconductor-like platform that can be tailored at the time of growth. The large growth parameter space makes it challenging to use intuition to optimize growth conditions for quantum performance. In this work, we use supervised machine learning to train regression models using different synthesis parameters in over 100 quantum diamond samples. We train models to optimize NV−defects in diamond for high sensitivity magnetometry. Importantly, we utilize a magnetic-field sensitivity figure of merit (FOM) for NV magnetometry and use Bayesian optimization to identify critical growth parameters that lead to a 300% improvement over an average sample and a 55% improvement over the previous champion sample. Furthermore, using Shapley importance rankings, we gain new physical insights into the most impactful growth and post-processing parameters, namely electron

irradiation dose, diamond seed depth relative to the plasma, seed miscut angle, and reactor nitrogen concentration. As various quantum devices can have significantly different material requirements, advanced growth techniques such as plasma-enhanced chemical vapor deposition (PE-CVD) can provide the ability to tailor material development specifically for quantum applications.

AI/ML/Autonomous Experimentation for Thin Films Processing
Room 317 - Session AIML2-ThA

AI/ML-enhanced RHEED in Thin Film Growth

Moderators: Mr. Dorien Carpenter, University of Alabama at Birmingham, **Prof. Martin Seifrid**, North Carolina State University

3:30pm **AIML2-ThA-6 Turning RHEED into a Tool for Stoichiometry Analysis and Real-time Control of Epitaxial Film Growth Using Machine Learning**, ***Ryan Comes,*** University of Delaware **INVITED**

Progress in materials synthesis increasingly depends on combining real-time characterization with data-driven analysis and feedback. Reflection High–Energy Electron Diffraction (RHEED) offers a unique capability for monitoring thin film growth during deposition, yet its broader utility is constrained by limited dynamic range, signal saturation, and challenges in extracting quantitative information from diffraction images. To address this, we have developed a robust and extensible methodology to improve RHEED image quality, enable quantitative analysis, and support feedback-aware synthesis workflows. Weshowed that deep convolutional neural networks trained on RHEED patterns could accurately predict the cation stoichiometry of $SrTiO_3$ thin films during growth, with explainable AI tools revealing previously unrecognized correlations between diffraction streak intensity ratios and reciprocal-space spacing.[1] These results establish RHEED as a viable surrogate measurement for film stoichiometry.

To identify and track structural evolution during growth, we have also applied unsupervised machine learning approaches, including principal component analysis and k–means clustering, to time-resolved RHEED image sequences. Image drift correction and precise alignment of the specular reflection enable reliable frame-to-frame comparisons for $LaFeO_3$ and $SrIrO_3$ films synthesized by molecular beam epitaxy. These preprocessing and analysis steps establish a foundation for automated recognition of growth modes and cross-material comparisons.[2]

Our ongoing work focuses on the development of software for real time analysis of videos to provide ML-driven feedback to the human operator of the MBE system using reinforcement learning. This framework incorporates a pathway toward real-time synthesis feedback by integrating enhanced RHEED video streams with growth metadata such as fluxes, shutter states, chamber pressure, and substrate information. By combining unsupervised learning, deep neural networks, and real-time diagnostics, this work lays the groundwork for closed-loop thin-film synthesis capable of quantitative interpretation, adaptive control, and accelerated materials discovery.

[1] S.B. Harris, et al. *Nano Letters*, **25**, 5867–5874. (2025)

[2] P.T. Gemperline, et al. *JVSTA,* **43**, 032701 (2025)

4:00pm **AIML2-ThA-8 AI-Driven Recognition of RHEED Pattern Features for MBE Monitoring**, ***Vadim Gorshanov,*** DCA Instruments Oy, University of Turku, Finland*; Markku Rajala,* DCA Instruments Oy, Finland*; Milica Todorović,* University of Turku, Finland

Reflection High-Energy Electron Diffraction (RHEED) is a standard in situ characterization technique used to monitor surface crystal structure during thin film deposition methods such as Molecular Beam Epitaxy (MBE). RHEED patterns contain rich information about the surface ordering, but their interpretation is often manual or restricted to simple intensity tracking, which fails to fully capture the evolution of the surface. This work presents an approach to automating RHEED pattern analysis using semantic segmentation (pixel-wise labeling) to detect and classify diffraction features, including spots, streaks, and Kikuchi lines.

To enable such analysis, we compiled and annotated a ground-truth dataset of diverse RHEED patterns. This dataset was utilized to conduct a comparative study of modern deep learning architectures, benchmarking Convolutional Neural Networks (CNNs) and Transformer-based architectures paired with various encoder backbones. The goal of this comparison is to identify and optimize the architecture that maximizes accuracy to ensure reliable pattern monitoring. Results demonstrate that the optimized models robustly isolate diffraction features from complex backgrounds. Furthermore, the method exhibits strong generalization capabilities, successfully recognizing RHEED patterns of different material systems and imaging conditions not present in the training data. In addition, the image processing achieves frame rates suitable for real-time monitoring. The procedure enables the extraction of quantitative diffraction features from raw RHEED images and videos, paving the way for automated control in industrial RHEED workflows, as well as facilitating post-growth analysis.

4:15pm **AIML2-ThA-9 Toward LLM Driven Agentic Automation of RHEED Diagnostics in Thin Film Deposition**, ***Asraful Haque,*** *Rama Vasudevan, Christopher Rouleau, Sumner Harris,* ORNL

Real-time interpretation of reflection high-energy electron diffraction (RHEED) patterns during thin film growth remains a bottleneck for fully autonomous deposition systems. While individual machine learning tools have demonstrated promise for isolated RHEED analysis tasks, integrating them into a coherent, decision-capable framework has been challenging. Here we present an agentic automation architecture that orchestrates multiple AI/ML modules for RHEED diagnostics using large language model (LLM)-based agents as the reasoning backbone. The system integrates: (i) a YOLO (You Only Look Once) based object detection and classification pipeline for real time identification of RHEED pattern features including spot geometry, streak morphology; (ii) a structural similarity (SSIM) based algorithm for automated sample alignment and beam registration in RHEED; and (iii) an FPGA-DAC (Field Programmable Gate Array and Digital to Analog Converter) controlled electron beam deflection subsystem enabling automated rocking curve acquisition. The LLM agent layer interprets outputs from each module, coordinates decision logic across the diagnostic pipeline, and interfaces with the deposition control system to enable closed-loop feedback.

We demonstrate proof of concept autonomous operation where the agent sequences alignment, real-time pattern classification, and real-time rocking curve measurements without human intervention. This modular, agent-orchestrated approach represents a scalable path toward self-driving thin film growth platforms where natural language reasoning and computer vision together manage the complexity of in-situ diagnostics. This research was conducted at the Center for Nanophase Materials Sciences (CNMS), which is a DOE Office of Science User Facility at Oak Ridge National Laboratory.

Advanced Microelectronic Materials and Devices Mini-Symposium
Room 318 - Session AM+EM+TF-ThA

ALD Fundamentals to Devices & Flash Session

Moderators: Prof. Andrew Meng, University of Missouri, **Prof. Dr. Greg Parsons**, North Carolina State University

2:15pm **AM+EM+TF-ThA-1 When Growth Has Not Yet Begun: Nucleation and Interface Control in Atomic Layer Deposition**, ***Zsófia Baji,*** Centre for Energy Research, Hungary*; Zsófia Bérces,* Centre for energy research, Hungary*; Zoltán Szabó,* Centre for Energy Research, Hungary **INVITED**

Atomic layer deposition (ALD) is generally described as a self-limiting thin-film growth technique producing conformal and compositionally controlled layers with atomic-scale precision. However, in the earliest stages of growth, precursor adsorption, surface chemistry, and substrate-dependent reaction pathways limit growth. These phenomena become increasingly important in the deposition of ultrathin functional films for emerging electronic technologies, where the target thickness often lies entirely within the nucleation regime. Understanding the atomistic and chemical mechanisms governing the transition from isolated nuclei to continuous films is therefore essential for the development of next-generation memory, logic, and two-dimensional device architectures.

The classical nucleation behaviour of oxide ALD systems is largely influenced by the chemistry and crystallinity of the substrates: the initial ALD cycles are controlled not only by precursor saturation but also by the density and distribution of chemically active surface sites and lattice matching. The role of precursor size, ligand configuration, and available hydroxyl density in determining growth-per-cycle behaviour and nucleation efficiency can be examined using phenomenological nucleation models. The comparison between experimental film morphologies and theoretical growth descriptions give insight to the initial stages of film growth. Mathematical nucleation modelling used to analyse the transient growth

behaviour can be used to derive the unknown boundary conditions governing the initial deposition stages.

The difference between precursor chemistries can be demonstrated by oxide and sulfide nucleation pathways. Sulfide growth is fundamentally hindered by the mismatch between conventional hydroxyl-terminated oxide substrates and sulfur-based film chemistry, therefore sulfide ALD repeatedly re-enters a renucleation regime during the early cycles, resulting in delayed film closure and poor ultrathin continuity.

To overcome these limitations, different nucleation-enhancement treatments can be employed to increase the density of reactive surface sites and enhance nucleation. The hydroxylation of the surface enhances the nucleation of oxide films, while controlling other growth chemistries requires a chemically engineered approach for the targeted functionalisation surfaces. Thus, nucleation must be considered as an interface-controlled process governed by the compatibility between precursor chemistry and surface termination.

2:45pm **AM+EM+TF-ThA-3 MoO_2Cl_2 as an alternative Mo ALD Precursor for MoS_2 with Improved Thin Film Properties**, ***Nihal Khatiwoda,*** University of Michigan*; Ian Campbell,* IMEC USA*; Pierre Morin,* IMEC Belgium*; Benjamin Groven,* IMEC, Belgium*; Ageeth Bol,* University of Michigan

ALD of MoS_2 is a promising route for scalable and conformal synthesis of 2D semiconductors for nanoelectronics applications. However, it is often limited by small grain sizes and out-of-plane features, which degrade device electrical properties. In this work, we investigate MoO_2Cl_2 as a novel molybdenum precursor for ALD of MoS_2. Compared to conventional Mo precursors, MoO_2Cl_2 exhibits enhanced vapor pressure, leading to more efficient precursor delivery. Additionally, its chlorine-based chemistry introduces the possibility of in-situ etching which can help suppress undesirable nucleation, out of plane growth, and thus facilitate lateral expansion of domain features.

Both thermal and plasma-enhanced ALD processes were developed using MoO_2Cl_2 and H_2S as co-reactant. For the thermal process, a stop-flow approach was implemented to increase co-reactant residence time and enhance the reaction kinetics.

In-situ spectroscopic ellipsometry reveals that MoO_2Cl_2 exhibits a substrate enhanced transient growth regime during the initial ALD cycles, characterized by rapid nucleation. This is followed by a slower homo-deposition growth where the system enters a steady state growth regime. This behavior suggests the possibility of tailoring the precursor-substrate chemistry to reduce nucleation density and enhance lateral growth.

Ex-situ characterizations further support the effectiveness of this precursor system. XPS confirms the absence of chlorine incorporation in the resulting films, indicating clean ligand removal and absence of unwanted chlorine doping into the films. AFM reveals improved surface morphology with increased grain size and, notably, absence of out-of-plane features.

Overall, this study demonstrates that MoO_2Cl_2 is a promising precursor for ALD of high-quality MoS_2. Its favorable volatility, combined with chlorine-mediated surface chemistry, enables improved control over film morphology and crystallinity. These findings highlight a viable pathway toward overcoming longstanding challenges in ALD MoS_2 growth, advancing its potential for integration into next generation nano-electronic devices.

3:00pm **AM+EM+TF-ThA-4 Impact of Ti Adhesion Layer and ALD Al_2O_3 Thickness on Interfacial Energy Barriers in metal/insulator/metal (MIM) Devices**, ***Jessica Haglund,*** *John Conley,* Oregon State University

Control and understanding of interfacial energy barriers at metal insulator contacts is essential for designing MOS and MIM based devices. These barriers depend not only on the details of the metals and dielectrics used, but also on processing conditions, deposition order, and structure of the interface. To use noble metal electrodes, a thin interfacial metal is essential for good adhesion. Thin interfacial metals have also been investigated as a way to tailor barrier heights. Ultrathin dielectrics are needed for MOS gates and high capacitance MIM capacitors. However, the dielectric constant, density, and optical refractive index of ALD Al_2O_3 have all been reported to be a function of film thickness. In this work, we investigate the impact of Ti adhesion layer and ALD Al_2O_3 film thickness on interfacial electron energy barriers in Pt/Ti/Al_2O_3/TiN MIM devices.

100 nm TiN bottom electrodes were reactive ion sputtered. ALD with TMA and H_2O was used to deposit Al_2O_3 using 50, 75, 100, 125, 150, 175, and 200 ALD cycles in a Picosun R150 and 100 and 200 cycles in a Picosun R200. Following ALD a thin Ti IL (0.5, 1, 2, 5, 10 nm) and a 10 nm Pt top electrode were deposited via electron beam evaporation using a shadow mask. CV and IV measurements were taken on the completed MIM structures. Energy barriers were measured suing internal photoemission (IPE) spectroscopy using a house-built system.[1] Top gate voltage was swept from 0 to 2 V and 0 to -2 V using 0.1 V steps. At each bias, incident photon energy was swept from 1.7 to 5.5 eV. IPE thresholds were determined at each voltage using yield plots and zero field barriers were determined using Schottky plots.

Both the top Pt/Al_2O_3 and bottom TiN/Al_2O_3 electron barriers were a function of Al_2O_3 thickness. While both electron barriers were roughly constant at ~3.6 eV for Al_2O_3 films ≥ 12 nm thick, both decreased by roughly 0.5 eV as Al_2O_3 thickness decreased down to 5 nm. For Ti, a 0.5 to 1.0 nm thick interfacial layer was sufficient to completely dominate the electron energy barrier of the Pt/Ti stack. Insertion of a Ti layer also resulted in band tailing, likely due to oxygen scavenging, but had no impact on the bottom Al_2O_3/TiN electrode barrier. The degradation of electron barriers with insulator thickness and dominance by a very thin layer of metal at the interface are important considerations for the prediction and optimization of leakage currents and performance in these devices. Additional measurements on Ga_2O_3 will be discussed.

[1] J. Haglund, T. Mimura, J.F. Ihlefeld, and J.F. Conley, Jr., ACS Appl. Electron. Mater. **6**(5), 3249–3256 (2024)

3:15pm **AM+EM+TF-ThA-5 Evaluation of Barium-Based Precursors for Atomic Layer Deposition of Barium Titanate Thin Films**, ***Aenakshi Sircar,*** Boise State University*; Peter Micah,* boise State University*; Steven Hues, Elton Graugnard,* Boise State University

Atomic Layer Deposition of Barium titanate (BTO) has been a topic of interest for its potential application in high-k dielectric and ferroelectric material for energy-efficient logic and low-voltage memory devices. It is a perovskite ferroelectric with a low coercive field and switchable polarization at room temperature. Several deposition methods have been explored for integrating conformal BTO thin films into high-aspect-ratio structures for advanced memory applications. Among these, atomic layer deposition (ALD) stands out due to its ability to achieve highly conformal low-temperature growth through self-limiting surface reactions using reactive precursors. Despite these advantages, the development of a comprehensive ALD process for barium titanate remains challenging, particularly due to the limitations associated with barium precursor chemistry. The low volatility and poor thermal transport of many barium-based precursors limit the ALD process window. Additionally, most barium-based precursors are extremely hygroscopic in nature and often form $Ba(OH)_2$, which can readily react with carbon-containing compounds to form $BaCO_3$. This introduces unfavorable conditions for the formation of BTO, since $BaCO_3$ and TiO_2 require higher energy to form BTO compared to $Ba(OH)_2$ and TiO_2. This behavior further complicates film characterization and can also negatively impact the electrical properties of the films.

Here, we report progress toward precursor selection for carbon-free barium titanate deposition. We investigate three different barium-based precursors: isopropyl [$Ba(iPr_3Cp)_2$], tertbutyl [$Ba(tBu_3Cp)_2$], and a novel imidazolate-based precursor, [Ba-Zttt]. The deposition cycles are optimized over several parameters, including the ALD temperature window (250–350 °C), growth per cycle, and film structure. The films are further characterized for thickness, density, roughness, phase composition, and dielectric properties to assess the feasibility of the different precursors for ALD of BTO and their potential contribution toward quaternary barium-based oxides.

3:30pm **AM+EM+TF-ThA-6 Deposition of Metastable ZrO_2 Crystalline Films at Low Temperatures by Electron-Enhanced Atomic Layer Deposition (EE-ALD)**, *Zachary Sobell,* ***Steven George,*** University of Colorado at Boulder

The metastable cubic and tetragonal ZrO_2 crystalline phases are important as high-k dielectric materials.Electron-enhanced atomic layer deposition (EE-ALD) was used to grow metastable ZrO_2 crystalline films with thicknesses of ~30 nm at low temperatures < 100 °C.This EE-ALD process employed alternating exposures of tetrakis(ethylmethylamido)zirconium (TEMAZr) and low energy (~70-100 eV) electrons concurrent with an oxygen (O_2) reactive background gas (RBG).ZrO_2 EE-ALD displayed rapid nucleation on silicon native oxide and linear growth in the steady state region.

The ZrO_2 EE-ALD was performed using an electron beam from a hollow cathode plasma electron source (HC-PES) with sample currents of ~30 mA over 10 cm^2.The electron beam can desorb surface species by electron stimulated desorption.The electron beam also travels through the O_2 RBG in the reactor at pressures of ~1-3 mTorr.Electron induced dissociation can form ions and radicals that facilitate the growth and oxidation of the ZrO_2

film.In addition, a negative bias voltage (-30 V) can be applied to the sample.This negative bias is believed to pull positive ions to the surface to enhance the film crystallinity and refractive index (RI).

With no applied sample bias and 5 s electron exposures, ZrO_2 EE-ALD proceeded at 1.2 Å/cycle and displayed an RI of 1.63 at 589 nm. Moderate crystallinity was observed by grazing incidence X-ray diffraction (GI-XRD) as shown in **Figure 1**. Increasing the electron exposure time increased the crystallinity and RI. A 10 s electron exposure increased the RI to 1.75. The crystallinity also increased significantly as displayed in **Figure 2**.The ZrO_2 EE-ALD growth rate was measured at 0.8 Å/cycle.

For the shorter electron exposure of 5 s, the application of a -30 V sample bias also increased the RI and crystallinity slightly versus no bias.The RI was measured at 1.70 and the EE-ALD growth rate was 0.8 Å/cycle. Increasing the electron exposure to 15 s with the simultaneous application of a -30 V bias increased the RI further and produced the most pronounced crystallinity as shown in **Figure 3**.A growth rate of 0.9 Å/cycle was measured along with an RI of 1.9.

The crystallinity and RI of the metastable ZrO_2 crystalline films with thicknesses of ~30 nm grown by EE-ALD depends on electron beam exposure time and negative sample bias voltage.The primary incident electrons may increase film crystallinity and RI by enhancing surface atomic mobility.The negative sample bias voltage may increase crystallinity and RI by facilitating oxidation by attracting O_2^+ positive ions to the sample.

3:45pm **AM+EM+TF-ThA-7 Zirconium Phosphate ALD Electrolyte for TiO2-Channeled H+ ECRAM***, **John Hoerauf**, David Stewart,* University of Maryland, College Park*; A. Alec Talin,* Sandia National Laboratories, USA*; Gary Rubloff,* University of Maryland, College Park

Artificial Intelligence (AI) computing energy demands are on pace to surpass global energy production. Analog in-memory computing (IMC) hardware development represents a paradigm shift to reduce the energy required for these calculations by up to six orders of magnitude. Electrochemical RAM (ECRAM) is a promising non-volatile three-terminal transistor technology to realize physical neuromorphic IMC circuits. To program information, ECRAM utilizes reversible electrochemical reactions between the gate and drain terminals to change the conductance of the channel material between the source and drain terminals, representing the state of information during read-out. ECRAM transistors that utilize H^+ as the electrochemically active species are compatible with CMOS devices, offer faster programming speed, and have increased cycle durability compared to Li^+ ECRAM. Due to the mobility of protons, H^+ ECRAM also provides an excellent platform for studying the underlying phenomena that govern informational state retention across all ECRAM chemistries, but further studies require a solid-state electrolyte with properties not yet reported in thin-film electrochemistry.

Zirconium Phosphate (ZrP_xO_y) is a promising electrolyte with the requisite properties, including a composition-dependent H^+ conductivity. This presentation discusses a novel atomic layer deposition (ALD) development for ZrP_xO_y and the successful application of this thin-film electrolyte in H^+ ECRAM. ALD ZrP_xO_y was deposited using both super-cycling and phosphate plasma polymerization to alter the phosphorous to zirconium ratio between 1.5:1 and 4.2:1. This change in composition resulted in a one decade change in proton conductivity (3e-10 to 4e-9 S/cm) while exhibiting electronic conductivities below the measurement resolution limit (<1e-11 S/cm), ideal for studying state retention in ECRAM. The higher conductivity $ZrP_{2.6}O_{6.6}$ electrolyte was applied to an ECRAM singe-transistor platform that utilizes TiO_2 between the source and drain for readout. Two decades of programming range were demonstrated with a projected 4-hour state retention time. This represents the first successful demonstration of a full solid-state H^+ ECRAM transistor with an anhydrous ALD electrolyte. Additionally, a novel electrochemically-induced phase transition at the composition $H_{0.01}TiO_2$ was observed in Titania, as confirmed both through cyclic voltammetry and a metal-to-insulator behavior between the source and drain terminals. This phase transition is similar to that observed in the Li-TiO_2 system and is the key to understanding how H^+ conductivity in the electrolyte affects informational state retention in future studies.

4:00pm **AM+EM+TF-ThA-8 Unique Optical and Electrical Properties of Ald Deposited Zno on Top of Poly(3-Hexylthiophene)***, **Anil Yadav**, Aditya Sadhanala,* Indian Institute of Science, India

Vapor Phase Infiltration (VPI) is a technique used to infuse the inorganic material inside porous films. It is inspired by the well-established Atomic Layer Deposition (ALD) process, which is typically performed on flat substrates such as silicon and glass. Here, we demonstrate the deposition of ZnO onto poly(3-hexylthiophene) (P3HT) thin films using a custom-built infiltration chamber. We are exploiting the infiltration process to explore the optical and electrical properties of the well-studied semiconducting polymers, such as P3HT. The sub-surface deposition of metal oxide, along with surface deposition, alters the optical and electrical properties of polymers. The hybrid material exhibited distinct and unique electrical and optical signatures, with applications in solar cells and organic light-emitting diodes (OLEDs). The UV suppression at the UV absorption peak indicates a distortion in the crystallinity of the semicrystalline P3HT thin film. Other characterizations showed that ZnO is predominantly deposited in the amorphous region, which improves the material's electrical properties.

Atomic Scale Processing Mini-Symposium
Room 316 - Session AP+EL+MS+PS+TF-ThA

Advancing Atomic Scale Processing Through Novel Sources and Pulsing Methods

Moderators: Dr. Keren Kanarik, Lam Research Corporation, **Prof. Dr. Han-Bo-Ram Lee**, Incheon National University

2:15pm **AP+EL+MS+PS+TF-ThA-1 High-Throughput Silicon ALE via Rapid Matchless Power Modulation***, **Banks Peete**,* North Carolina State University*; Jeremy Mettler,* University of Houston*; Paul Melnik,* EHT Semi*; Shreeyansh Rastogi, Zuhair Khan,* University of Houston*; Chris Bowman, James Prager, Timothy Ziemba,* EHT Semi*; Steven Shannon,* North Carolina State University*; Vincent Donnelly,* University of Houston

By leveraging rapid, multi-level power modulation, we have expanded the self-limiting window of continuous gas flow atomic layer etching (ALE) of silicon to higher chlorine flow rates enabling much quicker ALE cycle periods. ALE offers superb controllability, but it is limited in speed by the time it takes to purge and switch gases from the chamber. Previously, a continuous flow of argon and chlorine gases were injected into continuously-powered, inductively-coupled plasma (ICP) while the bias power to the substrate stage was pulsed on for 0.2 s and off for 1 s. When the chlorine flow was kept in a narrow window, the silicon chloride surface layer was removed by argon ions faster than the surface can re-chlorinate. At higher chlorine flow rates, this process collapsed into traditional reactive ion etching.

In this work, we expand this “ALE window” by modulating the ICP power in sync with the bias-on period. This was accomplished using a matchless power generator (EHT Semi “Orion”), capable of rapidly changing power levels by an order of magnitude in microseconds. The matchless capabilities ensure that power is still delivered efficiently during the large change in plasma impedance. Time-resolved hairpin probe measurements confirm electron density transition times between power states in the hundreds of microseconds time-scale, far faster than would be possible with a traditional matching network based power delivery system. By operating the ICP at 300W during the bias-off period and at higher powers (600 W to 1.5 kW) during the bias-on period, the ALE window can be expanded to higher chlorine flow rates. During the bias off phase, the higher chlorine flow rates re-chlorinate the surface faster, decreasing the total ALE cycle time. Time-resolved optical emission spectroscopy of the SiCl (280.75 nm) line was used as a real-time monitor of the relative etching rates. At higher chlorine flows, the line exhibited a “spike and decay” profile indicative of ALE, unlike the previous work with constant 300 W power, which showed a square wave-like response to the bias turning on that is associated with simple pulsed reactive ion etching. This confirms that syncing the bias with a higher level ICP power enables higher chlorine flow rates while still outrunning re-chlorination.

2:30pm **AP+EL+MS+PS+TF-ThA-2 Etching Commercially-Relevant Materials Using Tailored Waveform Biasing***, **Benjamin Harris**, Daryl White, Kate Stokes, Matthew Loveday, James Ellis, Geoffrey Hassall,* Oxford Instruments Plasma Technology, UK

Control of the ion energy distribution function (IEDF) in a plasma is essential for optimising etch processes, such as atomic layer etching (ALE) and reactive ion etching (RIE). If the ion energy is too low, ions will fail to etch the surface of a material. If the ion energy is too high, ions may induce subsurface damage by sputtering material below the surface layer. Between these two boundaries lies the optimal range for ion energies, where ion utilisation is maximised and subsurface damage is minimised. Historically, a radio-frequency, sinusoidal bias is applied to the wafer table to control the IEDF near the wafer surface. This produces bimodal IEDFs with characteristic widths on the order of tens of eV, which is often wider than the optimal window for etching industrially-relevant materials [1]. Tailored

waveform biasing (TWB) provides an alternative to radio-frequency biasing that offers enhanced control over the width and mean energy of the IEDF.

In this study, TWB is used to sputter etch commercially-relevant materials. A retarding field energy analyser is used to measure IEDFs, and on-wafer outcomes are investigated with a suite of metrology tools, including atomic force microscopy and scanning electron microscopy. The results are compared with radio-frequency biasing, showing the benefits of TWB for enhanced process control.

[1] Faraz, T., Verstappen, Y.G., Verheijen, M.A., Chittock, N.J., Lopez, J.E., Heijdra, E., van Gennip, W.J., Kessels, W.M. and Mackus, A.J., 2020. Precise ion energy control with tailored waveform biasing for atomic scale processing. *Journal of Applied Physics*, *128*(21).

2:45pm **AP+EL+MS+PS+TF-ThA-3 Precise Ion Energy Control Using Advanced Pulse Modulation for Thin Film Deposition and ALD***, Yejin Shin,* WONIK IPS CO., LTD., Republic of Korea*; Junghoon Kim, Tae Cho,* WONIK IPS CO., LTD.*; Hyun-Joug Woo, YongBaek Jeon, GyuTai Kim, TaeJoon Kim,* WONIK IPS CO., LTD., Republic of Korea

As semiconductor device dimensions continue to shrink, advanced thin film deposition processes increasingly require precise control of ion energy and ion flux to achieve void-free filling in narrow-pitch and high aspect ratio structures. In particular, lateral gap-fill processes for next-generation semiconductor architectures demand highly controlled plasma-surface interactions to improve bottom coverage, suppress seam and void formation, and maintain film uniformity within confined geometries. Conventional RF plasma technology often provides limited flexibility for controlling ion bombardment conditions, motivating the development of advanced waveform engineering approaches.

In this work, an advanced pulse modulation was adapted to precisely control ion energy characteristics during RF plasma deposition processes through tailored voltage waveform. To enable this capability, the bottom components of a system were extensively modified, including the integration of a redesigned junction module and an optimized RF grounding architecture. The modified structure was specifically designed to improve transient voltage response, reduce parasitic effects, and support consistent pulse modulation under plasma load. Particularly, the hybrid junction module was designed to have minimized reflected power fluctuation and enabled more stable waveform delivery to the substrate electrode, which is critical for precise ion energy control during deposition processes. These hardware enhancements enabled more accurate control of sheath voltage evolution and allowed dynamic tuning of ion bombardment energy at the substrate surface. Using the developed platform, various pulse modulation conditions were investigated to evaluate their influence on plasma stability, ion energy distribution, and deposition characteristics. Experimental observations which were made using the advanced PEALD tool manufactured by Wonik IPS expects that advanced pulse shaping can significantly influence ion acceleration dynamics and plasma-surface interactions without substantially perturbing bulk plasma stability. In particular, the ability to manipulate transient sheath behavior enabled improved control of ion-assisted deposition compared with conventional continuous-wave RFs as a 13.56 or 27.1MHz.

This work establishes a hardware and process framework for future investigation of advanced deposition applications, focused on evaluating the effectiveness of this approach for next-generation conformal film deposition. The presented approach provides a promising pathway toward plasma processing for advanced semiconductor manufacturing applications requiring precise control of plasma-surface interactions.

3:00pm **AP+EL+MS+PS+TF-ThA-4 Characterizing Inductively Coupled Plasmas in Ar/N2/H2 Mixtures for Plasma Enhanced Atomic Layer Deposition of Crystalline Films***, David Boris, Jeffrey Woodward, Virginia Wheeler, Michael Johnson, Mackenzie Meyer, Scott Walton,* U.S. Naval Research Laboratory

Low temperature plasmas containing mixtures of Argon, Nitrogen, and Hydrogen are widely used in the plasma enhanced atomic layer deposition of crystalline metal nitrides (e.g. AlN) at low temperatures (<500C).Generally, the addition of H_2 is beneficial in that it facilitates the removal of precursor ligands and leads to films with low carbon content (<1%). In addition, if the process conditions are properly chosen, highly crystalline metal-nitride films can be grown in $Ar/N_2/H_2$ mixtures.However, the effects of H_2 addition on the downstream plasma properties near the substrate are not well understood in remote, inductively coupled plasma (ICP) geometries.As such, a better understanding of the downstream plasma properties in this gas chemistry will be the focus of this presentation.

In this work, we use a combination of Langmuir probes, a retarding field energy analyzer, and optical emission spectroscopy (OES) to examine the effects of varying process parameters on the physical characteristics of $Ar/N_2/H_2$ plasmas generated in a remote, ICP geometry.In particular, a range of applied RF powers, gas flows, and pressures are explored with a focus on the resulting changes in atomic species density, plasma density, plasma potential, and the energy and flux of ions at the substrate.Of particular interest is the effect H_2 has on the ion flux and ion energy distribution at the substrate. These changes in plasma properties are then tied to changes in the characteristics of AlN thin films grown via plasma-enhanced ALD using a remote ICP employing $Ar/N_2/H_2$ gas mixtures. This work was supported by the NRL Base program through the Office of Naval Research.

3:15pm **AP+EL+MS+PS+TF-ThA-5 Direct Atomic Printing of High-K Dielectric Thin Film Oxide Materials** *, Tesfalem Welearegay, Nandan Singh Ruhela, Simone Santucci, Mira Baraket, Maksym Plakhotnyuk,* ATLANT 3D Nanosystems, Denmark

The rapid scaling up of CMOS microfabrication combined with growing demand for wide- and ultrawide-bandgap power electronics (GaN, SiC, β-Ga_2O_3), and the integration of high memory and neuromorphic devices have placed high-k dielectric thin films at the centre of modern semiconductor technology. High-k dielectric oxide thin films such as HfO_2, ZrO_2, Al_2O_3, Ta_2O_5, Nb_2O_5, and Ga_2O_3 are predominantly as-deposited by conventional atomic layer deposition (ALD) and spatial ALD techniques. Although ALD offers sub-nanometre control and excellent conformality, its low throughput, vacuum-based batch operation, high precursor consumption, and lack of in-line patterning have become major bottlenecks for the development and scale-up of next-generation high-k materials. These limitations become significant when device roadmap require sub-nm equivalent oxide thickness, and ultralow defect density to fine tune the film's intrinsic properties required for rapid materials screening with high throughput and precision..

We, therefore, present Direct Atomic Layer Processing (DALP®) technique — a spatial, atmospheric-pressure ALD technology platform that enables direct atomic printing of oxide thin films with monolayer-level precision and higher throughput while significantly reducing precursor waste. By spatially separating the precursor and oxidant zones under inert-gas exposures, DALP® technology combines the self-limiting surface chemistry of ALD with the speed and selective-area capability of a direct-write process. The platform offers unique versatility in fine-tuning the film composition, property and and structure, thereby enabling to control over the targeted properties of the film. The capability is demonstrated on two selected high-k oxide materials. GaOx deposited from its spatial precursor Galai™ (air liquide) with H_2O at relatively low temperatures of 150–240 °C under open atmosphere conditions. The as-deposited oxide films follows an ALD-like deposition window at 180–210 °C with growth per pass (GPP) of 0.35–0.5 Å/pass. Moreover, NbOx (Nb_2O_5) thin films were grown from its spatial precursor Nautilus 2™ (Air liquide) with H_2O at relatively low-temperature ALD window of 180 - 240 °C with GPP of 0.41 - 0.43 Å/pass, producing high-purity amorphous films suitable for different applications including DRAM capacitors, Mott memristors, and high-index optical coatings. These results establish DALP® technology as a versatile, sustainable, and high-throughput platform for the rapid development and manufacturing of high-k dielectric thin films for power electronics, memory, and quantum-device applications.

3:30pm **AP+EL+MS+PS+TF-ThA-6 Plasma-Enhanced ALD of TaC_xN_{1-x} Tailored for Superconducting Quantum Technologies Through Ion Energy and Other Plasma Control Knobs***, Silke Peeters, Arthur De Jong, Adrie Mackus, Erwin Kessels,* Eindhoven University of Technology, Netherlands*; Harm Knoops,* Oxford Instruments Plasma Technology, Netherlands

Tantalum nitride compounds are emerging materials for superconducting quantum circuits due to their reduced surface oxidation compared to Ta, which is used in state-of-the-art devices. However, the synthesis of electrically conductive tantalum nitride compounds is challenging. Moreover, these circuits require sharp material interfaces with minimal impurities to achieve state-of-the-art performance.

Ar-H_2 plasma has enabled the preparation of superconducting TaC_xN_{1-x} through atomic layer deposition using the metalorganic $Ta[N(CH_3)_2]_3[NC(CH_3)_3]$ precursor. In previous work[1,2], we have shown that the quality of TaC_xN_{1-x} and $Nb_xTi_{1-x}N$ films can be substantially improved through ion-energy control, achieved via application of a radiofrequency (RF, 13.56 MHz) substrate bias during low-pressure, remote plasma exposure. In this work, we explore the novel method of tailored-waveform

(TW, 200 kHz) biasing[3,4] and variation of the Ar-H_2 plasma composition to tune film properties for application in superconducting quantum devices.

Compared to RF biasing, TW biasing offers more precise control over the ion energy. Consistent with earlier RF-bias results, application of TW biasing up to an ion energy of 140 eV enhances grain growth and grain boundary quality through increased adatom mobility and preferential removal of weakly-bonded surface species. As a result, room-temperature electrical resistivity is improved from (9.6 ± 0.5)*10^4 μΩ cm for an 11 nm film to (3.8 ± 0.2)*10^2 μΩ cm for a 7 nm film. A decrease of the H_2-dilution in the Ar-H_2 gas mixture supplied to the plasma further enhances TaC_xN_{1-x} electrical conductivity and crystallinity, and promotes (111) texturing. A decrease in blistering, which can occur at high-stress, H-containing interfaces, is observed at the Si(100) substrate interface. The balance between Ar and H species significantly affects crystal grain growth. Ar species more effectively stimulate near-surface atomic rearrangement through physical bombardment, while H species act as reducing agents. However, H species can also reduce adatom mobility through over-passivation of dangling bonds and accumulate in the film.

This work shows that accurate understanding and control of plasma properties is necessary to tailor TaC_xN_{1-x} films to superconducting quantum technologies. Using the developed toolbox, we demonstrate successful integration of TaC_xN_{1-x} thin films in superconducting quantum technologies.

[1]S. A. Peeters et al. *Appl. Phys. Lett.* 123, 132603 (2023)

[2]S. A. Peeters et al. *AVS Quantum Sci.* 7, 026801 (2025)

[3]T. Faraz, A. A. De Jong et al. *J. Vac. Sci. Technol. A* 44, 033004 (2026)

[4]A. A. De Jong, S. A. Peeters et al. *to be published*

3:45pm **AP+EL+MS+PS+TF-ThA-7 Direct Atomic Layer Processing (DALP®): Spatially Localized, Multi-Material Fabrication for Next-Generation Devices from Discovery to Manufacturing**, ***Mira Baraket***, ATLANT 3D Nanosystems, Denmark

Progress in next-generation advanced electronic and functional devices, based on complex heterostructures and advanced materials integration, is increasingly constrained by the rigidity of conventional thin-film processing and patterning workflows. While these approaches deliver high material quality and uniformity, they offer limited flexibility for spatially localized, multi-material fabrication, three-dimensional thickness engineering, and rapid experimentation at the nanoscale within a single process flow.

ATLANT 3D introduces Direct Atomic Layer Processing (DALP®), a nanofabrication technology enabling digitally controlled, spatially localized deposition of multiple materials with atomic-scale precision. DALP allows different materials to be deposited sequentially and locally in a unified workflow, enabling manufacturing of complex material stacks, heterostructures, interfaces, and thickness gradients without intermediate lithographic patterning steps.

This presentation describes the DALP process architecture and its role in both combinatorial materials discovery and targeted device manufacturing for next-generation devices. By enabling programmable material placement, controlled thickness variation, and repeatable execution within a single platform, DALP supports accelerated materials exploration while also enabling the direct production of device-ready structures as part of broader manufacturing flows. Representative examples include multi-material nanoscale structures for advanced semiconductor and functional material applications, where precise interface control, spatial selectivity, repeatability, and manufacturability are critical. DALP expands the accessible design space of nanoscale fabrication and provides a a direct pathway from materials discovery to device-ready, manufacturable structures.

4:00pm **AP+EL+MS+PS+TF-ThA-8 From Plasma to Process: Understanding Dielectric Barrier Discharges for Spatial Atomic Layer Deposition**, ***Ralph Houben***, *Antoine Salden, Jente Wubs, Richard Engeln, Erwin Kessels, Julian Held, Bart Macco,* Eindhoven University of Technology, The Netherlands

Atomic layer deposition (ALD) is a thin-film deposition technique based on sequential, self-limiting reactions. Plasma-enhanced ALD (PE-ALD) extends this concept by leveraging non-equilibrium plasmas to enable low-temperature processing, wider choice in materials, and enhanced film properties. Advancing PE-ALD requires a detailed understanding of plasma chemistry and the role of reactive species from the plasma in driving surface reactions.

Spatial ALD (SALD), in which precursor and reactant zones are separated in space rather than time, enables high-throughput and large-area processing, making it attractive for low-cost and high volume applications such as photovoltaics and batteries. SALD often operates at atmospheric pressure in linear slit geometries, making dielectric barrier discharges (DBDs) a natural plasma source. However, the high-pressure environment introduces strong collisionality that fundamentally alters plasma chemistry compared to low-pressure PE-ALD. For example, for O_2 plasmas, rapid three-body reactions favor ozone (O_3) formation over atomic oxygen (O). The gas temperature plays a crucial role here, as it directly affects the rate coefficients of the ozone-forming reactions. Furthermore, power dissipation occurs through filamentary microdischarges rather than a uniform glow — both aspects that have no direct analogue in conventional low-pressure PE-ALD.

The oxidative species composition governs surface chemistry in oxide ALD. Quantifying O_3 and O with absolute densities — and linking them to plasma parameters through models — is essential for process control, yet such data for atmospheric DBDs in an ALD context are scarce.

In this work, ozone densities have been determined using broadband UV absorption spectroscopy, yielding absolute concentrations on the order of 10^{15} cm^{-3} under typical operating conditions. The density depends on dissipated power, gas temperature, and O_2 input in the gas mixture. We further present cavity ring-down spectroscopy (CRDS) as technique for probing the forbidden transition of atomic oxygen near 630 nm, providing calibration-free, absolute quantification of atomic oxygen densities. These measurements are supported by plasma chemistry modeling, which shows that the O_2/N_2 ratio governs whether ozone or atomic oxygen dominates — a critical distinction for ALD surface reactivity.

Furthermore, the species generation predicted by the model is directly tied to how power is dissipated in the discharge. Power dissipation analysis reveals the filamentary nature of the discharge and how it governs species generation. These insights are essential for rationally designing plasma-assisted SALD processes.

Advances in Battery Engineering, Interface Design, and Characterization Mini-Symposium
Room 319 - Session BT-ThA

Advanced Characterization of Battery Interfaces

Moderators: Dr. Samantha Rosenberg, Kairos Power, **Prof. Dr. Xiao-Ying Yu**, Oak Ridge National Laboratory, USA

2:15pm **BT-ThA-1 Designing Materials for High Performance Energy Storage Applications at Solid-Solid and Solid-Liquid Interfaces**, ***Ajay Karakoti***, Pacific Northwest National Laboratory **INVITED**

The performance of energy storage materials is fundamentally governed by interfacial phenomena, where ion transport, nucleation, and chemical degradation dictate cycle life and energy density. Probing these buried, dynamic interfaces requires combining advanced characterization, computational modeling, and augmented by data-driven workflows. This talk highlights two complementary efforts that leverage multiscale characterization, in-situ probes, and emerging computational frameworks to elucidate and engineer interfaces in next-generation solid-state and grid-scale lead-acid batteries.

The first part of the talk demonstrates a discovery framework for designing solid–solid interfaces in lithium-ion solid-state batteries by coupling state-of-the-art machine learning potentials with physics-based simulations on cloud high-performance computing. Screening across millions of candidate compositions yielded a tractable, shortlisted set of promising solid electrolyte candidates that were subsequently synthesized and experimentally validated. Postmortem characterization of cycled cells using SEM-EDS, XPS, and PXRD reveals how cathode–electrolyte interfacial stability and structural evolution govern long-term performance, informing design rules for composite electrolytes.

The second part of the talk identifies opportunities for utilizing data-driven frameworks to bridge our understanding of failure mechanisms in lead-acid batteries. The complex chemistry of this system necessitates probing reactions using a multi-modal toolkit spanning in-situ atomic force and optical microscopy, solid-state NMR, XPS, and synchrotron methods that link macroscopic failure modes, such as, irreversible sulfation and electrolyte stratification to atomic-scale interfacial structure. The rich, multimodal datasets emerging from these studies present a unique opportunity to bridge length scales and provide inputs for future machine learning and autonomous workflows aimed at formulating an overarching mechanistic understanding of battery failure and accelerating the discovery of new materials.

2:45pm **BT-ThA-3 Advances in Neutron and X-Ray Imaging and Tomography Methods for in Situ Characterization of Lithium-Ion Batteries at NIST***, **David Jacobson**, Jacob LaManna, Elias Baltic, Daniel Hussey,* National Institute of Standards and Technology (NIST) **INVITED**

Neutron imaging has played an important role in characterizing electrochemical systems in the last 20 years. Neutrons penetrate metallic components of battery systems yet remain sensitive to changes in lithium concentration and/or hydrogenous electrolyte concentration, thanks to the large attenuation cross-section for ^{6}Li and H. When combined in operando with X-rays, it is possible to obtain a multi-modal picture of the electrochemical system, allowing for phase separation that is not possible with individual probes alone.

At NIST, the neutron imaging program operates two instruments, both with simultaneous neutron/X-ray tomography capabilities: the BT2 NIST Neutron Imaging Facility (NNIF), and the NG6 Cold Neutron Imaging Instrument (CNII).

In this presentation, we will discuss the current status of these facilities, planned future upgrades, the impacts on battery characterization, and examples of the techniques as applied to imaging lithium batteries. During the NIST Center for Neutron Research (NCNR) shutdown, we performed experiments at other facilities that will be discussed here. In addition, we have pursued upgrades to the NIST imaging facilities to improve spatial resolution, field-of-view, data acquisition, and data analysis speeds.

Because neutron sources are lower in intrinsic brightness than synchrotron X-ray sources, they require longer data collection times for 3D data sets. To improve neutron data acquisition speeds NIST has deployed machine-learning methods to reduce image noise allowing for shorter image acquisition times. NIST is also incorporating a high-speed server and network to provide near real-time data analysis to facility users. Furthermore, we will discuss new cold neutron imaging methods for multi-scale characterization and the status of the NIST neutron microscope project.

3:15pm **BT-ThA-5 Solid Electrolyte Interphase Formation between a Li-Metal Anode and an Ionic Liquid Electrolyte Using an Ab Initio Molecular Dynamics Approach***, **Hafsa Ashraf**, Luis A. Selis,* Texas A&M University*; Jorge M. Seminario,* texas A&M University

Understanding and controlling lithium-metal interfacial phenomena is critical for developing safe, high-performance next-generation batteries. In this study, ab initio molecular dynamics simulations are used to investigate solid–electrolyte interphase (SEI) evolution and electrochemical interfacial stability for an ionic-liquid electrolyte in contact with a lithium-metal surface. The electrolyte consists of 1-ethyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide with 1 M LiTFSI. To improve interfacial performance, tetrafluoroborate is partially introduced as a counterion, and ethylene carbonate is included as a functional additive. The simulations show limited interfacial reactivity, suggesting strong chemical stability of the electrolyte formulation. Decomposition pathways indicate that lithium fluoride is the dominant SEI product, highlighting the potential of this IL-based electrolyte system to stabilize lithium-metal interfaces for advanced battery applications.

3:30pm **BT-ThA-6 ASSD Student Award Finalist Talk: Strategies for Tof-Sims of Buried Interfaces in Solid Polymer Electrolyte Batteries***, **Reyhane Shavandi**, Meghan Burns, Neelam Sunariwal,* University of Illinois at Chicago*; Sanja Tepavcevic,* Argonne National Laboratory*; Luke Hanley,* University of Illinois at Chicago

The solid electrolyte interphase (SEI) formed at lithium metal interfaces plays a critical role in determining the stability and performance of solid state batteries with polymer-based electrolytes. Time-of-flight secondary ion mass spectrometry (ToF-SIMS) combined with ion sputtering was used here to investigate the composition and spatial distribution of the buried SEI formed with a mixed of bis(fluorosulfonyl)imide (LiFSI) and poly(ethylene oxide) (PEO) electrolytes between lithium electrodes, Li|PEO-LiFSI-$LiNO_3$|Li. Gaseous cluster ion beam (GCIB) sputtering revealed that the SEI remained adhered to the Li electrode rather than to the polymer electrolyte, indicating its mechanical robustness and chemical stability. Depth profiles from ToF-SIMS analyses further revealed that addition of small amounts of $LiNO_3$ to the LiFSI/PEO electrolyte led to the formation of a nitrogen-rich SEI layer adjacent to the Li electrode surface, characterized by a strong CN^- signal identified by high mass accuracy peak assignment (S.R. Shavandi, *et al*., *J. Vac. Sci. Technol. B* 44, 2026, 012401). The presence of CN^- signal indicated the presence of nitrogen-containing species within the inner SEI and a corresponding reduction of LiF-content within the SEI. Based on these findings, an anode free system using a Cu electrode, which both less expensive and nonflammable was examined. The Cu electrode was coated with a thin Au layer and Al_2O_3 nanoparticles were incorporated into the solid-state electrolyte to form Li|PEO-LiTFSI-$LiNO_3$+Al_2O_3|Au/Cu. $LiNO_3$ was added to create a nitrogen-rich interfacial layer with excellent Li-ion transport ability, while Al_2O_3 nanoparticles served to mechanically reinforce the pure polymer electrolyte. Li plating onto bare Cu during electrochemical cycling is hindered by a large nucleation overpotential that leads to non-uniform and dendritic growth, but the Au coating onto Cu is thought to create a lithiophilic interface by forming Au–Li intermetallics that reduce the nucleation barrier and enable uniform Li deposition. Current efforts focus on combining the benefits of the nitrogen-rich interface with this lithiophilic Au-alloying strategy to better understand where Li preferentially plates and how the nitrogen-rich layer forms and evolves on Au/Cu versus metallic Li surfaces. ToF-SIMS directly probed Li nucleation and interfacial chemistry with depth profiling using either O_2 or GCIB sputtering guns to achieve high sensitivity to Li and buried interfacial species. Both two-dimensional depth profiling and three-dimensional chemical imaging were utilized to resolve the spatialdistribution of Li relative to the Au interlayer.

3:45pm **BT-ThA-7 Correlative Imaging and Surface Analysis of Air-Sensitive Materials***, **Lu Ping**,* Thermo Fisher Scientific, USA*; Hsiang-Han Tseng, Helen Oppong-Mensah, Tim Nunney,* Thermo Fisher Scientific, UK

Understanding complex materials increasingly requires the correlation of structural, morphological, and chemical information acquired across multiple analytical platforms. Imaging techniques such as scanning electron microscopy provide essential context on microstructure, defects, particles, and regions of interest, while surface-sensitive spectroscopies such as X-ray photoelectron spectroscopy reveal local chemistry, bonding, and elemental composition. For air-sensitive materials, however, transferring specimens between instruments can alter the very surfaces and interfaces under investigation, making reliable correlation especially challenging.

This presentation describes recent developments enabling vacuum-protected transfer between electron microscopy and surface analysis instrumentation. The approach combines SEM-based imaging and site selection with subsequent XPS analysis using a two-way vacuum transfer capability, allowing selected regions to be analyzed while minimizing atmospheric exposure. The ability to move samples between instruments under controlled conditions supports iterative, correlative investigation without compromising reactive surfaces.

Examples will be presented from air-sensitive materials, including Li-ion battery components, where preservation of native surface chemistry is critical for interpreting degradation, interphase formation, and chemistry-structure relationships. These results illustrate how vacuum-integrated correlation of imaging and spectroscopy can provide a completer and more reliable picture of materials that are difficult to characterize using isolated techniques alone.

4:00pm **BT-ThA-8 Correlating Surface Chemistry and Subsurface Structure in Battery Degradation Layers via XPS, HAXPES, AES, and TOF-SIMS***, **Sarah Zaccarine**,* Physical Electronics USA*; Isaiah Oladeji,* Sisom Thin Films*; Jacob Schmidt, Juergen Scherer, Amy Ferryman,* Physical Electronics USA

Understanding the formation and evolution of degradation layers at battery interfaces is critical for improving electrochemical performance, safety, and lifetime. These interphases are chemically complex and highly heterogeneous, requiring complementary, surface-sensitive analytical techniques to fully resolve their structure and composition. In this work, X-ray Photoelectron Spectroscopy (XPS), Auger Electron Spectroscopy (AES), and Time-of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS) are combined to investigate both surface and subsurface features of degradation layers in advanced battery materials.

XPS provides quantitative elemental and chemical state information from the top ~1–10 nm, enabling identification of key inorganic and organic species within interphase layers and their evolution during electrochemical cycling. The use of hard X-ray photoelectron spectroscopy (HAXPES) further extends the probing depth into the subsurface (up to 30 nm), allowing non-destructive characterization of buried interfaces while maintaining chemical state sensitivity. AES offers high spatial resolution at the nanoscale, making it particularly effective for resolving compositional variations across interfaces and within localized degradation features. TOF-SIMS complements these approaches with ultra-high sensitivity to trace species and molecular fragments, along with 3D chemical imaging and sputter depth profiling capabilities, that reveal the layered structureand distribution of degradation products below the immediate surface.

Overall, the synergistic application of XPS, AES, and TOF-SIMS provides a comprehensive toolkit for correlating surface chemistry, subsurface composition, and interfacial structure in battery degradation layers. These insights are essential for guiding the design of more stable electrode–electrolyte interfaces and enabling next-generation energy storage technologies.

4:15pm **BT-ThA-9 Airless Transfer for Battery Materials: Preserving Native Surface Chemistry for Analysis**, ***Forrest Nichols,*** *Dan Sullivan,* Eurofins EAG

Analysis of materials that react with atmospheric chemicals, such as batteries, require airless preparation and airless transfer into the materials analysis tools. In this paper we describe the sample preparation to remove a cathode from a Li ion battery in a glove box in a dry room and placed into an airless transfer box. The sample is airlessly transferred into an XPS tool for analysis. This is followed by exposure of the sample to air for one minute and then another XPS analysis. The sample is then exposed to air for two days and a final analysis is performed. The change in the surface composition and chemistry is investigated as a function of air exposure time. Airless transfer enables accurate surface analysis of battery materials by preserving native chemistry.

Spectroscopic Ellipsometry
Room 320 - Session EL-ThA

Spectroscopic Ellipsometry Oral Session

Moderators: Dr. Andy Antonelli, Antonelli Research and Technology, **Dr. Ufuk Kilic**, University of Nebraska - Lincoln, **Dr. Nikolas Podraza**, University of Toledo, **Prof. Dr. Eva Schubert**, University of Nebraska - Lincoln

2:15pm **EL-ThA-1 Spectroscopic Ellipsometry for Advanced Semiconductor Metrology Applications**, ***Matthew Hilfiker,*** *Rostislav Grynko, Nick Keller,* Onto Innovation **INVITED**

Advanced logic and memory development continues to push device architecture well beyond the limits of traditional process control methods. As dimensions shrink and structures become increasingly complex, parameter correlation has increased, placing new demands on both metrology sensitivity and model robustness. While spectroscopic ellipsometry has long been a workhorse technique in semiconductor manufacturing, its effective use at advanced nodes requires broader spectral coverage, improved modeling approaches, and tighter control of measurement uncertainty.

This talk provides an overview of spectroscopic ellipsometry as it is applied to today's most challenging metrology problems. Measurements in the visible and ultraviolet remain critical for monitoring dimensional control at the atomic scale. At the same time, mid–infrared ellipsometry has emerged as an important complement, offering enhanced sensitivity to structural effects that are difficult to access at shorter wavelengths. Together, these capabilities allow metrology strategies to be tailored to the specific physics and correlations of a given process step.

As device architecture continues to evolve, improving metrology performance increasingly depends on combining advanced optical modeling with measurement approaches that remain stable across highly correlated parameter spaces. The role of rigorous coupled physical wave analysis (RCWA) enabling optical critical dimension analysis of complex three–dimensional structures will be discussed. The presentation will emphasize broader trends shaping spectroscopic ellipsometry as a critical enabler of advanced semiconductor manufacturing.

2:45pm **EL-ThA-3 In It to Thin It: Spectroscopic Ellipsometry for Native Oxide Measurement on Indium Thermal Interface Materials**, ***Maxwell Junda,*** *Biswas Subedi,* Covalent

Native oxide layers on metal surfaces critically impact performance across industry. In semiconductor advanced packaging, native copper oxide at Cu-Cu hybrid bond interfaces can inhibit both electrical connectivity and bond integrity. For batteries, oxide on current collector foils influences interfacial impedance, and, for medical implants, surface oxide on titanium dictates biocompatibility and corrosion resistance. Here, we present the case of indium-based thermal interface materials (TIMs) where native oxide degrades wetting, thermal, and mechanical properties at the bond interface, contributing to void formation during reflow. Excessive oxidation can ultimately lead to thermal hot spots and reduced device reliability, making oxide thickness a key quality metric.

There are only a few metrology options for native oxides on metals. Being non-destructive, fast, and compatible with production inspection workflows makes spectroscopic ellipsometry (SE) appealing. The reality is, however, that topography, grain structure, and oxide composition variability on production surfaces present challenges for SE. Additionally, accuracy requires managing correlation between the oxide thickness and optical properties of both the metal and oxide in the optical modeling.

Covalent has developed a reliable SE-based native oxide thickness measurement on indium TIM surfaces. To overcome the inherent variability of commercial indium surfaces, we collect many distributed individual measurements to yield statistical distributions of oxide thickness. This ensures that locally anomalous sites do not overly bias the representative characterization of the overall oxidation level. Optical constants for both the indium metal and its native oxide were established through simultaneous multi-sample fitting across samples of varying oxidation, producing a robust model in which only oxide thickness remains as a fit parameter for routine inspection. Results were validated against both cross-sectional TEM and XPS. Oxide thicknesses for minimally oxidized samples are typically on the order of 5 nm. We also applied this methodology to compare as-received to intentionally oxidized samples, successfully discriminating oxide thicknesses relevant to TIM quality control. TIM shelf life was also studied through repeated measurements over time. This methodology is now deployed for routine indium TIM inspection.

Finally, we will discuss plans to extend this work with imaging ellipsometry to investigate oxide thickness variation at the microscale, to understand how surface topography and grain boundaries contribute to the spatial variability observed in focused-spot SE measurements.

3:00pm **EL-ThA-4 Developing an Optical Database of Thermally Evaporated Cadmium Selenide Telluride Alloys for Machine Learning Enhanced Spectroscopic Ellipsometry**, ***Alex Bordovalos,*** *Nadeesha Katakumbura, Eva Mulloy, Bishal Shrestha, Suresh Chaulagain, Marie, Solange Tumusange, Balaji Ramanujam, Randy Ellingson, Ambalanath Shan, Nikolas Podraza,* University of Toledo

Machine learning techniques have shown great promise for performing rapid spectroscopic ellipsometry data analysis on simulated ellipsometric spectra in select case studies. It is critical that machine learning enhanced spectroscopic ellipsometry (MLSE) is applied to measured ellipsometric spectra collected for samples with varieties of layer structures to demonstrate its utility while developing a better understanding of transitioning MLSE from simulated ellipsometric spectra to measured ellipsometric spectra. To this end,the complex dielectric function ($\varepsilon = \varepsilon 1 + i\varepsilon 2$) spectra of thermally evaporated cadmium selenide telluride (CdSe(x)Te(1-x)) alloys are established for the purpose of simulating ellipsometric spectra that represent current fabrication techniques in CdSe(x)Te(1-x) photovoltaic (PV) devices.

A series of ten thermally evaporated CdSe(x)Te(1-x) alloys are deposited on commercial transparent conducting oxide glass. These alloys are measured with energy-dispersive X-ray spectroscopy to have Se content (x) of 0.00, 0.14, 0.25, 0.31, 0.36, 0.46, 0.62, 0.75, 0.85, and 1.00. A cadmium chloride ($CdCl_2$) heat treatment, standard to PV devices, is applied to the alloys which are then measured with X-ray diffraction to reveal a wurtzite crystal structure at $x \geq 0.62$ and a zinc blende crystal structure at $x \leq 0.46$. Spectroscopic ellipsometry measurements are performed on these alloys. $\varepsilon 2$ is determined using a background TaucLorentz oscillator, an Urbach tail, and a series of excitonic critical point parabolic band oscillators with common phase for a given crystal structure while $\varepsilon 1$ is determined from analytically solving Kramers-Kroning integration and a Sellmeier expression. A set of polynomial fits are then applied to each optical property parameter to establish the variations of each parameter as a function of Se content. These relationships reduce the number of model fit parameters by mapping these optical property parameters to x.

This optical model for CdSe(x)Te(1-x) alloys is well suited for simulating ellipsometric spectra for the purposes of developing MLSE for CdSe(x)Te(1-x) PV applications because it has a comparatively smally number of parameters and the model generated optical properties are representative of materials in current devices. The next steps include training an MLSE model using simulated ellipsometric spectra and then applying the MLSE to measured ellipsometric spectra collected from CdSe(x)Te(1-x)PV device stacks.

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3:15pm **EL-ThA-5 Spectroscopic Ellipsometry Studies of Materials for High Power Electronics**, ***Madan Kumar Mainali***, *Prabin Dulal, Bishal Shrestha, Suresh Chaulagain, Venkanna Kanneboina, Ambalanath Shan, Nikolas Podraza,* University of Toledo

Wide band gap materials 4H-SiC and 6H-SiC are two hexagonal crystal polytypes of silicon carbide. It is used in high power electronics as it has high thermal conductivity, high operational temperature, higher efficiency with lower power loss, and high switching frequency. Spectroscopic ellipsometry is used to characterize the optoelectronic properties of 4H-SiC and 6H-SiC (0001) single crystal samples from MTI Crop, over the infrared (IR) to vacuum ultraviolet (VUV) (0.05 – 8.5 eV) spectral range. Spectroscopic ellipsometry is a non-contact optical characterization technique sensitive to structural (bulk film thickness, interfacial layer thickness, surface layer thickness), optical properties (band gap, above band gap transitions, phonon modes), and electronic transport (resistivity, carrier concentration, carrier mobility, scattering time, and carrier effective mass) properties. Complex dielectric function ($\varepsilon = \varepsilon_1 + i\varepsilon_2$) spectra are obtained from reflection mode spectroscopic ellipsometry for backside roughened 4H-SiC and 6H-SiC. A single parametric model describing ε predominately for the ordinary directions is developed over the 0.05 – 8.5 eV for 4H-SiC and 6H-SiC with some contribution from the extraordinary direction of 6H-SiC in the IR region. Indirect band gaps for 4H-SiC and 6H-SiC are found to be 3.30 and 3.03 eV, respectively, and the corresponding direct optical gaps are at 4.46 and 4.42 eV. A model describing the optical response in the IR spectral range is created using a Drude expression with either transverse optical (TO) and longitudinal optical (LO) (TOLO) or Lorentz oscillator models. Free carrier concentration (N) is optically measured to be 3.7×10^{18} and 3.3×10^{18} cm^{-3} using TOLO and Lorentz oscillator models respectively, and the corresponding carrier mobility (μ) is 34 and 39 cm^2/Vs for 4H-SiC. For 6H-SiC, N is measured to 8×10^{18} cm^{-3} using either TOLO or Lorentz oscillator models and μ in the ordinary direction is 9 and 10 cm^2/Vs using the TOLO and Lorentz oscillator model, respectively, and 5 cm^2/Vs in the extraordinary direction using either model. For 4H-SiC, using the TOLO oscillator model, TO and LO phonon modes are obtained at 797.7 and 992.1 cm^{-1}, respectively. In 6H-SiC, TO modes in ordinary and extraordinary directions are found at 797.7 and 789.7 cm^{-1} and the corresponding LO modes are found at 992 and 984 cm^{-1}, respectively. The TO and LO modes obtained from the Lorentz oscillator model are consistent with modes obtained from TOLO model.

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3:30pm **EL-ThA-6 Photoacoustic Simulations for Acoustic Critical Dimension Metrology**, ***George Antonelli***, Antonelli Research & Technology; *Brian Daly,* Vassar College

Picosecond laser ultrasonics is a twenty year old high volume semiconductor metrology and continues to find new applications. One of the strengths of this technique is the deep connection between the development of the hardware and the multi-physics simulations that allow the extraction of critical parameters. As semiconductor devices continue their shift from 2D to 3D, analysis of photoacoustic data has become more challenging as the simulations are in general limited to planar stacks of films. The development of fast numerical methods for solving 3D light-matter interactions enabled the leap from films to structures giving birth to optical critical dimension (OCD) metrology.These numerical tools offer a template for a similar leap in photoacoustics. Acoustic critical dimension (ACD) metrology like OCD is an optical method, but it can non-destructively extract critical dimensions of 3D structures buried beneath an opaque surface. This method requires a new class of multi-physics simulation capable of performing tightly choreographed optical, electronic, and coupled opto-mechanical calculations. In this paper, previous work on this topic will be summarized and new algorithms realized in a software package under development will be presented. Two key components of this work are (1) the democratization of this complex analysis to facilitate its use by undergraduates and (2) a shift away from the structure definition as geometry found in OCD today and towards a process driven paradigm. Structures are therein defined by the way they are manufactured and fits on the structures can be linked back to the fundamental process parameters.

3:45pm **EL-ThA-7 Optical Modeling of Plasmonic Nanostructures**, ***Peter Petrik***, *Géza Szántó, Deshabrato Mukherjee, Chao Zeng, Máté Stift, Shayesteh Raeisi, Zoltán Lábadi,* Centre for Energy Research, Hungary; *Attila Bonyár,* Budapest University of Technology and Economics, Hungary; *Miklós Fried,* Centre for Energy Research, Hungary

Plasmonic nanostructures are utilized in many applications for sensing, photonics, and much more. General models in ellipsometry that focus on transfer matrix, effective medium, first principle oscillators, and analytical dispersion functions show difficulties when modeling such structures. In this work we present modeling approaches and applications for characterizing a broad variety of plasmonic and periodic nanostructures, including gratings, nanoparticles created by annealing, electrochemistry, as well as combinatorial sputtering. The formation of nanoparticles was monitored during annealing and electrochemistry. We utilized both through-liquid and Kretschmann-Raether cells for monitoring the growth of gold layers in an electrochemical cell, as well as the interaction between silk layers and analytes in Kretschmann configurations. We also studied the adsorption of flagellar filaments on nanostructured gold surfaces and their electrochemical sensing performance. The optical sensing properties of periodic gold nanostructures were also investigated in terms of measuring the ambient and thin overlayers, as well as the sensitivity for the determination of the dimensional parameters of the periodic structures. Using simplified hemispherical numerical models, we explained the sensing performance of annealed gold layers created by combinatorial sputtering. The sensitivity as a function of the initial amount of deposited gold and type of analyte was measured and explained by numerical finite element modeling of the gold nanostructures and adsorbed layers.

4:00pm **EL-ThA-8 Engineering Anisotropic Optical Properties in Hybrid Plasmonic Metamaterials**, ***Ufuk Kilic***, *Raymond Smith, Yousra Traouli,* University of Nebraska-Lincoln; *Christos Argyropoulos,* Pennsylvania State University; *Eva Schubert, Mathias Schubert,* University of Nebraska-Lincoln

Hybrid plasmonic metamaterials provide a powerful platform for tailoring light–matter interactions through structural control of their effective dielectric properties [1-3]. Here, we investigate the anisotropic optical response of bottom-up engineered Si–Ag hybrid plasmonic metamaterials fabricated using glancing angle deposition (GLAD). Sequential oblique-angle depositions combined with controlled substrate rotation enable deterministic control of nanocolumn geometry, optical anisotropy, and structural handedness over large areas [2-3]. The optical properties are characterized using Mueller matrix generalized spectroscopic ellipsometry (MM-GSE) from the near-infrared to the ultraviolet spectral range. Multi-layer anisotropic effective-medium approximation analysis is employed to extract the wavelength-dependent dielectric tensor elements and quantify the influence of plasmonic–dielectric hybridization on the effective optical response. The extracted dielectric functions reveal pronounced anisotropy and strong tunability arising from the engineered morphology, material composition, and structural handedness of the nanocolumn architectures.

Finite-element-method simulations are performed to establish the physical origin of the observed optical behavior. The simulations reveal strong polarization-dependent field localization and spin-dependent plasmonic mode coupling, producing enhanced optical anisotropy and broadband chiroptical activity, including pronounced circular dichroism extending from the near-infrared to the ultraviolet. Excellent agreement between experiment and theory validates the extracted dielectric functions and effective-medium analysis. **Complementary high-resolution imaging, crystallographic analysis, and compositional characterization, including scanning electron microscopy (SEM), transmission electron microscopy (TEM), and X-ray diffraction (XRD), confirm the formation of spatially coherent, compositionally distinct, and morphologically uniform hybrid nanocolumn arrays.**The combined experimental and theoretical investigation establishes a framework for engineering anisotropic dielectric functions in hybrid plasmonic metamaterials through nanoscale structural design. The demonstrated tunability of the effective dielectric response provides opportunities for polarization-selective photonics, broadband chiral platforms, optical sensing, and integrated nanophotonic technologies.

References:

[1] Carneiro, S. V., et al., *Materials Today Nano* 22 (2023): 100345.

[2] Kilic, U., et al., *Advanced Optical Materials* (2024): 2302767.

[3]Kilic, U., et al., *Nature communications* 15.1 (2024): 3757.

4:15pm **EL-ThA-9 From Disordered Nanoparticles to Periodic Gratings: A Unified Framework for High-Precision Plasmonic Metrology**, ***Deshabrato Mukherjee***, *Géza Szántó, Chao Zeng, Máté Stift, Shayesteh Raeisi, Zoltán Lábadi,* Centre for Energy Research, Hungary; *Attila Bonyár,* Budapest University of Technology and Economics, Hungary; *Miklós Fried, Peter Petrik,* Centre for Energy Research, Hungary

We developed a high-throughput screening and ultra-sensitive detection framework using two distinct architectures: a disordered graded gold nanoparticle platform for rapid process optimization and periodic gold gratings for predictable accurate performance.

The high-throughput combinatorial platform was created by depositing graded gold layers (0-20 nm) along the X-axis on fused silica using magnetron sputtering, followed by annealing up to 600°C. This led to the formation of self-assembled nanoparticles with laterally varying surface density from 2090 to 88 particles/μm^2, resulting in an evolution of morphology from oblate to hemispherical. This was followed by spatially resolved operando tracking using a modular Avantes fiber optic scanning spectroscopy system that mapped the transition of the localized surface plasmon resonances and volatile vapor pathways. The finite element method (FEM) calculations were modeled using JCMsuite to analyze nanoparticle formation and near-field properties. To detect ethanol, water layers via Peltier cooling, and chemisorbed MBA monolayers, we isolated specific thickness thresholds from 1.6 to 3.2 nm as the optical sensing regimes. These findings were evident due to the localized geometry and the near-field coupling due to the inter-particle gaps resulting in a surface-enhanced Raman spectroscopy (SERS) enhancement factor of 10^6 under confocal laser excitation.

Complementing this, we developed periodic gold gratings using a non-destructive metrology framework. The periodic gold gratings (CD between 70-130, thickness 60 nm, and period 200 nm) were fabricated using electron-beam lithography and reactive ion etching. These grating parameters were chosen for fabrication after multi-dimensional FEM simulations using JCMsuite to determine the changes or variations in the amplitude ratio represented by Ψ and the phase difference represented by Δ of the polarized reflection coefficients. The gratings were measured in reflection-mode with Woollam M-2000DI spectroscopic ellipsometer and fitted, and complemented with FEM modeling that enhances the traditional effective medium approximations. We demonstrated that the phase-sensitive parameter, Δ, provides superior sensitivity over the amplitude parameter, Ψ simulating across a five-dimensional parameter space that included the critical dimensions, period, thickness, wavelength, and angle of incidence. Using structural partial derivatives, we achieved a bulk refractive index limit of detection of 10^{-5} refractive index units, a critical dimension uncertainty in the picometer range, and a surface mass density limit of detection of 10 pg/mm^2 using De Feijter overlayer modeling.

Plasma Science and Technology
Room 315 - Session PS-ThA

Simulation for Plasma Processes

Moderators: Nobuyuki Kuboi, Sony Corporation, **Dr. Yu-Hao Tsai**, TEL Technology Center, America, LLC

2:15pm **PS-ThA-1 A Multi-Scale Simulation Methodology for Recipe Design in Semiconductor Etch Processes**, ***SeungMin Lee***, Samsung Electronics, Republic of Korea **INVITED**

As semiconductor device scaling approaches sub-nm regime and beyond, the synergy between plasma-surface interactions and feature-scale topography evolution has become increasingly non-linear and difficult to predict. Conventional technology computer-aided design (TCAD) and Monte Carlo-based topography simulations, while physically robust, often face a trade-off between computational cost and predictive accuracy, especially when accounting for complex plasma chemistries. This gap between theoretical precision and practical processing speed necessitates a fundamental shift in how we approach process modeling and feature-scale evolution.

To address these limitations, this presentation introduces a robust hybrid framework that integrates plasma physics, topography simulation, and artificial intelligence (AI). By bridging AI with domain-specific physics of plasma reactions and surface kinetics, we accelerate the coupling between equipment-level plasma distributions and feature-scale profile evolution. This methodology allows for the rapid prediction of etching and deposition profiles with maintaining the rigor or Monte Carlo-based transport models. Furthermore, we explore how AI-driven features extraction can identify hidden correlations between plasma reaction transitions and structural defects, providing insights that were previously inaccessible through traditional TCAD-based methods.

Ultimately, the fusion of AI with physical modeling provides a new paradigm for "Digital Twin" environments in semiconductor manufacturing. We demonstrate how this integrated methodology enables autonomous TCAD calibration and real-time optimization of process conditions to improve etching outcomes. This science-based AI approach not only enhanced our fundamental understanding of plasma process but also significantly accelerates the development cycle for the next generation of logic and high-density memory devices.

2:45pm **PS-ThA-3 GPU-Accelerated AMR Simulation of Charging-Driven Instability in Ion-Assisted Etching**, ***Takumi Ohmura***, *Satoshi Nakamura, Hisashi Kotakemori, Taishi Ikeda, Kenta Yashima, Yasuyuki Kayama,* Samsung Device Soltuions R&D Japan; *YunTae Lee,* Samsung Electronics, Republic of Korea; *Yukihide Tsuji,* Samsung Electronics, Japan; *Jaehoon Leem, Jaeyong Lee, Shinwook Yi, Moon-Hyun Cha, Jaehoon Jeong,* Samsung Electronics, Republic of Korea

Predictive modeling of high–aspect–ratio contact etching requires resolving three–dimensional geometries that involve surface reactions, surface charging, and long–timescale evolution, which remain computationally challenging.Our simulator combines adaptive mesh refinement (AMR) with GPU acceleration for both the Poisson solver and particle transport. The Poisson solver is accelerated by more than an order of magnitude (>10×) using an AMR–based multi–level multigrid solver on GPUs. Moreover, both charged and uncharged particle transport are further accelerated by more than 2× through hierarchical voxels. This advance enables high–resolution, long–term simulations.

Using a simplified ion–assisted etching model, we demonstrate that charging–induced electrostatic fields can cause morphological instability. Parametric studies indicate that striation formation is primarily driven by the low–energy ion population. These ions are reflected by a potential barrier that increases approximately linearly with feature depth and grows with higher electron temperature. We find that striations appear when the low–energy ion energy is comparable to the potential barrier, within a factor of two. In this regime, ion trajectories are strongly perturbed by the electrostatic fields. Meanwhile, when ion energies significantly exceed the potential barrier, striation formation is suppressed. However, lateral broadening is observed due to the angular spread of ion trajectories.

This work shows that GPU–accelerated AMR is suitable for feature–scale simulations incorporating surface charging, and it provides physical insight of interpreting charging–driven pattern formation. In addition, our finding is expected to provide useful guidance for realistic processing conditions and improve process-parameter optimization.

3:00pm **PS-ThA-4 Particle in Cell Monte Carlo Collision Simulations of Capacitive Ar/Cl_2 Discharges**, *Bahram Mahdavipour,* ***Jon Tomas Gudmunsson***, University of Iceland

Reactive gases mixed with rare gases in capacitively coupled discharges are often used in etching and deposition processes in microelectronic device fabrication. The chlorine discharge and its mixtures are frequently applied in the etching of semiconductors and metals. Here, capacitive discharges in Ar/Cl_2 mixture driven by sinusoidal rf voltage at 13.56 MHz with 2.54 cm discharge gap are explored using one-dimensional particle-in-cell/Monte Carlo collisional (PIC/MCC) simulations. The discharge model includes excited argon species and secondary electron emission, due to electron, ion and excited species impact on the electrodes. Chlorine is a highly electronegative discharge gas, whereas argon forms an electropositive discharge. By adding chlorine to an argon discharge, the plasma discharge can be transformed from being electropositive to become electronegative, and the electronegativity can be varied over a wide range. For pressure of 10 Pa the electronegativity can be varied from 0 - 107, while the electron energy distribution varies from bi-Maxwellian to Druyvesteyn like, as the Cl_2 fraction in the admixture is varied from 0 - 100 %. We will discuss how the electron power absorption mechanisms, the electronegativity, the electron energy distribution function, the reaction rates, and the composition of the discharge vary with the addition of chlorine to the argon discharge. Furthermore, we explore how the electron power absorption mechanisms, the electronegativity, the electron energy distribution function, and the discharge composition evolve with changes in pressure and driving voltage amplitude. In particular, we identify the discharge conditions where the electron power absorption transitions from the alpha-mode to the drift-

ambipolar (DA) mode to a combined DA and striation mode, as the pressure, and the Cl_2 fraction in the feedstock are increased.

3:15pm **PS-ThA-5 Verification and Validation of the Open-Source Code PICLas for Capacitively Coupled Plasma Discharges in Etching Applications**, ***Paul Nizenkov***, *Asim Mirza, Stephen Copplestone, Julian Beyer,* boltzplatz - numerical plasma dynamics GmbH, Germany*; Marcel Pfeiffer,* Institute of Space Systems, University of Stuttgart, Germany

Capacitively coupled plasma (CCP) discharges are widely used in plasma etching and surface treatment processes. Predictive simulation of such discharges is essential for reactor design, process optimization, and the development of new etching chemistries. In this contribution, we present the verification and validation of PICLas (https://github.com/piclas-framework/piclas), an open-source Particle-in-Cell with Monte Carlo Collisions (PIC-MCC) code released under GPLv3, for radio-frequency CCP discharges in argon relevant to plasma etching applications. PICLas provides a framework for kinetic plasma simulation using Particle-in-Cell, Direct Simulation Monte Carlo (DSMC), Bhatnagar-Gross-Krook (BGK), and Fokker-Planck methods, enabling detailed modelling of electron kinetics, plasma chemistry, and plasma-surface interactions in low-pressure processing environments. First, the 1D benchmark by Turner et al. (Phys. Plasmas 20, 013507, 2013) is employed for a systematic code-to-code comparison of argon CCP discharges at multiple operating conditions. Second, a 2D axisymmetric simulation of the Gaseous Electronics Conference (GEC) reference cell, a standardized reactor geometry representative of industrial etching tools, is performed and compared with available numerical results and experimental measurements. Key outputs include species- and time-resolved ion energy and angular distributions at the substrate and chamber walls, surface-charge tracking on dielectric boundaries, and secondary electron emission fluxes. These quantities can directly feed feature-scale etch models and surface chemistry frameworks. The verified simulation capability provides a foundation for predictive modelling of etching plasmas and plasma-surface interactions, supporting reactor-scale process development and optimization.

3:30pm **PS-ThA-6 Fully Kinetic Full-Chamber Modeling of ICP Discharges**, ***Daniel Main***, Silvaco, Inc.*; Seth Veitzer, Tom Jenkins, John Cary,* Silvaco Inc.

Low-temperature kinetic plasma simulations using particle-in-cell (PIC) and Monte Carlo methods (DSMC/MCC) for the chemistry can provide many advantages over fluid simulations, including self-consistent collisional heating at low pressure and correctly modeling sheaths without ad hoc assumptions. In addition, a fully kinetic approach can move beyond common assumptions made in fluid models, such as local conductivity or Maxwellian distributions of the plasma species. In this talk we present kinetic modeling results of inductively coupled plasmas (ICPs) in a 2D cylindrically symmetric geometry using the VSim[1] software package. We demonstrate how implicit methods can make these challenging simulations feasible, reducing compute times by factors of 20-200. We also demonstrate a method of providing constant power to the plasma, which further decreases the runtime needed to achieve steady-state discharges. We present several case studies which are based on process parameters discussed in Godyak et al. (2002)[2], showing good agreement with experimental measurements including plasma potential, plasma density, and electron temperature. Finally, we demonstrate the importance of a fully kinetic approach at low pressure (<~ 10 mTorr) to correctly model collisionless heating. We show that the simulated electron energy probability function compares well with experimental results, including the tri-Maxwellian features observed in Godyak et al.

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3:45pm **PS-ThA-7 Generalized RF Breakdown Surfaces and Avalanche Regimes in Dual-Frequency Argon CCPs: A 2D PIC/MCC Study**, ***Junesuk Kang***, KWT Solution, Republic of Korea

Single-frequency RF breakdown in argon capacitively coupled plasmas has often been represented as a breakdown curve versus pressure or *pd*. In dual-frequency CCPs, however, the breakdown boundary is inherently multidimensional because the high-frequency voltage, low-frequency voltage, frequency ratio, relative phase, and electrode surface properties can all modify the balance between electron multiplication and wall loss. In particular, the low-frequency field is not merely an additional contribution to an effective RMS voltage. Depending on the operating condition, it may increase electron drift loss to the electrodes and raise the required high-frequency breakdown voltage, or it may enhance ionization and surface-emission feedback and lower the threshold.We investigate these effects using a two-dimensional electrostatic PIC/MCC model of voltage-driven argon CCP breakdown. The simulations track electrons and Ar^+ ions, include electron-neutral elastic, excitation, and ionization collisions, Ar^+ collisions, and configurable surface reflection and secondary-electron-emission models. For each pressure, LF voltage, frequency pair, phase, and surface condition, the HF breakdown voltage is obtained by bisection using a growth-rate criterion based on $d(\ln N_e)/dt$, together with density-threshold crossing and self-sustained-growth confirmation. The resulting data are analyzed as generalized breakdown surfaces, $V_{HF,br}(p, V_{LF}, f_{HF}, f_{LF}, \theta, \text{surface})$. Ionization sources, electron wall fluxes, J·E, electron energy distributions, and secondary-electron-induced ionization are used to classify RF-avalanche, LF-loss-dominated, LF-assisted, surface-assisted, and mixed avalanche regimes. This framework provides a kinetic benchmark for RF startup windows and ignition-margin control in dual-frequency plasma processing reactors.

4:00pm **PS-ThA-8 Stochasticity in Advanced Plasma Etching**, ***Xingyi Shi***, *Han Luo, Jason Kenney, Shahid Rauf,* Applied Materials

As feature dimensions continue to scale, variability in plasma etching increasingly limits pattern fidelity. While intra-feature etch variations have traditionally been attributed to variations in incoming mask critical dimensions, emerging process regimes introduce additional sources of variability. Highly constrained plasma operating conditions can lead to ion-flux-limited etching, where stochastic effects become significant even for nominally uniform feature geometries. Under such conditions, measurable intra-feature variations may develop during etching despite minimal geometric nonuniformity at the start of the process.

In this work, we investigate the role of ion-driven stochasticity in governing intra-feature etch depth variations using feature-scale modeling. The study examines how process conditions and feature characteristics influence the evolution of etch front variability in ion-limited regimes. By comparing cases with different etching conditions and feature opening areas, the analysis highlights general trends linking stochastic transport and surface reaction processes to observed etch nonuniformity. Ongoing and forthcoming simulation results will be used to quantify these effects and to establish a qualitative framework for understanding and mitigating stochastic-induced variability in advanced plasma etching processes.

4:15pm **PS-ThA-9 Influence of Nitrogen Addition on Metastable Dynamics in a 2.45 GHz Ar-N_2 Plasmas**, ***Nafisa Tabassum***, *Duncan Trosan,* North Carolina State University*; Abdullah Zafar, Timothy Chen, Kelvin Chan,* Applied Materials, USA*; Steven Shannon,* North Carolina State University

A microwave-driven plasma operating at 2.45 GHz was studied using OES, LAS, probe diagnostics, and the plasma simulation package Zapdos [1]. The working gas was an Ar/N_2 mixture with a N_2 partial pressure range from 0 % to 25 % of total gas pressure (mTorr range) and a delivered power density (0.30 W/cm^3 -1.2 W/cm^3 range). Spatially resolved diode laser absorption spectroscopy of the Ar 696.7 nm transition $1s_5 \rightarrow 2p_2$ was used to probe the plasma. The line-integrated density and gas temperature were determined from the integrated absorption and broadening of the measured line shape. Relative concentrations of molecular N_2, ionized molecular N^+_2 and atomic N as well as bright Ar emission lines were obtained through optical emission actinometry as a function of N_2 partial pressure. The electron density and electron temperature were measured using Langmuir and hairpin probes. The metastable density decreases with increasing pressure, likely due to enhanced collisional quenching and reduced electron excitation out-weighing the production. In pure argon, it also decreases with delivered power, whereas the addition of N_2 leads to an opposite trend, with the metastable density increasing with power. The opposite power dependence likely results from modified plasma chemistry and surface interaction processes. Additionally, the experimental findings are compared with simulations conducted using CRANE and ZAPDOS plasma simulation applications in the Multiphysics

Object-Oriented Simulation Environment (MOOSE) platform.[1] PSST 32 (4), 044006

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Advanced Surface Engineering
Room 304 - Session SE-ThA

Advanced Surface Engineering Oral Session

Moderators: Prof. Dr. Diana Berman, University of North Texas, **Prof. Dr. Filippo Mangolini**, The University of Texas at Austin

2:15pm **SE-ThA-1 In-Situ Raman Spectroscopy of Adaptive Tribological Coatings**, ***Andrey Voevodin***, University of North Texas **INVITED**

In-situ Raman spectroscopy is a powerful method to investigate adaptive tribological surfaces. The in-situ Raman spectroscopy is shown to capture tribologically induced changes of adaptive coatings inside the lubricated sliding contact in response to applied mechanical and thermal stresses. For solid lubricated adaptive contacts, duplex plasma-electrolytic oxidation (PEO) and chameleon coating produced on Al alloys were investigated. These were composed of a 80-160 mm thick hard load-supporting Al-Si-O coating and a 5–8 µm top layer of a chameleon coating made of graphite or BN, MoS_2 or WS_2, and Sb_2O_3. For liquid contacts, 52100 steel coupons were tested under lubricant starvation regimes using low viscosity hydrocarbons. The counterpart pins were made of 52100 steel and Si_3N_4. The tests were performed at temperatures ranging from room (liquid lubrication) to 600 °C (solid lubrication). In-situ Raman spectroscopy revealed that the lubricating phases, i.e. MoS_2, WS_2, and graphite, were protected from oxidation by the porous PEO structure. It also revealed a gradual evolution of chameleon composition with diminishing orthorhombic Sb_2O_3 phase presence at the surface in favor of hexagonal lubricating phases of chameleon components. The low shear strength of MoS_2, WS_2, and graphite and the integration of the chameleon coating with the PEO sublayer were responsible for the ultra-low friction behavior. In all examples, the in-situ Raman spectroscopy was shown to reliably detect contact chemical change correlated with the observed friction behavior.

2:45pm **SE-ThA-3 Automated Characterization of Combinatorial Thin Films and Their Stress**, ***David Adams***, *Finley Haines, Amun Jarzembski,* Sandia National Laboratories, USA

Combinatorial sputter deposition techniques provide an ability to fabricate a large variety of thin films in a relatively short time thereby accelerating materials discovery. Indeed, past studies have reported methods that produce 10s or 100s of unique films in a single vacuum deposition. Despite these advances, new, high-throughput characterization techniques are needed to match the pace of combinatorial synthesis. In particular, automated techniques that accurately reveal the structure and the relevant properties of combinatorial films are of great interest.

Toward this end, we describe automated, ex-situ characterization of biaxial film stress wherein >100 individual, combinatorial thin films are probed in concert. Combinatorial, magnetron sputter-deposited Pt-Au and Pt-Ni films are interrogated using a k-Space Co. Thermal Scan instrument wherein samples are affixed inside a vacuum test cell. This instrument precisely moves a laser spot array to each specimen (before and after deposition) to determine wafer curvature changes. The application of Stoney's equation to determine the stress of combinatorial films from measured curvatures is discussed. Films are much thinner than the substrates (which satisfies one Stoney assumption), but a laterally graded thickness across each specimen moves away from at least one separate assumption used in the derivation of this often-used equation. Accounting for measured thickness gradients, we demonstrate accurate stress measurements over a range of temperatures up to +600C. Combinatorial Pt-Au and Pt-Ni films produced in single depositions exhibit a variety of stress responses that are ultimately correlated to measured film density and composition. Altogether, we determine their thermal expansion coefficients, pinpoint their onset of relaxation, and reveal changes occurring at high temperature tied to secondary phase formation. The gathered information augments an extensive library of process-structure-property relationships that underly their high-temperature performance.

Sandia National Laboratories is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

3:00pm **SE-ThA-4 Designing Defect Structure and Interfacial Strain in an Epitaxial VN Bilayer Film by Tailoring N Concentration**, ***Marcus Hans***, *Damian Holzapfel,* RWTH Aachen University, Germany; *Zhuo Chen,* Erich Schmid Institute of Materials Science, Austria; *Soheil Karimi Aghda, Michal Fečík,* RWTH Aachen University, Germany; *Daniel Primetzhofer,* Uppsala University, Sweden; *Zaoli Zhang,* Erich Schmid Institute of Materials Science, Austria; *Jochen Schneider,* RWTH Aachen University, Germany

A bilayer of $V_{0.49}N_{0.51}/V_{0.56}N_{0.44}$ has been grown epitaxially on MgO(001) by reactive high power pulsed magnetron sputtering in an industrial-scale deposition system at a temperature of 400 °C and it is demonstrated that the defect structure and interfacial strain are governed by the N concentration. Based on the lattice mismatch between MgO and $V_{0.49}N_{0.51}$ with V vacancies, an interfacial strain of -2.3(1)% is expected. From ab initio calculations, X-ray diffraction and transmission electron microscopy data it is inferred, that the $V_{0.49}N_{0.51}$ layer exhibits V vacancies, N Frenkel pairs and a high dislocation density of ~0.20 nm^{-2}, causing an interfacial strain of -1.4(5)% at the $MgO/V_{0.49}N_{0.51}$ interface. The phase formation of understoichiometric $V_{0.56}N_{0.44}$ is governed by N vacancy formation, while the dislocation density is reduced to ~0.04 nm^{-2} at the $V_{0.49}N_{0.51}/V_{0.56}N_{0.44}$ interface and to < 0.01 nm^{-2} within $V_{0.56}N_{0.44}$ at a distance of ~35 nm from the interface. Based on ab initio calculations, a strain of -1.7(6)% is predicted at the $V_{0.49}N_{0.51}/V_{0.56}N_{0.44}$ interface in very good agreement with the experimentally obtained value of -1.6(8)%. It is evident that control of the N concentration allows for the design of layered architectures with well-defined strained interfaces and tailored defect structures. Finally, the employment of only one transition metal is chemically simple and therefore, from a recycling point of view, also more sustainable than combining different transition metals as commonly done in layered architectures, including superlattices.

3:15pm **SE-ThA-5 Corrosion Behaviour of Zr-Ti-N Thin Films**, ***Jyoti Menghani***, Sardar Vallabhbhai National Institute of Technology SURAT, India; *k Baba Pai,* ITM UNIVERSE, India; *Nitin Jalgaonkar,* Seco Tools ,India

Zr–Ti–N coatings with varying thicknesses (1.5, 2.0, 2.5, and 3.0 µm) were deposited on 316 stainless steel substrates by cathodic arc evaporation using separate zirconium and titanium targets in a reactive nitrogen atmosphere. The influence of coating thickness on the microstructure and corrosion behavior of the films was systematically investigated. X-ray diffraction (XRD) analysis revealed the formation of crystalline Zr–Ti–N phases along with the presence of substoichiometric Ti_2N.

Surface and cross-sectional morphologies of the coatings were examined using scanning electron microscopy (SEM), which confirmed dense columnar growth of the deposited films. Cathodic arc-induced droplets were observed on the coating surfaces, and their presence was found to influence surface morphology and localized corrosion characteristics. Variations in coating thickness significantly affected coating compactness, defect density, and structural integrity.

The corrosion behavior of the coatings was evaluated in 0.1 N HCl solution using potentiodynamic polarization and electrochemical impedance spectroscopy (EIS). The acidic HCl medium was selected to simulate aggressive industrial corrosive environments. Electrochemical studies demonstrated that the corrosion resistance of the coatings improved with increasing coating thickness. The corrosion current density (Icorr) decreased from 136 µA/cm^2 for 1.5 µm Zr–Ti–N coating to 92.14 µA/cm^2 for 3.0 µm coating, indicating enhanced barrier protection and reduced electrolyte penetration. EIS results further confirmed the improvement in charge transfer resistance and protective efficiency with increasing coating thickness.

The study demonstrates that coating thickness, microstructural evolution, and cathodic arc droplet formation play a significant role in determining the corrosion performance of cathodic arc deposited Zr–Ti–N coatings for protective applications in aggressive acidic environments.

3:30pm **SE-ThA-6 High Throughput Thin Film Materials Synthesis via Laser Spike Annealing**, ***Drake Austin***, Air Force Research Laboratory (AFRL) **INVITED**

As the discovery of new materials and functionalities are occurring at an unprecedented rate, new strategies to accelerate the connection between material state or property to a desired application are necessary. Despite the availability of modern tools, the slow, tedious, and Edisonian research practices of the past are still the standard for areas such as thin films and coatings. The development of a new thin film requires either starting from a known, reported recipe, or the use intuition to determine a suitable starting condition. After thin film deposition is complete, there may be post-growth optimization and characterization, with many iterations of this

process necessary until the initial growth conditions match some desired end state.

Laser spike annealing (LSA) is a promising technique for rapidly investigating the modification of thin film materials due to thermal annealing. By scanning a focused, continuous-wave laser across a thin film surface, localized heating can be achieved with heating/quenching times as short as microseconds and temperatures exceeding 1000°C. The laser intensity, scan rate, and annealing environment can be varied, allowing thousands of distinct annealing conditions to be studied on a single sample, including dwell times several orders of magnitude shorter than what can be achieved with rapid thermal annealing. This approach can therefore be used for accelerated materials discovery and optimization by modifying existing thin films in a localized, high throughput manner.

In this work, LSA is applied to the oxidation of various thin film materials, including transition metals such as Hf and transition metal dichalcogenides such as MoS2. Tunable oxidation is achieved by varying the laser conditions in a controlled oxygen environment, enabling access to a wide range of effective temperatures and heating times. The resulting structural and compositional modifications are characterized using X-ray diffraction, Raman spectroscopy, ellipsometry, UV-vis absorption spectroscopy, and X-ray photoelectron spectroscopy. Applications in the study of optical and electronic materials are presented, including refractive index optimization and the development of materials for neuromorphic device applications.

4:00pm **SE-ThA-8 Towards Reliable X-Ray Photoelectron Spectroscopy: Understanding Fundamental Differences between Analyses Performed on Samples with and Without Electrical Contact to Spectrometer***, Grzegorz (Greg) Greczynski,* Linköping University, Department of Physics, Sweden

X-ray photoelectron spectroscopy (XPS) analyzes of insulators or inhomogeneous samples containing insulating phases are often done with specimens electrically isolated from ground and the surface potential controlled by the flood gun. While such approach offers the possibility of delivering non-distorted spectra, the consequences for the energy level alignment between sample and the spectrometer are often not considered. The present contribution highlights these aspects by discussing several, carefully selected, case studies that visualize fundamental differences between XPS analyses performed on samples with and without electrical contact to ground. Consequences for core level shifts, energy splitting between peaks from different samples, and spectra referencing are discussed in detail. It is shown that the choice of the measurement configuration (samples with *vs*. without contact to the spectrometer) determines to what extent binding energies of core level peaks from conducting and insulating samples (or conducting and insulating phases of the same sample) depend on the specimens' work function. Recognizing these aspects is crucial for the correct spectra referencing and interpretation of core level shifts for series of samples with varying work function.

4:15pm **SE-ThA-9 Lithography-Free Fabrication of Transparent, Durable Glass Surfaces with Embedded Functional Nanostructures***, Iliyan Karadzhov, Rubaiya Hussain, Alessia Mezzadrelli,* ICFO-Institut de Ciencies Fotoniques, Spain*; Wageesha Senaratne, Prantik Mazumder,* Corning Research and Development Corporation*; Valerio Pruneri,* ICFO-Institut de Ciencies Fotoniques, Spain

Glass is central to displays, touchscreens, medical interfaces, and public interactive systems. Integrating additional functions such as antimicrobial activity and mechanical durability to optical clarity is of significant commercial interest which, however, remains challenging. Lithographic techniques provide excellent control over nanoscale geometry and are widely used for surface patterning. However, for applications where random subwavelength features are acceptable, lithography-free routes based on self-assembled metal masks can reduce process complexity and improve compatibility with large-area glass processing.

Among candidate antimicrobial materials, Cu offers well-established ion-mediated antibacterial activity; however, exposed Cu nanostructures are susceptible to wear and optical degradation, limiting their practical use on transparent surfaces. Embedding Cu within glass nanostructures is therefore an attractive strategy to simultaneously enable durability and sustained functionality. In our previous work on abrasion-resistant antireflective glass, thermally dewetted Ag nanoparticles were used to form a Ni nanohole mask for dry etching subwavelength nanoholes into glass. While effective for creating durable antireflective textures, this approach was not suitable for embedding Cu because a selective etchant that could remove the Ni mask without attacking or degrading the embedded Cu could not be identified.

We overcome this limitation by replacing the Ni hard mask with a diluted polymer nanohole mask, enabling wet glass etching and subsequent lift-off of Ti/Cu nanodisks embedded below the glass surface. The resulting surfaces show 80–85% visible transmission, haze below 1%, and near-neutral color. Antimicrobial testing against *E. coli* OP50 shows approximately 99% bacterial reduction after 1 h, while crockmeter abrasion causes no measurable optical change. Future work will optimize geometry and Cu release to improve antimicrobial efficacy toward sanitizer-level benchmarks and validate performance against standard test strains.

Surface Science
Room 305 - Session SS-ThA
Rising Stars

Moderators: Prof. Liney Arnadottir, Oregon State University, **Dr. Dario Stacchiola**, Brookhaven National Laboratory

2:15pm **SS-ThA-1 Restructuring, Fluxionality and Dynamics of Heterogeneous Catalysts in Reaction Conditions from First Principles***, Philippe Sautet,* University of California at Los Angeles **INVITED**

The determination of the surface structure of heterogeneous catalytic systems in reaction conditions is a key aspect for a detailed understanding of the nature of active sites and for the rational design of efficient catalysts. However, catalysts are not static but dynamic, fluxional, metastable and they strongly evolve under reaction conditions, creating new active sites, not present for the as prepared catalysts.

We will show by atomistic modeling that rare, metastable catalytic sites play a paramount role to determine the activity of heterogeneous catalysts. These metastable active sites are created under reaction conditions and are not present for the as prepared catalysts. The first example will concern the nature of active sites for the zirconia on copper inverse catalyst under the conditions of CO_2 hydrogenation to methanol, on a model of highly dispersed Zr oxide clusters on Cu(111). The exploration of reaction-pathways on an ensemble of 83 formate configurations accessible under reaction conditions reveals that structural sensitivity is pronounced, and only 10 of the catalyst configurations are significantly active across the full pathway, with the energy of the methoxy intermediate as a key reactivity descriptor. As a second example we will consider large PtNi nanoparticles (more than 10,000 atoms) for which the 3D local atomic structure and chemical composition was determined by atomic electron tomography. The experimental 3D atomic coordinates have used by first-principles trained machine learning to identify the active sites of the nanocatalysts. A striking feature is the difference of the ORR activity by several orders of magnitude among the surface Pt sites on the nanocatalysts. As a third example we will present the dynamical behavior of large Pt nanoparticles for dehydrogenation and hydrogenation reactions. We found that hydrogen adsorption drives a size-dependent transformation from an amorphous to a crystalline structure, leading to sharp phase transitions for smaller nanoparticles and smooth transformations for larger ones. When modeling alkane dehydrogenation or ethylene hydrogenation, we show a marked discrepancy between the abundance of a surface site and its catalytic contribution, indicating that the active sites are rare, not the most common sites.

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2:45pm **SS-ThA-3 Probing Dynamic Catalytic Interfaces: Structure, Evolution, and Function***, Gengnan Li,* Center for Nanoscale Materials, Argonne National Laboratory

Catalytic reactions often occur at interfaces, which are inherently dynamic under operating conditions. Capturing the dynamic structural, electronic, and chemical evolution of these interfaces under relevant reaction environments is therefore critical for developing a fundamental understanding of structure-performance relationships in catalysis. Recent advances in multiscale in situ and operando characterization techniques have redefined the traditional structure – function paradigm by providing comprehensive insights into the local coordination environment, electronic

structure, and dynamic behavior of material surfaces and interfaces. In this talk, I will present our recent work on the controlled engineering of IrO_x-CoO_x interfaces in $IrCoO_x$ electrocatalysts to improve IrO_x dispersion and reduce the overall cost of hydrogen production. Combined spectroscopic and microscopic analyses reveal distinct electronic structures and surface arrangements arising from different interfacial architectures. In situ spectroscopic measurements further identify the catalytic interface as an active, dynamically evolving region that governs reaction activity and selectivity. We show that interfacial defect populations, coordination environments, and metal-support interactions reorganize in response to the reaction environment, leading to emergent structure-function relationships that cannot be deduced from post-reaction analysis alone. These measurements provide unprecedented opportunities to elucidate the underlying reaction mechanisms under operating conditions.

3:00pm **SS-ThA-4 Site-Specific Deuterium Adsorption in Nitrogen-Doped Graphene and Porous Carbon Materials**, *Buddhika S. Alupothe Gedara, Peter S. Rice, Prescott Evans, Tom Autrey, Bojana Ginovska, Mi Yeon Byun, Zdenek Dohnálek,* ***Zbynek Novotny,*** PNNL

Nitrogen-functionalized carbon materials are investigated as promising candidates for hydrogen activation and storage. However, the role of specific nitrogen functionalities in facilitating hydrogen adsorption and activation remains poorly understood. To address this scientific gap, we investigated deuterium adsorption on three model systems: N-doped highly-oriented pyrolytic graphite (N-HOPG), N-doped graphene/Ru(0001), and porous nitrogen-carbon (NC) synthesized by pyrolysis of glucose and graphitic carbon nitride. For the first two systems, a variable N concentration was introduced using ion irradiation. Nitrogen incorporation occurs preferentially in two configurations: graphitic N (GN; N substituted in the hexagonal C lattice), and pyridinic N (PN; substitutional N adjacent to a C vacancy). The relative concentrations of GN and PN can be controlled by varying the ion dose, annealing temperature, and the choice of substrate [1,2]. Atomic deuterium was generated by D_2 cracking over a hot tungsten filament. For all probed materials, X-ray photoelectron spectroscopy showed that D exposure at 220 K induces a shift of the PN peak (398.0 eV) to higher binding energy by +1.1 eV, while the GN peak (400.6 eV) remains unchanged, demonstrating that deuterium binds selectively to PN sites. A near complete saturation of PN sites with D atoms was observed for N-HOPG (85%). Only a partial saturation of PN sites was observed for N-doped graphene/Ru(0001) (30%, due to the necessity to cleave the N-Ru bond before D adsorption) and in porous NC (6%, consequence of limited accessibility due to pore confinement effects). Deuterium fully desorbed from N-HOPG above 900 K, whereas on N-doped graphene/Ru(0001), a complete D desorption from PN is observed at ~700 K, indicating that the Ru metal weakens the N-D bond strength [2]. Moreover, the NC exhibited nearly the same desorption behavior as N-HOPG, demonstrating that well-defined model systems can effectively capture the behavior of more complex N-doped carbon materials, providing insight into the role of nitrogen dopants in hydrogen activation at carbon surfaces and interfaces.

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3:15pm **SS-ThA-5 Developing a Nanoscopic Understanding of Electronic Metal-Support Interactions: From Model Systems to Powder Catalysts**, *Lindsey Penland, Hirushan Hetti Arachchige, Nadith Dissanayake,* ***Rachael Farber,*** University of Kansas

Electronic metal-support interactions (EMSI), characterized by charge transfer across the metal/support interface, are often cited as an origin of enhanced selectivity and efficiency for oxide-supported metal nanoparticle catalysts. The coexisting factors influencing EMSI makes it difficult to predict EMSI in oxide-supported metal nanoparticle systems. This presentation will highlight recent work investigating EMSI in **1)** model TiO_2(110) catalysts and **2)** Mo/KIT-6 powder catalyst samples.

Rutile TiO_2(110) was used as a model oxide support to determine the spatially resolved electronic consequences of Cu nanoparticle size and defect density on EMSI. Using a combination of scanning tunneling microscopy (STM), scanning tunneling spectroscopy (STS), and dI/dV mapping, a pristine and intentionally defected TiO_2(110) surface was characterized to reveal the relationship between local coordination environment and the observed local density of states (LDOS). On the pristine TiO_2(110) surface, STS measurements highlighted the attenuation of the LDOS at the Cu/TiO_2(110) interface and within a fixed distance of the Cu particle, suggesting that the region beyond the immediate metal/oxide interface may be significant for chemical activity. Ongoing work focuses on understanding how the increased defect density of the sputtered TiO_2(110) surface influences the thermal stability of Cu nanoparticles and the LDOS of the Cu/TiO_2(110) system. Preliminary results suggest increased thermal stability of adsorbed Cu on the sputtered TiO_2(110) surface while dI/dV mapping indicates unique electronic features due to the incorporation of Cu nanoparticles on the sputtered TiO_2(110) surface.

In an effort to bridge the materials gap between ideal systems and actual catalysts, powder Mo/KIT-6 catalysts, shown to be effective for propylene epoxidation, were investigated with STM and STS. STM data demonstrated that Mo nanoparticles decorate the KIT-6 surface for high loading (1.5wt%) catalysts while the low loading catalyst (0.5wt%) has dispersed Mo adsorbates. Interestingly, the low loading catalyst was shown to be more active towards propylene epoxidation, suggesting that isolated Mo sites are more active than Mo nanoparticles. STS data of KIT-6 and the Mo/KIT-6 powders demonstrate the emergence of electronic states within the bandgap of KIT-6 for both low and high loading catalyst samples, suggesting a surface-wide attenuation in the LDOS following the incorporation of Mo onto the KIT-6 support. These results contribute to the structural and electronic characterization of the Mo/KIT-6 surface, providing deeper insight into the origins of observed chemical activity.

3:30pm **SS-ThA-6 Reconciling Metal Coordination in g-C_3N_4-based Single Atom Catalysis: A Surface Science Study of Melem-Metal Interactions on Au(111)**, ***Faith Lewis,*** TU Wien, Austria*; Nicolò Allasia,* Polytechnic University of Milan, Italy*; Ola Alayan,* IMEM-CNR and Università degli Studi di Genova, Italy*; Moritz Eder, Viktoria Waidbacher, Margareta Wagner,* TU Wien, Austria*; Letizia Savio,* IMEM-CNR and Università degli Studi di Genova, Italy*; Gianvito Vilé,* Polytechnic University of Milan, Italy*; Gareth S. Parkinson,* TU Wien, Austria

Single-atom catalysis (SAC) is a rapidly growing field of research that combines the advantages of solid supports from heterogeneous catalysis with the tunability of active sites in homogeneous catalysis. SACs also lead to well-defined single-atom centers which can achieve high selectivity. Recently, graphitic carbon nitride (g-C_3N_4) has been identified as a framework to stabilize SACs that facilitate reactions such as the ORR and HER. The precursor, melem (2,5,8-triamino-heptazine) is typically polymerized, and the resulting structure features a network of 6-fold nitrogen pockets which stabilize the single atoms. The g-C_3N_4 framework is a common conceptual baseline for these catalysts, yet its structural specifics are increasingly debated, with recent studies directly challenging the prevailing model.[1] X-ray absorption spectroscopy (XAS) suggests a 4-fold metal coordination with equal bond lengths, a geometry that cannot exist within the often-proclaimed 6-fold pocket of g-C_3N_4.

In this work, we use the surface science approach to reconcile this contradiction through scanning probe microscopy (SPM) and X-ray photoelectron spectroscopy (XPS). On an Au(111) single crystal, melem forms a honeycomb overlayer that is stabilized through hydrogen bonding of the amino groups on the corners with the pyridinic nitrogens on the sides of the triangular molecule. When melem and metals, specifically Ni and Fe, were co-deposited at various temperatures onto Au(111), different overlayers formed. At lower temperatures, more densely packed regions of the same triangular features form next to the honeycomb structure. At higher temperatures, two different motifs form depending on the metal. With Fe, the densely packed regions observed at lower temperatures dominate, while for Ni a new structure appears in which the triangular melem molecules are no longer recognizable on the surface. We conclude this is the result of polymerization and formation of a 2D layer.

Our results indicate that, under these conditions, the Fe-melem species forms dimeric complexes centered by a metal atom. The resulting square-planar coordination environment aligns closely with recent XAS observations, offering a structural explanation for the 4-fold coordination.

1. Allasia, Nicolò, Shuai Xu, Sadaf Fatima Jafri, et al. 2025. “Resolving the Nanostructure of Carbon Nitride-Supported Single-Atom Catalysts.” *Small* 21 (23): 2408286. https://doi.org/10.1002/smll.202408286.

3:45pm **SS-ThA-7 Exploring Reactive Oxygen Species for Epoxidation on AgCu Bimetallic Surfaces**, ***Ashleigh Baber,*** James Madison University

Surface science provides a powerful framework for exploring the fundamental nature of model heterogeneous catalysis, with the goal of enhancing reactivity, improving selectivity, and identifying active sites. Our research group utilizes ultrahigh vacuum temperature-programmed

reaction spectroscopy to probe catalytic reactivity, complemented by low-temperature scanning tunneling microscopy for atomic-scale visualization of model catalysts. We explore the role of hydroxyl groups as reactive oxygen species in the epoxidation of ethylene and propylene over Ag/Cu(111) model catalysts. The presence of Ag and hydroxyls promotes selective partial oxidation to epoxides while suppressing overoxidation to combustion products. By elucidating the relationship between surface structure and catalytic activity, this work contributes to the rational design of more efficient catalysts for industrial applications enhancing performance, reducing waste, and mitigating CO_2 emission.

4:00pm **SS-ThA-8 Peter Mark Award Talk: Tip-Enhanced Raman Spectroscopy with Scanning Ion-Conductance Microscopy**, ***Naihao Chiang***[1], University of Houston **INVITED**

Tip-enhanced Raman spectroscopy (TERS) combines the single-molecule chemical sensitivity of surface-enhanced Raman spectroscopy with the nanoscale spatial resolution of scanning probe microscopy. Over the last decade, TERS has achieved Angstrom-scale spatial resolution under ultrahigh-vacuum conditions, making it a powerful tool for investigating surface-bound species. To extend this technique to soft samples in an electrolytic environment, such as *in vitro* biological samples, scanning ion-conductance microscopy (SICM) was selected as the platform for integrating TERS. In this presentation, I will provide the background and instrumentation design principles that enable SICM-TERS, along with examples of proof-of-concept systems. Additionally, the plasmonically enhanced near-field in SICM-TERS can be used to deliver intracellular cargo with single-cell precision; examples on human T-cells will be discussed. In the future, we expect this newly developed SICM-TERS platform to provide chemical information at interfaces in regimes that conventional techniques find challenging to access.

Vacuum Technology
Room 321 - Session VT-ThA

Vacuum Technology Flow and Pumps

Moderators: Dr. Marcello Juni Ferreira, ESS, **Marcy Stutzman**, Jefferson Lab

2:15pm **VT-ThA-1 Vacuum Technology in Cork Science: From Permeability to TCA Desorption**, ***Orlando Teodoro***, Nova School of Science and Technology, Portugal **INVITED**

Natural cork has been used for centuries as a high–performance sealing material for wine bottling due to its elasticity, durability, tightness to liquids, and naturally low gas transmission. In addition to being a renewable and recyclable material, cork combines mechanical resilience with a unique cellular structure that enables long-term sealing performance. However, the cork industry has historically faced important challenges related to the variability of sealing performance at the cork–bottle interface and to the presence of trace contaminants responsible for wine defects, particularly 2,4,6–trichloroanisole (TCA), the main compound associated with cork taint. TCA is of particular concern because it can migrate from cork to wine, producing sensory defects at concentrations as low as 2–3 ng/L.

This work presents several applications of vacuum technology developed and introduced for cork science and industrial processing over the last two decades. The first topic addresses the characterization of gas and vapor permeation through cork using vacuum-based methods. Permeability measurements performed under controlled pressure conditions enabled the study of transport mechanisms in natural cork and supported the development of transport models accounting for the permeation of gases and vapors through the cellular cork structure.

The second topic focuses on the sealing performance of cork stoppers in bottlenecks and on the role of surface treatments and lubricants. Vacuum-based leak testing methods were used to characterize sealing performance at the cork–glass interface, revealing leak rates ranging from below 10^{-7} mbar·L/s for well-sealed stoppers to above 10^{-5} mbar·L/s for poor sealing conditions.

The third topic concerns the interaction of TCA with cork and the development of large-scale vacuum-based thermal desorption processes for contaminant removal. Experimental studies combining controlled heating, vacuum exposure, and gas analysis provided insight into the desorption behavior of TCA and its interaction with the cork structure. These studies contributed to the development of industrial processes capable of efficiently reducing TCA contamination while preserving the physical integrity and performance of the cork.

The work illustrates how vacuum technology evolved from a laboratory research tool into an enabling industrial technology in the cork sector. These developments contributed to substantial improvements in cork quality control, contaminant removal, and sealing consistency, playing a significant role in the modernization of the cork industry over the last decades.

2:45pm **VT-ThA-3 Gas Transport in 3D-Printed Polymers: Linking Microstructure to Outgassing and Permeation Behavior**, ***Sefer Avdiaj***, University of Prishtina, Kosovo; *Zgjim Rrustemi,* University of Prishtina. Department of Physics, Kosovo; *Ramiz Hoti,* University of Prishtina. Department of Chemistry, Kosovo; *Partizan Malkaj,* Polytechnic University of Tirana. Department of Physics, Albania; *Zeqe Tolaj,* University of Prishtina. Department of Physics, Kosovo; *Makfire Sadiku,* University of Prishtina. Department of Chemistry, Kosovo

Additive manufacturing is opening new possibilities for producing polymer components with complex and customized geometries. However, their use in vacuum environments is still limited by gas transport effects such as diffusion, permeation, and outgassing. In this study, we investigate how the microstructure created during 3D printing influences gas transport behavior in commonly used polymers.

Samples are being fabricated using fused deposition modeling (FDM), with systematic variation of key printing parameters such as infill density, layer thickness, and raster orientation. These parameters are expected to significantly affect the internal structure of the materials, including porosity, interlayer bonding, and anisotropy. Gas diffusion and permeation are being measured using steady-state and time-lag methods, while outgassing behavior is evaluated under controlled vacuum conditions.

Preliminary results indicate that gas transport properties are strongly influenced by printing-induced microstructure. Early observations suggest that increased porosity and weaker interlayer bonding lead to higher permeation and outgassing, while optimized processing conditions reduce gas release. Ongoing work is focused on obtaining quantitative relationships between processing parameters, microstructure, and transport properties.

The expected outcomes of this study will provide a deeper understanding of gas transport mechanisms in 3D-printed polymers and establish guidelines for improving their performance in vacuum and low-pressure applications. This work aims to support the development of additively manufactured components suitable for vacuum technology.

3:00pm **VT-ThA-4 Study on the Influence of Different Combinations of Roots Pump Sets on Flow Characteristics**, ***Shengquan Yang***, *Kun Liu,* Northeastern University, China

Abstract: The multi-stage series Roots pump set has broad application prospects in fields such as nuclear fusion vacuum systems, semiconductor manufacturing, aerospace environment simulation, and large-scale scientific devices due to its advantages of high pumping speed, high compression ratio, no oil pollution, and suitability for high flow gas transportation. By operating in series with multi-stage pump bodies, the working pressure range of the pump group can be significantly expanded, the ability to extract light gases can be improved, and the demand for efficient pumping under complex working conditions can be met. However, the internal flow process of multi-stage Roots pump sets is complex, and phenomena such as gas transport, pressure distribution, and reflux leakage between stages are coupled with each other. The matching relationship between different stages has a significant impact on the pumping speed, compression ratio, and operational stability of the pump set. Especially under conditions of high speed, large pressure difference, and light gas, significant issues such as increased flow loss, uneven inter stage flow field, and local temperature rise are prone to occur within the pump unit, which in turn affects the overall pumping performance and long-term operational reliability. This study is based on computational fluid dynamics methods to establish a transient flow model for multi-stage Roots pump sets. Numerical simulations were conducted on the inter stage flow field, pressure distribution, and gas transport process of the pump sets, and the flow characteristics and pressure distribution laws of different combinations of pump sets under different operating conditions were analyzed. The research results indicate that as the compression ratio increases from 10 to 1000, the inter stage pressure difference significantly increases, and the clearance reflux velocity and reflux rate significantly increase; The heat generation effect of gas compression is enhanced, and the inter stage temperature at a compression ratio of 1000 is significantly higher than that at a compression ratio of 10; And the highest temperature occurs in the

[1] **Peter Mark Memorial Award Winner**

stage before the exhaust stage, not in the final exhaust stage, indicating that this stage has undergone the strongest gas compression and thermal accumulation; The gap between Roots rotors decreases, resulting in a decrease in leakage, but the reflux velocity increases, leading to an increase in inter stage pressure. This study provides a theoretical basis

3:15pm **VT-ThA-5 NAVAC Vacuum Technology: Old Problems. New Architecture. NAVAC HelixDrive Screw Pumps and NAVAC ShieldDrive Mag-Coupled Rotary Vane Pumps***, Evan Sawyer,* NAVAC

Part One: HelixDrive Series — Dry Screw Technology Reimagined

Dry screw vacuum technology has existed for decades. Two intermeshing rotors trap and compress gas without contact — no oil, no sealing fluid. The concept is sound. The execution has historically been the problem. Traditional dry screw pumps are large, thermally complex machines with gearboxes and couplings that demand as much management attention as the processes they serve.

The HelixDrive series starts differently. Its coaxial design integrates motor and pump along a shared axis, eliminating mechanical interfaces and achieving the smallest dry screw form factor at this performance level.

The HD series reaches an ultimate pressure of 7.5×10^{-4} torr — challenging oil-sealed rotary vane pumps and exceeding most dry screw designs. A proprietary internal coating provides chemical resistance in corrosive, moisture-laden environments, sustaining performance over time. Thermal management is integrated: smaller models use onboard air cooling; the HD100 uses water cooling limiting surface temperature rise to under 50°F, keeping performance predictable.

Maintenance is largely eliminated. No tip seals means no wear, no particulate, no contamination risk. No oil means no changes, no mist filters, no backstreaming.

Part Two: ShieldDrive SDi Series — Rotary Vane Done Right

Oil-sealed rotary vane technology is proven but carries known liabilities: shaft seal leakage, oil mist in the workspace, messy maintenance, and degradation in chemically aggressive environments.

The SDi series engineers those problems away. A magnetic drive coupling replaces the dynamic shaft seal entirely, creating a hermetic boundary with no leakage path. An integrated oil mist filter — built into the pump body — captures exhaust droplets and doubles as an exhaust muffler, with tool-free quick-change access. An integrated drip tray handles maintenance mess. A detachable oil reservoir replaces drain plugs with a clean swap. Due to the magnetically coupled seals, there is no need for the "Cookie sheets" underneath the rotary pump. Additionally, the simple addition of the oil reservoir allows for a quick oil change without having to move the pump or use a separate container to trap the oil.

Gas ballast is adjustable for condensable vapor processes. The variable-frequency drive enables Eco Mode, reducing speed, energy draw, and noise during lower-demand operation. Another innovation that allows for lower energy consumption when the pump doesn't need to run at full capacity.

3:30pm **VT-ThA-6 From Experiment to Grid: A Systems Engineering Approach to Vacuum Pumping Systems in Stellarators***, Danah Garcia,* Type One Energy Group, Inc.

The fusion industry sits at a pivotal point in its trajectory from experimental reactors to power plant devices. The Infinity Two Stellarator is currently in design by Type One Energy. Part of the risk mitigation platform on Infinity Two will be conducted with the Infinity One device, a smaller scale stellarator that will help reduce physics and engineering uncertainties in fusion power plant design. Employing systems engineering fundamentals is crucial for mobilization of the industry, and special attention should be paid to systems that are integral to the power output of the device, namely the vacuum pumping system (VPS). The VPS interfaces with the plasma chamber and the tritium plant, linking the fuel processing system with the main reaction chamber of the device. As this link, the VPS is responsible for continuous exhaust of deuterium, tritium, helium and other plasma impurities, and helps maintain a burning plasma in the reactor, which is necessary for net energy out of the power plant. Type One Energy's VPS on the Infinity One fusion device will serve as an integrated design verification testbed for the Infinity Two stellarator, with demonstration of plasma particle exhaust as a key objective. The Wendelstein 7-X (W7-X) stellarator is the largest, most technologically advanced stellarator in the world, however its design is best suited for exploration of magnetic configurations, rather than particle exhaust. Demonstration of enhanced particle exhaust in Infinity One over W7-X will help solidify Infinity One's purpose of risk reduction, with emphasis on increased particle flux out of the plasma chamber and achieving target subdivertor pressures. With respect to the VPS, advancing the technology readiness level of high throughput vacuum pumping systems with fusion fuel present is critical. This work will demonstrate the scalability of the VPS from the Infinity One device to a reactor-scale device, exemplifying the need for risk mitigation in the transition of the fusion industry from the laboratory to the grid.

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3:45pm **VT-ThA-7 Measuring Rf Surface Resistance of Non-Evaporable Getter Coatings***, Eleni Marshall, Oleg Malyshev, Daniel Seal, Reza Valizadeh,* STFC Daresbury Laboratory, UK

A new method for measuring the RF surface resistance of non-evaporable getter (NEG) coatings on tubular samples has been developed at Daresbury laboratory.

NEG coatings are vital for achieving good pressures in vacuum systems with limited conductivity but will reduce the RF surface conductivity of the vacuum chamber when compared with the substrate material. For purposes such as particle accelerator chambers, this is important as the increased surface resistance can cause a loss in beam energyand increase in beam energy spread.

With this method, both the surface resistance and the NEG pumping properties can be measured from the same sample, allowing a full quantification of NEG properties.

This study compares samples of TiZrV of different thickness and microstructure, to see the relationship between NEG surface resistance and pumping properties.

4:00pm **VT-ThA-8 Feasibility of Turbomolecular Deceleration as an Intrinsic Measurement of System Pressure***, Andrew Chew, Paul Smith, Sam Lodge,* Edwards Ltd, UK*; James Healy,* University of Bristol, UK

When the drive power to a turbomolecular pump (TMP) is halted the TMP decelerates at a rate dependent upon various parameters/variables. These include TMP impeller mass, original rotational speed, suspension type, inlet and exhaust pressure and pumped gas type. Also and crucially, the TMP pumping configuration in terms of number of turbomolecular blade rows and drag stage numbers and types. We will report measurements of dependency of different TMPs on these variables and the feasibility of indicative pressure readings.

Patent Application: GB1902564.2

4:15pm **VT-ThA-9 Single-Stage Vacuum Pump Performance Measuring Method***, Xiaoyu Chi, Kun Liu, Dechun Ba, Yuanhua Xie,* Northeastern University, China

Traditional dry pump measurement devices usually focus on the entire vacuum pump performance parameters other than vacuum pump interior flow situation .This paper propose a performance test method for testing a single stage of a vacuum pump, concentrating on four basic physical quantities ; flow, vacuum degree ,temperature and rotating speed. For a better description of the measurement method , this test method is divided into six modules: the pump inlet test doom module, the pump outlet test doom module, the pressure measurement module, the temperature measurement module,the flow measurement module and the rotating speed measurement module. This method ensures the normal operation and parameter measurement of the single-stage vacuum pump by adjusting the pressure range of the front and rear vacuum dooms so that we can measure the flow field inside the single rotor and the specific measurement parameters to fit pumping speed - pressure curve and other parameter curves. The pressure, flow, temperature and rotating speed measurement ranges of the test method are 10^{-3}~10^{5} Pa, 20 SCCM~5000 SLM , 20℃~300℃and 100 rad/s~3000 rad/s. Compared with the traditional vacuum pump measurement method, the measurement method of the single-stage vacuum pump proposes a performance parameter to measure the internal flow field of the first-stage rotor of the multi-stage vacuum pump and the related parameters to provide design reference and experimental data support and rotor profile design for the rotor combination of the multi-stage vacuum pump.

2D Materials
Room Ballroom A - Session 2D-ThP
2D Materials Poster Session

2D-ThP-1 Electrochemical Lithium Intercalation Cycling-Induced Phase Transition of 2H-MoS_2 to 1T and delayed Reversion to the 2H Phase, ***Yerin Hong***, *Juhwan Lim, Jinhong Min,* University of Michigan, Ann Arbor, Republic of Korea*; Nishkarsh Agarwal,* University of Michigan, Ann Arbor, India*; Robert Hovden,* University of Michigan, Ann Arbor*; Ageeth Bol,* University of Michigan, Ann Arbor, Netherlands*; Yiyang Li,* University of Michigan, Ann Arbor

In this study, we investigated the phase transition behavior of molybdenum disulfide (MoS_2) during and after repeated lithium intercalation and deintercalation cycles, motivated by its potential for energy storage and electronic applications. MoS_2 undergoes a phase transition from the 2H (trigonal prismatic) to the 1T (octahedral) phase upon lithium insertion. After cycling with galvanostatic cycling with potential limitation (GCPL) and using Raman spectroscopy, we confirmed that the 1T phase persisted even after most lithium was removed. Interestingly, a spontaneous reversion of the 1T phase to the 2H phase was observed over time. Raman spectroscopy results showed a significant decrease in 1T phase peaks for cycled MoS2, with the phase converted to 2H after resting periods for several days. Additionally, electrochemical cycling of the cycled MoS_2 flakes revealed lithium potential profiles was comparable to pristine MoS_2, reinforcing the evidence of spontaneous phase reversion. These results demonstrate the metastable nature of the 1T phase and structural evolution of MoS_2 upon and after lithium intercalation cycling. In addition, these findings can provide key insights into the potential strategies of the precise phase control for energy storage and electronic applications, or to synthesize endotaxial structure with distinct quantum states.

2D-ThP-2 Controlling Sputtering Energy Threshold in TMD Plasma Processing via Surface Functionalization and Cryo Temperatures, ***Yury Polyachenko***, *Sofiia Yarytska,* Princeton University*; Yuri Barsukov, Shoaib Khalid, Igor Kaganovich,* Princeton University Plasma Physics Lab

Transition metal dichalcogenides (TMDs) are a novel class of quasi-2D materials with potential applications in smaller semiconductor chips, nanoscale piezoelectric biosensing, and more. However, their manufacturing consists of many steps and poses various currently unsolved challenges.

In this study [1], we perform a computational investigation of a TMD manufacturing stage with low-energy plasma-assisted desorption and etching of MoS_2. First, we systematically select an appropriate level of theory and employ a combination of equilibrium and non-equilibrium ab initio molecular dynamics (AIMD) simulations to identify the geometric regions of MoS_2 that exhibit the highest susceptibility to damage induced by plasma particles. We provide energy thresholds for sputtering and investigate their dependence on the incident angle. We show how oxidation and fluorination of MoS_2 into MoS_2O and MoS_2F can lower the sputtering energy thresholds from ~30eV to ~10eV. Such functionalizations expand the energy range where plasma is expected to desorb the target TMD top layer without damaging the metal scaffold. Additionally, the threshold values for MoS_2O and MoS_2F exhibit distinct dependencies on temperature and impact angle, indicating that variation of these parameters could enable precise and selective etching.

We predict a previously unobserved temperature-dependent behavior of the sputtering threshold in MoS_2O at cryo temperatures ~100-200K. We propose a multistage sputtering mechanism to explain this newly observed trend by its connection to threshold sensitivity to impact angle: from ~14eV for a normal $\theta \approx 0°$impact to ~7eV for a $\theta \approx 20°$impact. We validate the underlying hypothesis through numerical AIMD simulations. We further demonstrate that the proposed mechanism is not restricted to MoS_2 but is also operative in $MoSe_2$, WS_2, and WSe_2.

Acknowledgment: This research was supported by the U.S. Department of Energy, Office of Science, Fusion Energy Sciences and Basic Energy Sciences, as part of Microelectronics Science Research Center (MSRC) through the Plasma-enabled 2D Materials project at the Princeton Plasma Physics Laboratory (PPPL), under contract number No. DEAC02-09CH11466.

[1] Yury Polyachenko, Yuri Barsukov, Shoaib Khalid, Igor Kaganovich; J. Phys. Chem. Lett. 2026, 17, 18, 5207–5214 , https://doi.org/10.1021/acs.jpclett.6c00348

2D-ThP-3 Graphene/MoS_2 Au Nanoparticle Floating-Gate Memristor Arrays for Low-Power Neuromorphic Systems, ***Sabeen Hong***, *Woo Jong Yu,* Department of Electrical and Computer Engineering, Sungkyunkwan University, Republic of Korea

Recent progress in neuromorphic computing has highlighted the need for device platforms capable of performing memory and computation in an energy-efficient manner. In conventional von Neumann architectures, the physical separation of memory and processing units causes data-transfer bottlenecks and considerable energy waste, ultimately limiting computational speed. As an alternative approach, memristive devices have attracted attention because their tunable conductance states can emulate synaptic weight modulation. In this work, we demonstrate a low-power neuromorphic system based on gold nanoparticle floating-gate memristors (AuNp-FGMs).

The AuNp-FGM is designed using graphene as the floating gate and MoS_2 as the channel material. By inserting gold nanoparticles between the floating gate and tunneling oxide, a two-terminal memristor structure was fabricated. The device operates within the ±3 V range, and its conductance modulation is governed by changes in the Fermi energy level (E_f) of graphene. Owing to this floating-gate-based charge modulation mechanism, the AuNp-FGM exhibits reliable memory behavior and analog switching characteristics suitable for neuromorphic applications.

The fabricated device shows an on/off ratio exceeding 10^6, data retention for over 9 hours, and endurance over 80,000 cycles. In addition, the device exhibits low cycle-to-cycle variability, with a Cv of 3.6% measured from 90 cycles, where Cv = σ/μ, σ is the standard deviation, and μ is the mean value. The synaptic update characteristics were further evaluated through multi-level potentiation and depression. For 100-level potentiation using +4 V pulses with a duration of 0.5 s, the non-linearity factor ranges from 0.1 to 0.6. For 100-level depression using −3 V pulses with a duration of 0.2 s, the non-linearity factor ranges from 2.3 to 4.6, measured from 15 devices. Similar modulation behavior was also observed when the number of input pulses was varied to 50, 100, 200, 300, and 400.

To evaluate the applicability of the AuNp-FGM to system-level neuromorphic operation, a neuromorphic array composed of 2 neurons and 32 synapses was constructed. The array was tested using three input patterns: horizontal, vertical, and diagonal. Through 40 learning simulations, the total energy consumption was calculated to be 70 μJ. This corresponds to a 97% reduction in energy consumption compared with previous experiments. These results indicate that graphene/MoS_2-based AuNp-FGM arrays provide a promising platform for low-power neuromorphic systems by combining reliable floating-gate memory characteristics with efficient synaptic weight modulation.

2D-ThP-4 Inhibition of Alumina Atomic Layer Deposition on Modified 2D van der Waals Material $CrPS_4$, ***Marissa Piña***, *Andrew Teplyakov,* University of Delaware

$CrPS_4$ is a 2D van der Waals material in the ternary transition metal chalcogenide (TTMC) class of compounds. As an A-type antiferromagnetic semiconductor, thin $CrPS_4$ flakes a few layers thick can display net or zero magnetization depending on whether there is an odd or even number of layers. The combination of 2D magnetic materials such as $CrPS_4$ with topological insulators such as atomic layer deposition (ALD)-grown alumina has potential as a magnetic tunnel junction in spintronics devices including magnetic RAM, but has seldom been studied to date.

We have analyzed the atomic layer deposition of alumina on mechanically exfoliated $CrPS_4$ flakes before and after modification with acetylacetone (acacH) at room temperature and at 140 °C. The modifications seem to result in inhibited alumina growth, which was very unexpected considering alumina grows rapidly on most surfaces. In both cases, the alumina grown on the modified $CrSP_4$ surface may experience a growth delay of over 1 nm [determined by ToF-SIMS depth profiling after 60 cycles of water and trimethylaluminum (TMA) at 130 °C] and a smoother surface compared to alumina grown on the unmodified surface.

The difference in unmodified versus modified alumina growth is likely related to defects which provide nucleation sites for ALD growth. The defects are potentially passivated by the acacH modification. The acac-containing fragments, including $Cr(acac)^+$, that indicate a successful modification appear uniformly across the $CrPS_4$ flakes in ToF-SIMS ion images. Additionally, AFM of the $CrPS_4$ flakes after these modifications and after alumina ALD reveal a nearly atomically smooth surface, possibly indicating uniform coverage.

The alumina growth could be more efficient on unmodified surfaces because TMA decomposes or builds up at the defects, as we observed clusters of CH^- and AlO_2^- fragments on the $CrPS_4$ surface by ToF-SIMS that become larger after higher numbers of ALD cycles. This means that the acacH modification could result in a more perfect interface and a better alumina film. This process also has potential applications in area-selective ALD, since alumina growth on $CrSP_4$ can be slowed with a simple modification, especially when you couple the current findings with the fact that the number of $CrPS_4$ layers can be controlled by an atomic layer etching (ALE) process.

2D-ThP-5 Investigation of Phase Separation of Mixture of Oil and Water in Monte Carlo Simulation, ***Mehabaw Fikrie***, Gondar, Ethiopia; *Tibebe Birhanu,* Catholic University of Korea, Ethiopia

Phase separation, the spontaneous segregation of a homogeneous mixture into distinct phases with different physical and chemical characteristics, is a fundamental phenomenon in soft matter physics, materials science, and energy-related technologies. Understanding the microscopic dynamics of immiscible fluid systems such as oil-water mixtures is increasingly important for advancing enhanced oil recovery (EOR), chemical processing, and emerging computational material design. In this study, Monte Carlo (MC) simulation techniques were employed to investigate phase separation behavior in mixed oil-water particle systems under varying thermodynamic and spatial conditions. Simulations were performed for particle systems ranging from 500 to 2,500 particles with interval 500 within square simulation domains of side lengths 25–40 units with 5 unit interval. Critical parameters including box size, particle density, interaction strength, and simulation time were systematically analyzed to evaluate their effects on phase evolution and stability. The findings reveal that a system with box size L = 30 and particle number N = 2000 exhibits the clearest and most stable phase-separated structure. Increased particle interactions and larger system sizes significantly enhance the transition from homogeneous dispersion to well-defined phase domains. Furthermore, extended equilibration times improved the sharpness and stability of interfaces, with optimal separation observed at MCstep = 10^6. The results provide valuable computational insights into molecular-scale phase dynamics, wettability control, and interfacial phenomena. This work demonstrates the growing role of computational modeling and simulation in emerging trends of science and technology, particularly in energy optimization, advanced materials research, and intelligent fluid-system engineering.

Keywords: Oil-water mixture; Phase separation; Monte Carlo simulation; Box size; Particle number

2D-ThP-6 Strain-Tunable Mid-Infrared Optical Absorption in Bilayer Silicon for Silicon-Compatible Photonics, ***Kumar Vishal,*** Wright University

Two-dimensional bilayer silicon (BLSi) offers a silicon-compatible platform for extending integrated photonics into the mid-infrared, but its optical response remains strongly governed by strain-induced structural and electronic transitions. In this work, density functional theory calculations are used to evaluate the strain-dependent optical properties of AA-stacked BLSi under biaxial in-plane tensile strain, with optical absorption and refractive index calculated for in-plane polarization by including interband and intraband transitions.The results show that tensile strain drives a structural transition from a low-buckled bilayer lattice to a buckle-free honeycomb configuration at approximately 5.17% strain. This transformation removes the out-of-plane buckling and produces an abrupt increase in the refractive index, demonstrating the strong coupling between atomic geometry and optical response. In the buckle-free phase below the large-strain bandgap-opening threshold, the optical absorption edge remains pinned near 1.14 μm, indicating a strain-resistant transition at the M point. When the strain exceeds approximately 12.26%, both direct and indirect energy bandgaps open, and the direct-gap-associated interband transition moves into the mid-infrared. By increasing strain, the absorption peak redshifts across a broad wavelength range from about 1.5 to 11.5 μm, while the refractive index increases sharply and exhibits mid-infrared dispersion linked to these interband transitions.These findings identify strain as an effective tuning parameter for controlling the mid-infrared optical behavior of bilayer silicon. The predicted broadband tunability, silicon compatibility, and strong strain-dependent absorption suggest that BLSi could provide a pathway toward CMOS-compatible mid-infrared photodetectors and integrated silicon photonic components without relying on heterogeneous III-V or II-VI absorber integration.

2D-ThP-7 Nanoscale Friction in Exfoliated SnSe and $SnSe_2$ Two-Dimensional Materials, ***Mehmet Ozdogan,*** *Thomas Iken, Deniz Cakir, Nuri Oncel,* University of North Dakota

Two-dimensional layered materials are promising candidates for solid-state lubrication because weak interlayer van der Waals interactions can enable low-resistance sliding at micro- and nanoscale contacts. While graphene and transition-metal dichalcogenides have been widely studied in this context, the tribological response of layered tin chalcogenides remains comparatively unexplored. Here, we investigate the nanoscale frictional properties of mechanically exfoliated SnSe and $SnSe_2$ nanoflakes using atomic force microscopy-based lateral-force microscopy, supported by X-ray photoelectron spectroscopy and first-principles calculations.

SnSe and $SnSe_2$ flakes were exfoliated onto SiO_2 substrates and measured under ambient conditions using calibrated lateral-force microscopy. Graphene flakes of comparable thickness were measured under the same conditions as a reference solid lubricant. Friction maps and load-dependent lateral-force measurements show that both SnSe and $SnSe_2$ exhibit low friction coefficients, with values of 0.023 ± 0.004 and 0.027 ± 0.019, respectively, compared with 0.042 ± 0.060 for graphene. These results indicate that Sn-based layered chalcogenides can provide frictional performance comparable to or better than commonly studied two-dimensional lubricants under ambient conditions.

To understand the microscopic origin of the measured friction trends, density functional theory calculations were performed for pristine and oxygen-modified SnSe and $SnSe_2$ surfaces. Potential-energy-surface calculations indicate that pristine $SnSe_2$ should possess lower intrinsic sliding barriers than SnSe, consistent with its weaker interlayer interaction. However, XPS analysis reveals the presence of thin native oxide layers on both materials after air exposure. Incorporating oxygen-induced surface distortion into the calculations reverses the predicted friction trend, producing higher sliding barriers for oxidized $SnSe_2$ than for oxidized SnSe. This result explains the experimentally observed lower friction of SnSe relative to $SnSe_2$ and highlights the strong influence of surface chemistry on the tribological behavior of two-dimensional materials.

These findings establish SnSe and $SnSe_2$ as low-friction layered chalcogenides and show that the measured ambient friction response is strongly influenced by native surface oxidation. The intrinsic calculations further suggest that $SnSe_2$ could exhibit even lower friction when surface oxidation is suppressed, making surface control essential for evaluating its true lubricating potential [1].

[1]. *ACS Appl. Nano Mater.* ***2025****, 8, 14713−14719.*

2D-ThP-8 Influence of Sapphire Annealing Conditions on Terrace Formation and TMD Nucleation and Growth Kinetics, ***Morteza Sheibani Karkhaneh,*** Boise State University

The controlled synthesis of high-quality two-dimensional transition metal dichalcogenides (2DTMDs) is essential for the development of next-generation electronic, optoelectronic, andcatalytic devices. In order to grow high quality monolayer TMD thin films, many researchershave demonstrated the need to control the surface properties of the substrate. Specifically,terrace formation and the resulting step heights of c-plane sapphire has been shown to be acritical component of growing unidirectional TMD crystals and achieving thin films with minimalto no grain boundaries. However, while many papers have shown various ways to achievedifferent terrace formations, there is a need to understand how different processing conditionsimpact terrace formation, step heights, and ultimately the kinetics of TMD crystal growth.In this study, c-plane cut sapphire substrates were annealed at various temperatures,processing gases, pressures, and ramp/dwell conditions to obtain different terrace formationswith varying step heights using AFM. We demonstrate how these different factors impact thereordering of the sapphire surface and then explore how CVD growth conditions may inducereordering of the surface, even after pretreatment of the sapphire and ultimately impacting TMDcrystal growth.In this regard, we utilized pretreated sapphire to show how different surface properties impactTMD nucleation and growth. To understand the impact of the sapphire surface on TMD growth,we characterize the TMD samples using various techniques including Raman spectroscopy,TERS, photoluminescence, XPS, and AFM.The results demonstrate that substrate annealing plays a critical role in controlling TMDnucleation and growth kinetics. These findings provide important insights into substrate engineering for the scalable growth of high-quality TMDs that may expand to other 2D materials,offering a practical route toward wafer-scale integration of TMD-based devices.

2D-ThP-9 A New Metric to Assess the Rashba Spin-Orbit Coupling in Undulated 2D Materials, *Zhicheng Li, Favian Sun,* ***Sunny Gupta****, Boris Yakobson,* Rice University

Wrinkles and undulations are ubiquitous in two-dimensional (2D) materials. By breaking mirror symmetry, such topographical deformations can enable spin-orbit coupling and Rashba spin splitting, allowing spin precession with important implications for spintronic devices. The Rashba parameter, α_R, is commonly used to quantify the strength of Rashba spin splitting, with larger α_R generally associated with shorter spin-precession lengths. However, using first-principles electronic-structure calculations, we show that α_R can be an inadequate metric for materials with non-parabolic bands and higher-order Rashba spin-orbit interactions. To address this limitation, we propose a new dimensionless metric, L_{pr}, where L_{pr} is the spin-precession length and κ is the curvature of undulation. This metric directly captures device-relevant spin-precession behavior and enables more meaningful comparison and ranking of materials by Rashba-effect strength. Finally, using transport calculations, we demonstrate current modulation arising from spin precession in undulated 2D materials and show how this effect can be controlled in realistic device geometries.

2D-ThP-10 Ultra-Thin ALD-Based Conformal Coatings for Corrosion and Moisture Protection in High-Density Advanced Packaging, ***Rakesh Kumar****,* Specialty Coating Systems, Inc.*; Shuichi Sawada,* Daisan Kasei Co., Ltd, Chiba, Japan

The continued evolution of advanced packaging, encompassing high-density substrates, fine-pitch interconnects, microvias, and microBGA architectures, is enabling increasingly complex, high-performance electronic systems. Yet as feature sizes shrink and packaging densities rise, ensuring long-term reliability against corrosion and moisture ingress becomes a critical manufacturing challenge. This creates a compelling need for ultra-thin conformal coatings capable of delivering near-hermetic protection without compromising the dimensional and electrical tolerances demanded by advanced packaging designs.

Atomic Layer Deposition (ALD), introduced in the late 1990s, offers a uniquely precise solution: nanometer-scale films of metals and metal oxides deposited with exceptional conformality and thickness control. However, its broader adoption in electronics manufacturing has historically been limited by elevated processing temperatures incompatible with sensitive substrates and assembled components.

This paper presents a room-temperature ALD-based conformal coating process directly applicable to printed circuit boards, advanced packaging substrates, and sensitive electronic assemblies. The coating can be deployed as a standalone layer or in conjunction with Parylene, enabling flexible integration into existing packaging workflows. Corrosion resistance was evaluated through 21-day mixed flow gas (MFG) testing using Cl_2, H_2S, NO_2, and SO_2, conditions representative of harsh field environments. Results confirm robust protection in aggressive corrosive atmospheres, alongside strong substrate adhesion and excellent electrical insulation. Critically, when combined with Parylene C, the ALD coating improves the water vapor transmission rate by 63–100 times, establishing it as a high-impact materials solution for the reliability and protection requirements of next-generation advanced packaging

2D-ThP-11 Multifunctional GO-Based 2D Materials for Auranofin Combination Therapies, ***Diego La Mendola****, Lorenzo Chiaverini, Luca Famlonga,* University of Pisa, Italy*; Cristina Satriano,* University of Catania, Italy*; Tiziano Marzo,* University of Pisa, Italy

Graphene oxide (GO) has emerged as a promising two-dimensional nanomaterial for drug delivery due to its large surface area, biocompatibility, and versatile surface chemistry. GO can efficiently load therapeutic agents through π–π stacking, hydrogen bonding, and electrostatic interactions, enabling high drug-loading capacity and controlled release. These properties make GO-based nanocarriers attractive for applications in cancer therapy, anti-inflammatory treatments, and multifunctional nanomedicine.

In this work, graphene oxide was investigated as a two-dimensional platform for the loading and delivery of Auranofin (AF), a gold-containing compound originally developed for rheumatoid arthritis and currently attracting significant interest for its anticancer, anti-inflammatory, and redox-modulating properties. In particular, GO nanosheets were employed for the development of AF-based combination systems, including AF–NAC (Auranofin-N-acetylcysteine) and AF-NPX (Auranofin-Naproxen).

The study focused on the physicochemical interactions between GO and the different therapeutic agents, exploiting the high adsorption capability and oxygen-containing functional groups of graphene oxide. The resulting hybrid nanostructures were subjected to comprehensive physicochemical characterization, including UV–Vis spectroscopy, Fourier-transform infrared spectroscopy, dynamic light scattering, zeta potential analysis, and atomic force microscopy, in order to evaluate structural, morphological, and surface properties. In addition, drug-loading efficiency and stability in physiological conditions were assessed to correlate structural features with functional performance. The developed systems were further analyzed in terms of loading efficiency, stability, and potential synergistic effects associated with oxidative stress modulation and anti-inflammatory activity. Special attention was devoted to the AF–NAC system for the investigation of redox-regulation mechanisms, while the AF–NPX formulation was designed to combine the pharmacological activity of Auranofin with the anti-inflammatory properties of Naproxen.

Preliminary findings indicate that graphene oxide represents a promising 2D nanocarrier for improving drug stability, controlled release, and multifunctional therapeutic performance. These results further support the potential of GO-based platforms in advanced nanomedicine and combination drug delivery strategies, although challenges related to toxicity, biodegradation, and long-term biosafety still require careful investigation for future clinical translation.

2D-ThP-12 Transport and Dielectric Interface Engineering in ALD-Grown MoS_2 Transistors, ***Alberto Martinez****,* University of Granada, Spain*; Francisco Gamiz,* Univeristy of Granada, Spain*; Carlos Marquez,* University of Granada, Spain

The electrical performance of MoS_2 transistors is strongly determined by how the 2D semiconductor is grown and coupled to surrounding dielectrics. Plasma-enhanced atomic layer deposition (PE-ALD) is attractive for CMOS-oriented integration because it enables direct, conformal growth over large areas and can be followed by dielectric deposition without transfer steps. However, ALD-grown MoS_2 is not a direct equivalent of CVD-grown material. Its nanocrystalline morphology, small grain size, grain-boundary density, and growth-dependent stoichiometry can promote ambipolar or weakly polarity-selective operation, defect-assisted conduction, and hopping-like transport. Understanding these mechanisms is essential for reliable encapsulation and gate-stack design.

Here, we investigate ALD-grown MoS_2 field-effect transistors with emphasis on transport mechanisms, contact effects, and dielectric integration. Back-gated devices are used as diagnostic structures to evaluate the intrinsic channel response. Their transfer characteristics show no systematic preference for n-type or p-type operation, suggesting localized states, grain-boundary conduction, and hopping-assisted transport through defects.

To separate channel and contact contributions, we analyze device arrays with different geometries and extract sheet and contact resistance. These parameters allow us to assess how ALD growth and dielectric processing affect both the MoS_2 channel and the metal/MoS_2 interface. The results indicate that the dielectric environment strongly influences channel conductivity and device variability, highlighting the role of surface states, trapped charge, and dielectric-induced doping.

We then evaluate in situ dielectric encapsulation using Al_2O_3- and Si_3N_4-based layers deposited directly on MoS_2. Encapsulation is considered not only as passivation, but also as a functional interface for front-gate devices. Electrical measurements, bias-stress experiments, and low-frequency characterization are used to probe charge trapping, interface stability, and dielectric coupling, providing insight into how deposition conditions influence hysteresis, noise, drift, and robustness.

Finally, selected dielectric stacks are extended to front-gated MoS_2 transistors, where the encapsulation layer also acts as the gate insulator. By comparing back-gate and front-gate operation, we evaluate the transition from diagnostic test structures to local-gate architectures. Overall, this work connects ALD growth, defect-assisted transport, resistance extraction, and dielectric interface engineering, providing guidelines for scalable ALD-grown MoS_2 transistors compatible with CMOS-oriented fabrication.

2D-ThP-13 Nanoscale Imaging of Layer-Parity and Twist-Dependent Magnetism in CrSBr, ***Aalok Tiwari***, Carnegie Mellon University, USA; *Shubhada Patil,* Helmholtz-Zentrum Berlin für Materialien und Energie, Germany; *Ravi Kumar Bandapelli,* Carnegie Mellon University, USA; *Alevtina Smekhova,* Helmholtz-Zentrum Berlin für Materialien und Energie, Germany; *Wenhao Liu,* University of Texas at Dallas; *I-Hsuan Kao, Zhenhong Cui, Brandon Tran,* Carnegie Mellon University, USA; *Zixin Zhai,* University of Texas at Dallas; *Raghvendra Posti, Sandy Adhitia Ekahana,* Carnegie Mellon University, USA; *Alexander X. Gray,* Temple University; *Bing Lv,* University of Texas at Dallas; *Florian Kronast Kronast,* Helmholtz-Zentrum Berlin für Materialien und Energie, Germany; *Simranjeet Singh, Jyoti katoch,* Carnegie Mellon University, USA

Van der Waals (vdW) antiferromagnetic semiconductors offer the potential for innovative energy-efficient spintronics at atomic thickness. The advent of twist engineering further enables tailored arrangement of spins yielding emergent magnetic ground states via competing interactions. Chromium sulfide bromide (CrSBr) serves as an ideal platform for understanding the interplay between atomic thickness and twist-angle-dependent emergent spin texture at micrometer length scales. We carry out x-ray magnetic circular and linear dichroism (XMCD/XMLD) combined with photoemission electron microscopy (PEEM) to resolve the magnetic order at nanoscale resolution in atomically thin and 90° twisted CrSBr. We demonstrate layer-parity-dependent magnetic order persisting from bulk through monolayer limit. The remanent state shows strong temperature and layer number dependent coercivity. By twisting two CrSBr ferromagnetic monolayers with in-plane magnetic easy axes by 90°, we observe a superlattice effect in the twisted region leading to new emergent order.

2D-ThP-14 Impact of Air Exposure on the Stability and Resistivity of TaS_2 and $TaSe_2$ Films, ***Tinsae Alem***, *Michael Hann, Kory Burns, Stephen McDonnell,* University of Virginia

Transition metal dichalcogenides (TMDs) are promising for next-generation electronic, optoelectronic, and flexible device applications due to their tunable bandgaps, optical anisotropy, and mechanical flexibility. However, most TMDs, particularly Ta- and Nb-based thin films, are limited in practical use due to environmental instability; this is because ambient exposure can degrade their structural and electronic properties via oxidation and surface adsorption. In this study, we investigate the air stability of molecular beam epitaxy (MBE)-grown TaS_2 and $TaSe_2$ thin films (~5-10nm) by examining oxidation during sequential air exposure. Oxide-layer formation was estimated using X-ray reflectivity (XRR), while electrical resistivity measurements and X-ray photoelectron spectroscopy (XPS) tracked changes in resistivity and chemical composition. We compare degradation behavior between sulfide and selenide films, as well as the influence of substrate choice (SiO_2/Si and sapphire). Our results show that the TaS_2 grown on SiO_2/Si exhibits minimal changes in resistivity, outperforming both TaS_2 grown on sapphire and $TaSe_2$ grown on SiO_2/Si under identical ambient conditions. We further observe a gradual increase in resistivity with exposure time in $TaSe_2$, culminating in a complete transition from selenide to oxide after ~437hr of sequential air exposure. These findings correlate oxidation evolution with electrical transport degradation, providing insight into stability trends and degradation mechanisms in Ta-based TMD thin films. Understanding the oxidation rate and its relationship with resistivity could provide insight into improving the reliability and integration of TMD thin films for potential environmental sensing applications.

2D-ThP-15 Functional Agents for Functional Materials, ***Bogdan Dryzhakov***, *Emily Herron,* Oak Ridge Natinal Laboratory

Two-dimensional materials and heterostructures exhibit rich spatially varying optical responses, but interpreting hyperspectral spectroscopy datasets from these systems often requires expert-driven feature assignment and time-intensive comparison to prior literature. CHUNKS, or Cross-modal Hypothesis Understanding for Nanoscale Knowledge in Spectroscopy, is a domain-aware, retrieval-augmented agentic workflow that addresses this challenge by connecting experimental spectra to materials-science literature context. By integrating raw hyperspectral data to materials science corpus of >119K full text articles, CHUNKS generates actionable insights, including hypotheses, spectral feature classifications, and parameter initialization for downstream analysis. This workflow supports rapid, informed decision-making during initial materials characterization and provides a pathway toward experiment automation by making spectral interpretation more systematic and knowledge-guided. Here, we demonstrate CHUNKS on a hyperspectral scanning electron microscope cathodoluminescence dataset from a 2D heterostructure stack.

2D-ThP-16 Synthesis of Graphene Quantum Dots by Alkali Metal Intercalation and Exfoliation of Anthracite Coal, *George Bepete,* Concordia University, Canada; ***Gothamie Ratnayake***, *David Emanuel Sanchez, Zhuohang Yu, Edgar Dimitrov, Andres Fest Carreno,* The Pennsylvania State University; *Maykol Christian Damasceno Oliveira, Bartolomeu Cruz Viana, Francisco Eroni Paz Santos,* Federal University of Piauí, Brazil; *Mauricio Terrones,* The Pennsylvania State University

Leveraging the abundance and low cost of anthracite coal, a sustainable and scalable synthesis route is developed to produce graphene quantum dots (GQDs). Through this approach GQDs are collected as powders or slurries and redispersed in common solvents, enabling integration into diverse solution–processed platforms. Briefly, the process involves intercalating naturally sourced anthracite coal with potassium metal and exfoliating it in N-methyl-2-pyrolidone (NMP) to yield reduced GQDs of 2.5-3.5 nm in diameter. This method offers a practical path towards scalability with an isolated yield of ~ 28% GQDs based on the starting anthracite coal mass. Notably, the resulting GQDs feature a 3.4 eV direct bandgap, excitation–dependent photoluminescence, and thermo–optical properties (thermal diffusivity of $(6.4 \pm 0.3) \times 10^{-8}$ m^2/s and nonlinear refractive index of -4.69×10^{-9} cm^2/W). These intriguing thermo-optical properties along with improved scalability of the synthesis of GQDs motivate their use in future photothermal and nonlinear optical systems. Overall, this work reframes coal as a sustainable, low-cost precursor for quantum nanomaterials with applications in sensing, energy, and thermal management.

2D-ThP-17 Al–Pd Dual-atom Sites on N-doped Defective Graphene for CO_2 Activation: A DFT Study of 2D Catalytic Surfaces, ***Radhey Bhattarai***, *Yirong Mo,* University of North Carolina at Greensboro

Two dimensional materials provide a powerful platform for surface-site engineering because of their fully exposed atomic planes, tunable defect chemistry, and strong electronic sensitivity which enable precise control of adsorption and catalytic reactivity. The solid carbon materials have emerged as a promising option as these are affordable and have high surface area allowing them to capture small molecules like CO_2 and release it as other chemically valuable products using less heat, particularly when controlled with nitrogen structure. To make carbon capture much cheaper, easier and designing catalyst that generates most controllable active sites, two metal atom system containing main group elements and transition metal elements are paired which will be dispersed on the 2D carbon material. The density functional theory (DFT) is used to investigate Al-Pd dual-atom catalysts system where metal atoms are anchored on defective N-doped graphene as model 2D catalytic surfaces for electrochemical CO_2 reduction. To understand how defect structure and heteronuclear site geometry influence catalysts stability, charge redistribution, and surface intermediates binding, two local coordination environments are examined.

The data obtained from the calculation shows that Al-Pd pair generates an asymmetric active site on the graphene surface which shows cooperative bifunctional role where Al promotes polarization of CO_2 while Pd modulates charge transfer and the binding strength of reaction intermediates. From the electronic structure analysis, including charge redistribution and projected density of states, confirms that both the 2D support and the local coordination environment strongly leads the reactivity of this catalysts system. The free energy analysis and transition state analysis further gives insight into CO_2 reduction selectivity and its competition with hydrogen adsorption.

This work demonstrates how cheap, affordable, versatile, and defect engineered graphene can host atomically dispersed bimetallic sites and how the first principle surface science can guide the design of low-dimensional catalytic 2D materials for carbon conversion.

Actinides and Rare Earths
Room Ballroom A - Session AC-ThP
Actinides and Rare Earths Poster Session

AC-ThP-1 The Application of Occam's Razor to Bremsstrahlung Isochromat Spectroscopy, ***J G Tobin***, University of Wisconsin - Oshkosh

In philosophy and science, Occam's Razor is the problem-solving principle that recommends searching for the simplest possible explanation, consistent with the facts. [1] As put forth by Ptolemy (circa AD 90 -180): "We consider it a good principle to explain the phenomena by the simplest hypothesis possible." [2] More colloquially, "When you hear hoofbeats, think of horses not zebras," as suggested by Theodore Woodward. [3] In the

case of Bremsstrahlung Isochromat Spectroscopy (BIS), [4-9] there have been many different interpretation methods based upon different theoretical models. Here, a simple picture will be presented, founded upon one underlying principle: the 5f electrons of the actinides are a slightly perturbed jj-coupled system. [10-15] This simple picture will include (1) the demonstration that many uranium systems are 5f3-localized and (2) a model for 5f mixing and delocalization. [16 -17] ACKNOWLEDGEMENTS: JGT wishes to thank the University of Wisconsin - Oshkosh for its on-going support. It is a gem set beside the Fox River and Lake Winnebago. References1.https://en.wikipedia.org/wiki/Occam%27s_razor2.Franklin, James (2001). The Science of Conjecture: Evidence and Probability before Pascal. The Johns Hopkins University Press. Chap 9. p. 2413.Sotos, John G. (2006) [1991]. Zebra Cards: An Aid to Obscure Diagnoses. Mt. Vernon, VA: Mt. Vernon Book Systems. ISBN 978-0-9818193-0-3.4.J.K. Lang and Y. Baer, Rev. Sci. Instrum. 50, 221 (1979).5.Y. Baer and J. Schoenes, Solid State Commun. 33, 885 (1980).6.Y. Baer and J.K. Lang, Phys. Rev. B 21, 2060 (1980).7.Y. Baer, Physica 102B, 104-110 (1980).8.E. Wuilloud et al., Phys. Rev. B 29, 5228 (1984).9.Y. Baer, "Electron Spectroscopy Studies," Chapter 4, "Handbook of the Physics and Chemistry of the Actinides," eds. A.J. Freeman and G.H. Lander, North Holland, Amsterdam (1984)10.J. G. Tobin et al., Phys. Rev. B 105, 125129 (2022).11.J.G. Tobin et al., Solid State Sciences 160, 107779 (2025).12.J. G. Tobin, "An Empirical Analysis of alpha-U Bremsstrahlung Isochromat Spectroscopy," MRS Advances 7, 783-788 (2022).13.J.G. Tobin et al., Phys. Rev. B 72, 085109 (2005).14.A. L. Kutepov, J. G. Tobin, S.-W. Yu, B. W. Chung and P. Roussel, J. of Phys.: Cond. Matter, 36, 045601 (2024).15.J. G. Tobin et al., MRS Bulletin 47, 1078–1083 (2022).16.J.G. Tobin, J. Vac. Sci. Technol. A 43, 063206 (2025).17.J.G. Tobin and A. Kutepov, J. Electron Spect. Rel. Phen. 284, 147577 (2026).

AC-ThP-2 Uranium 2D Ferromagnetism at Ambient Temperatures in Layered Zintl Phase UCu_2P_2, ***Ladislav Havela**, Alexandre Kolomiets, Volodymyr Buturlim,* Charles University, Czechia*; Fuminori Honda,* Kyushu University, Japan*; Fabrice Wilhelm,* ESRF Grenoble, France*; Jiri Prchal,* Charles University, Czechia*; Andrei Rogalev,* ESRF Grenoble, France

Light-actinide magnetism is based on 5*f* electronic states, which are typically involved in metallic bonding, in contrast with the localized 4*f* states in lanthanides. Hence they are rather an analogy to transition-metal 3*d* materials, characterized by itinerant character. There is, however, a special ingredient in actinides, the strong spin-orbit interaction. It gives rise to orbital magnetic moments, yielding the strong anchor to the crystal lattice, providing thus new functionalities, as enormous magnetocrystalline anisotropy or giant magnetoresistance effects.

However, weaker Coulomb *U* restricts the 5*f* magnetism to the low temperature range. Combining with 3*d* metals, efficiently enhancing ordering temperatures in compounds with rare earths, does not work with actinides, as the 3*d* and 5*f* band states coexist at similar energies and hybridize between each other, suppressing typically both 3*d* and 5*f* magnetism.

There exists an alternative route of further reducing the 5*f* delocalization in compounds with large U-U spacings and weak 5*f*-ligand hybridization. The trick is to use polar bonding to reduce also the 5*f*-6*d* hybridization by withdrawing the U-6*d* states from the energy range of 5*f*'s by the bonding to an anion in Zintl phases. The most successful case is UCu_2P_2, a layered compounds with trigonal crystal structure, formed by alternating slabs of U (cation) and Cu-P (polyanion). The interactions can be further tuned by hydrostatic pressure, increasing the Curie temperature from 216 K to 296 K at pressures reaching 15 GPa. To describe variations of Curie temperature and spin and orbital moments, we applied X-ray magnetic circular dichroism at U-$M_{4,5}$ edges (ID 12 at ESRF) using perforated diamond anvil cells, minimizing the absorption in diamond. The results are in a good agreement with ab-initio calculations by means of the GGA+*U* method, which reveal other surprising features of the compound.

This work was supported by the Czech Science foundation under grant No. 25-16339S.

AC-ThP-3 Recent Studies of Actinide Materials by Soft X-Ray Synchrotron Radiation Methods, ***David Shuh**,* Lawrence Berkeley National Laboratory*; Haisley Windsor, Cambell Conour,* Department of Chemistry, University of California Berkeley*; Emma Archer, Nic Cicchetti, Olivia Gunther,* Lawrence Berkeley National Laboratory*; Jennifer Wacker,* Lawrence Berkeley National Lab*; Sergei Butorin,* Uppsala University, Sweden*; Polly Arnold,* Department of Chemistry, University of California Berkeley*; Hendrik Ohldag, Matthew Marcus,* Lawrence Berkeley National Laboratory

The capability to conduct x-ray synchrotron radiation spectroscopy on actinide materials has led to marked improvement in the fundamental understanding of *f*-electron behavior and chemistry of *f*-electron materials. Specialized beamlines and endstations capable of utilizing the unique spatial resolution, energy resolution, and intensity provided by the advent of near and third generation synchrotron radiation x-ray beams from storage ring user facilities, coupled to new sample holding techniques, has provided unmatched opportunities to characterize the chemical and physical properties for a range of actinide materials. This has been particularly evident in the soft x-ray region of synchrotron radiation where the scanning transmission x-ray microscope (STXM) has been used to determine electronic structure from the ligand perspective via ligand K-edge spectroscopy and resonant inelastic x-ray scattering (RIXS) has been employed to garner information about actinide metal centers Both have emerged as uniquely powerful tools to elucidate the electronic structure of actinide materials.

The results of recent actinide soft x-ray STXM and RIXS studies will be presented. These will include recent studies of the actinyl tris(benzoate) complexes with a range of donating/withdrawing substituents studied using scanning transmission x-ray microscopy (STXM) and time dependent density functional theory (TDDFT). The results from RIXS studies of the Am oxides will be recapped and prospects for future studies highlighted. Lastly, an update on the status of the laboratory-based x-ray absorption system used for f-element studies at LBNL will be presented.

AC-ThP-5 5f Electronic Structure of van der Waals Uranium-Tellerium Alloys, ***Jonathan Denlinger**,* Lawrence Berkeley National Laboratory*; Christopher Broyles, Justin Shotton, Sheng Ran,* Washington University, St. Louis

Low dimensionality of magnetism and of correlated f-electron physics are current high interest research topics in condensed matter. Here, we compare and contrast the properties of two layered van der Waals uranium alloys with a focus on the diversity of their U 5f electronic structures measured by angle-resolved photoemission (ARPES), and on new f-spectroscopic features not previously reported.

UOTe crystallizes in (Te-U-O-U-Te) quintuplet layers and exhibits bilayer (uddu) antiferromagnetic ordering of local moments below 165K [1]. The U 5f states are found to be well localized at ~1 eV below E_F similar to UO_2, but with an additional weak satellite peak at -0.2 eV of unexplained origin that exhibits a Kondo-like temperature dependence. Moreover, the AFM ordering has a distinct effect on the relative energy alignment of the localized f-states between the zone center and the zone boundary. ARPES of UOTe also exhibits unusual superstructure replicas of the Fermi surface that result from an exotic incommensurate structural modulation of its vdW gap between Te layers.

The UTe_3 crystal structure contains two Te square-net planes that ubiquitously promote charge density wave (CDW) formation in the rare-earth tritellurides. Here strong U 5f character near E_F with strong temperature-dependent Kondo coherence is found in a shallow electron pocket whose high density of states is consistent with its ferromagnetic ordering below 20K [2]. The strong f-scattering dominates the otherwise delicate imperfect Fermi surface nesting of light mass Te p-bands, that results in the suppression of CDW ordering. Finally, an unusual momentum-dependent 'negative' spectral weight profile for zone-folded Te p-bands is observed and discussed as an interference phenomena.

[1] C. Broyles *et al.*, Adv. Mater. **37**, 2414966 (2025).
[2] J. Shotton *et al.*, arXiv: 2603.03509 (2026).

AC-ThP-6 Development of a Novel Aerogel-Assisted Ssntd for Automated Fissile Isotope Identification, *Rami Babayew, Yaacov Yehuda-Zada,* Nuclear Research Center Negev, Israel*; Galit Bar,* Soreq Nuclear Research Center, Israel*; Noam Elgad,* Nuclear Research Center Negev, Israel*; Danny Dayan,* Ben Gurion University Be'er Sheva, Israel*; Jan Lorincik,* Centre Řež, Czech Republic*; Itzhak Orion,* Ben Gurion University Be'er Sheva, Israel*; Shay Dadon,* Nuclear Research Center Negev, Israel*; Aryeh Weiss,* Bar Ilan University, Israel*; Galit Katarivas Levy, **Itzhak Halevy**,* Ben Gurion University Be'er Sheva, Israel

Accurate identification of fissile isotopes is a central challenge in nuclear forensics and safeguards. Fission Track Analysis (FTA) using solid-state nuclear track detectors (SSNTDs) provides high sensitivity but is limited by manual processing and restricted isotopic discrimination. This work presents an automated, physics-informed framework for fissile isotope characterization combining Monte Carlo simulations, synthetic data generation [1], and image-based analysis.

GEANT4 simulations were performed for ^{235}U, ^{233}U, and ^{229}Th to model fission fragment transport and cluster formation in LEXAN® SSNTDs with

silica aerogel spacers. Synthetic track images were generated to study the effect of aerogel thickness on cluster morphology. Results show that increasing aerogel thickness enhances cluster separation and improves signal-to-noise ratio up to an optimal range, beyond which performance saturates due to pixel-resolution constraints and track truncation effects.

An automated image-processing pipeline (FTA-Finder) was developed to identify fission sites, separate overlapping clusters, and suppress background tracks. The fraction of well-resolved clusters increases with aerogel thickness, indicating improved reconstruction robustness.

Isotopic discrimination was evaluated using reconstructed track-length histograms and double-Gaussian fits for heavy and light fission fragments. A complementary analysis based on Real Flight Path (RFP) distributions showed clear isotope-dependent peak shifts. For 0.1 μm grains embedded in 50 μm aerogel (ρ = 0.033 g/cm^3), ^{235}U exhibited higher RFP peak positions than ^{233}U, while ^{229}Th showed the lowest values due to differences in fission-fragment energy and mass distributions.

Statistical analysis over 30 synthetic realizations showed significant separation between ^{235}U and ^{229}Th at ~3σ, while discrimination between ^{235}U and ^{233}U approached the resolution limit (~1σ). Peak deviations remained below 0.69%, confirming stable reconstruction performance.

All results are based on simulation and synthetic data. Future work will focus on experimental validation using neutron irradiation in reactor environments and extension to additional detector configurations. The proposed framework provides a scalable pathway toward quantitative isotopic fingerprinting for nuclear forensic and safeguards applications.

Reference:

[1] R. Babayew, Y. Yehuda–Zada, N. Elgad, J. Lorince, I. Orion, A. Weiss, G. Katarivas Levy, I. Halevy, *Simulation tools for improvement of the fission track analysis method for nuclear forensics* (2024), JRNC, Akadémiai Kiadó, Budapest, Hungary, DOI: 10.1007/s10967-023-09313-5.

AI/ML/Autonomous Experimentation for Thin Films Processing

Room Ballroom A - Session AIML-ThP

Poster Session

AIML-ThP-1 Ai-Based Real-Time Ashing Rate Estimation and Anomaly Detection Using Equipment Sensor and OES Data in Semiconductor Manufacturing*, Taekyung Ha,* ***You Tack Suh****,* PSK, Republic of Korea

The semiconductor industry is currently undergoing rapid transformation driven by the expansion of artificial intelligence (AI) technologies. AI is not only increasing the demand for advanced semiconductor devices, but is also becoming a key enabler of innovation in semiconductor manufacturing processes. As semiconductor devices become more sophisticated with higher integration density and smaller process nodes, wafer fabrication costs continue to rise significantly. Consequently, unexpected process failures or abnormal equipment conditions can result in substantial financial losses and reduced production yield.

Despite the increasing complexity of semiconductor manufacturing, many plasma-based processes such as etching and ashing still lack direct in-situ methods to determine whether the process is proceeding normally in real time. In current manufacturing environments, abnormal process conditions are typically monitored through post-process sampling inspections and offline metrology techniques. However, these approaches have inherent limitations, including delayed feedback, increased inspection costs, and the risk of missing transient process anomalies.

To address these challenges, this study proposes an AI-based process monitoring framework for semiconductor ashing equipment. The proposed approach utilizes both equipment sensor signals and Optical Emission Spectroscopy (OES) measurement data collected during the ashing process to estimate the ashing rate and detect abnormal process conditions in real time. By integrating multiple process-related data sources, the model aims to improve process visibility and enable early detection of equipment or process deviations.

For the development of the predictive models, machine learning methodologies including XGBoost and Long Short-Term Memory (LSTM)-based neural network algorithms were investigated and compared. Experimental results demonstrated that the XGBoost-based models achieved the best overall performance among the evaluated approaches. The proposed model achieved an ashing rate estimation accuracy of 89% and a process anomaly detection rate of 95%, indicating strong potential for practical deployment in semiconductor manufacturing environments.

The results of this study suggest that AI-driven virtual metrology and anomaly detection technologies can significantly enhance process stability, reduce inspection dependency, and minimize yield loss in advanced semiconductor fabrication processes.

AIML-ThP-2 ASSD Student Award Finalist Poster: Leveraging Convolutional Neural Networks (CNN) for the Real-Time Classification of Melt-Fraction of Phase Change Materials (PCMs) Using Infra-Red (I.R.) Imaging*, Nishit Pachpande, Anusree Sen, Debjyoti Banerjee,* Texas A&M University

Phase Change Materials (PCMs) are attractive candidates for incorporation in the Latent Heat Thermal Energy Storage (TES/ LHTES) Systems due to their high latent-heat capacity. Despite their attractive performance, PCMs (especially salt hydrates) often pose reliability issues. Salt hydrates (as PCMs) suffer from debilitating complications due to supercooling issues, i.e. the tendency of PCMs to stay in liquid phase at a temperature lower than the melting temperature (during the solidification portions of thermal cycles involving repeated melting and freezing). Also, the traditional methods for analyzing the thermal properties of PCMs are often time-consuming, expensive and require specialized protocols (where the measured properties are dependent on the measurement techniques).

Machine Learning (ML) techniques can be leveraged to address these issues by enhancing the reliability of PCMs with minimal effect on their performance.The objective of this study is to predict the amount of energy stored in a PCM-based TES using ML techniques (CNN model). An experimental apparatus which was developed in this investigation for performing experimental validations of the computational predictions. These model predictions were also compared with that of a pre-trained model ("EfficientNetB0"/ TensorFlow). The PCM (PureTemp 29^{TM}) was melted in a vertically graduated cylinder using a nichrome coil. Digital image acquisition (GoPro HERO8) of the melting PCM was performed for obtaining the corresponding melt-fraction values based on the height of meniscus in the melt pool. For training and testing the CNN model ~1660 I.R. images were acquired at 1-minute intervals (using FLIR One camera) during melting. The classification model was trained for classification classes corresponding to 10 melt-fraction bands (0-10%, 11-20%, ..., 91-100%). The CNN model predictions yielded a test accuracy of 93.98%, thus performing better than the pre-trained model (93.73%). These results demonstrate the efficacy of implementing deep learning based image analyses models as a fast, low-cost, reliable, accurate, robust, resilient and scalable tool for the real-time monitoring, prediction and characterization of PCM based TES systems.

KEYWORDS: latent heat thermal energy storage, TES, LHTES, machine learning, ML, artificial intelligence, AI, thermal management

AIML-ThP-3 Machine Learning-Assisted Pulsed Laser Deposition Based on Plasma Optical Emission Signatures*, Dorien Carpenter, Roman Luckett, Zahra Nasiri, Shiva Gupta, Rodion Mayatskiy,* University of Alabama at Birmingham*; Sumner Harris,* Center for Nanophase Materials Sciences, Oak Ridge National Laboratory*; Renato Camata,* University of Alabama at Birmingham

Growth of thin films by pulsed laser deposition (PLD) is governed by the formation, transport, and condensation of a transient laser-generated plasma plume. During ablation, the target is converted into a complex mixture of atoms, ions, molecules, clusters, droplets, and particulates, whose relative populations depend on target chemistry, constituent vapor pressures, and laser-material coupling. As the plume expands, its ionization state, temperature, particle flux, and kinetic energy distribution are further shaped by laser-plasma interactions, ablation geometry, and collisions with background gas. These coupled processes determine the composition, arrival rate, and energy of growth precursors reaching the substrate, thereby strongly influencing nucleation, phase formation, crystallinity, morphology, and ultimately thin film properties.

Optical emission spectra (OES) acquired during PLD encode rich information about the plasma processes that mediate thin film growth. Because OES can provide real-time, noninvasive measurements of plume composition, excitation, and plasma evolution, it offers actionable data streams that machine-learning workflows can harness to guide thin film growth on synthesis-relevant timescales. This could enable autonomous control of PLD and open new pathways for fabricating nonequilibrium materials that remain difficult to realize using conventional approaches.

In this work, we explore how representations of plasma temperature (*T*) and ionization fraction (*Xe*) can be constructed using Gaussian Process

Bayesian Optimization (GPBO) from a limited number of experiments. These quantities are extracted from OES of Fe-rich plumes. A GP regression model is trained on progressively accumulating experimental data to generate surrogate models of the underlying *T* and *Xe* as a function of laser fluence and spot size. We assess the impact of different acquisition functions and GP kernels against baseline random sampling. Model performance is evaluated using synthetic datasets from coupled laser ablation-fluid dynamics simulations, where *T* and *Xe* serve as ground-truth quantities.

We discuss results for PLD of iron, over a fluence range of 2-10 J/cm^2 and spot area of 0.2-13 mm^2 obtained from 1000 independent GPBO trials initialized with random three-point seed pairs of fluence, spot area, and *T* or *Xe.* We quantify the rate of convergence of the optimization to regions of interest in the (*T*, *Xe*) space, with respect to the choice of kernel and acquisition function. We then show how the surrogate models for *T* and *Xe* evolve in time and how they can be used to guide PLD to little explored plume ionization and temperature conditions for thin film growth.

AIML-ThP-4 Role of Oxide Phase and Surface Facets on Self-Limiting Thermal Atomic Layer Etch in High-k Oxides , ***Michael Nolan****, Rita Mullins,* Tyndall National Institute, University College Cork, Ireland

Thermal Atomic Layer Etching (ALE) is of high interest for its potential to deliver atomic level control over the etch of many materials and shows potential for use in future CMOS nodes with requirements for sub-nm levels of control on complex structures. It is performed using sequential surface modification and volatile release reactions. For metal oxides, HF fluorinates the initial surface to form a MF4 layer (M = metal) which undergoes ligand-exchange with precursors such as TiCl4 or SiCl4, which volatilizes the MF4 layer. The question of the role of the phase and surface facets in a deposited high-k metal oxide film has received little attention but can be addressed with first principles atomistic simulations. In this contribution we use density functional theory and molecular dynamics simulations to explore the effect of the phase and surfaces of HfO2 and ZrO2 on the HF modification half-cycle of ALE. The models used in this study representing polycrystalline materials are the (111) and (001) surface facets of monoclinic, orthorhombic and tetragonal HfO2 and ZrO2. Our thermodynamic analysis shows that for polycrystalline HfO2 and ZrO2, the HF pulse reacts in a self-limiting manner, and is preferred up to processing temperatures that are sensitive to the phase and surface. Models of HF coverage are used to compute calculated theoretical etch rates for the different oxide phases and surface facets and these show a strong dependence on both the crystal phase and the surface so that if different phases and facets are present an uneven etch profile will be seen. The stability, geometry and surface atomic coordination environments drive this dependence.

AIML-ThP-5 Automated Experimentation Reveals Co-Spacer Design Rules for Targeted Phase Selection in Quasi-2D Halide Perovskites*, **Elham Foadian****, Mahshid Ahmadi,* University of Tennessee Knoxville

Targeted phase control in quasi-2D halide perovskites (HPs) is essential for tailoring their optoelectronic properties, yet remains challenging since phase formation is governed by the coupled effects of spacer chemistry, precursor assembly, and crystallization kinetics. Despite rapid advances in quasi-2D HPs, the identification of spacer design rules still relies largely on manual trial-and-error synthesis, limiting mechanistic understanding and reproducible phase selection. Here, we present a multimodal, closed-loop autonomous experimentation workflow for targeted phase selection in quasi-2D HPs using co-space engineering. We investigate a ternary 3D:2D compositional space composed of 3D $FAPbI_3$ and two Dion–Jacobson co-spacers, 1,4-butanediammonium (BDA) and 3-(aminomethyl)piperidinium (3AMP), to identify compositions that converge toward a stable 3D-like phase. In situ photoluminescence (PL) spectroscopy reveals that BDA promotes rapid crystallization and early formation of 3D-like emissive domains, whereas 3AMP slows crystallization and favors the persistence of lower-n quasi-2D phases. By systematically regulating the BDA:3AMP co-spacer ratio, the crystallization pathway can be tuned to balance fast framework formation with sufficient structural relaxation, enabling convergence toward the target phase. These kinetic insights are integrated with automated high-throughput synthesis, time-dependent PL characterization, X-ray diffraction similarity scoring, and Gaussian process–Bayesian optimization to navigate phase homogeneity and stability. This work establishes co-spacer engineering as a design strategy for targeted phase selection in kinetically governed quasi-2D HPs.

AIML-ThP-6 Toward Autonomous Discovery of UV-Activated Small-Molecule Inhibitors for Area-Selective Atomic Layer Deposition*, **Lucas R. Kuehnel****, Campbell A. Sweet, Anthony A. Khoury, Erick A. Gutierrez-Monje, Matthias J. Young,* University of Missouri-Columbia

Recent work from our group has demonstrated functional group lithography to nucleate atomic layer deposition (ALD) for patterned deposition on non-growth surfaces like MoS_2 and highly oriented pyrolytic graphite. An analogous approach could enable patterned deposition on growth surfaces through UV-activated inhibition to further develop the dry functional group lithography tool set. However, it is unclear what chemistries might enable UV-activated inhibition. To efficiently search chemical space for UV-activated inhibitors, we developed a high-throughput screening framework for machine-learning-guided discovery. As a model system, we focus here on identifying inhibitors for ZnO ALD from diethylzinc and water on alumina surfaces. Quartz crystal microbalance measurements are used to monitor adsorption, desorption, and film growth dynamics, enabling quantitative assessment of nucleation delay and related mass change metrics. These experimentally derived metrics are used as targets in an initial exploratory active learning phase to generate a diverse seed dataset. We employ a suite of machine learning models for predicting vapor pressure, melting point, boiling point, pK_a, and oxidation potential to screen candidate molecules for physical processing feasibility within the constraints of the experimental system. These experimental constraints, imposed by a high-throughput design, place inherent biases on the searchable chemical space. For example, choosing to eliminate precursor heating enables more rapid testing, but favors smaller, more volatile molecules. Practically speaking, careful consideration of the imposed constraints can favor the discovery of molecules that are more likely to be industrially viable. The success of this discovery framework would provide a first step toward establishing dry functional group lithography as a tool for nanofabrication.

AIML-ThP-7 Toward Autonomous Screening of oMLD Thin Films for Next-Generation Lithium-ion Battery Materials*, **Campbell A. Sweet****, Kim A. Gerhard, Blaine D. Kelly, Lucas R. Kuehnel, Matthias J. Young,* University of Missouri

Organic conductive polymers with high lithium-ion redox capacities are promising as sustainable positive electrode materials and as performance-enhancing coatings for established cathodes such as lithium iron phosphate. Oxidative Molecular Layer Deposition (oMLD) enables the delivery of conformal organic conductive polymer thin films on porous powder substrates with precise thickness control, making it a promising platform for this application domain. However, exploration of oMLD chemistries remains limited because the experimental workflows are time-intensive and require substantial manual intervention. Given the large chemical design space of organic precursors, traditional oMLD workflows are not readily scalable for rapid materials discovery. Here, we discuss progress to date on establishing a rapid and autonomous workflow for screening oMLD thin films as organic positive electrode coating materials for lithium-ion batteries. We specifically describe our efforts to accelerate deposition, automate precursor handling, and streamline electrochemical characterization and analysis. Workflow analysis revealed key bottlenecks including low precursor volatility, slow performance characterization, and inefficient chemical data mapping and search. We report progress toward autonomous workflow operation using LLM agents to manage repetitive and cumbersome tasks. These advances provide a framework for accelerating oMLD-driven materials discovery and may extend to other challenging-to-accelerate workflows.

AIML-ThP-8 Small Science Agentic Models for Automated Perovskite Thin Film Exploration via Monte Carlo Decision Trees and Delayed Bayesian Optimization Feedback*, Elham Foadian, **Sheryl Sanchez****, Mahshid Ahmadi,* University of Tennessee Knoxville

Autonomous materials discovery requires decision frameworks capable of handling process-dependent outcomes, delayed feedback, and sparse experimental data. We introduce Small Science Agentic Models (SSAMs), a distributed architecture for self-driving laboratories in which scientific reasoning is embedded across narrow, physically interpretable models tied directly to the experimental workflow. Implemented as an event-driven, agent-based closed loop, the SSAM framework integrates hypothesis generation, protocol construction, characterization-derived state representation, machine-learning decision-making, and orchestration, treating each experiment as an evolving process trajectory rather than an isolated parameter evaluation. We apply this framework to discover an effective Dion–Jacobson (DJ) organic spacer for stabilizing the photoactive 3D-like phase of $FAPbI_3$. Through agent-guided hypothesis formation

employing Socratic reasoning and Tree-of-Thought branching, furan-2,5-diyldimethanammonium (FuDMA) was identified as a previously unexplored DJ spacer compatible with the perovskite lattice. The binary $FAPbI_3$/$FuDMAPbI_4$ compositional system was then explored autonomously using a Monte Carlo decision tree with delayed-reward updating. Over ten iterations, the system achieved 95% predictive agreement between predicted and measured film quality, identified the highest-performing sample within three iterations, and converged toward focused exploitation by approximately seven iterations. Optimal film formation was localized to FA based compositions of 60–80% within a tightly constrained spin-coating and annealing regime. Complementary Nuclear Magnetic Resonance Spectroscopy (NMR), Fourier Transform Infrared Spectroscopy (FTIR), and time-resolved photoluminescence (TRPL) analysis revealed two composition-dependent FuDMA interaction regimes. At intermediate spacer concentrations, FuDMA acts as a lattice-stabilizing additive that extends carrier lifetimes and suppresses non-radiative recombination, while at higher fractions it drives quasi-2D phase formation accompanied by accelerated fast-decay dynamics. These results establish SSAMs as a transparent, workflow-grounded approach to trajectory-aware autonomous experimentation in dynamic materials systems.

AIML-ThP-9 Revolutionizing Sem Image Analysis: Deep Learning vs. Classical Restoration for Enhancement and Segmentation, ***Amanda Georgina Nieto Sánchez,*** Universidad Anáhuac México*; Leon Hamui,* School of Engineering, Universidad Anáhuac México

Scanning electron microscopy (SEM) images frequently suffer from noise, blur, low contrast, and acquisition artifacts that complicate automated microstructure analysis and segmentation. While classical restoration approaches such as Wiener filtering, Richardson–Lucy deconvolution, CLAHE enhancement, and unsharp masking are commonly used, their impact on downstream AI-based segmentation tasks remains insufficiently explored.In this work, we investigate a deep learning-based image restoration framework for SEM post-processing using convolutional autoencoders trained with synthetically degraded SEM datasets. The degradation pipeline incorporates Gaussian blur, additive and multiplicative noise, and contrast perturbations designed to emulate realistic SEM acquisition conditions. The restored images are subsequently evaluated both through image-quality metrics and automated segmentation performance.A comparative study was performed between the proposed convolutional autoencoder and four classical restoration techniques: Wiener filtering, Richardson–Lucy deconvolution, CLAHE, and unsharp masking. Restoration quality was quantified using PSNR and SSIM metrics. In addition, segmentation performance was evaluated using U-Net architectures trained separately on degraded and restored SEM images.Although classical metrics showed moderate variations between restoration methods, segmentation-oriented evaluation revealed significant differences in model behavior. Quantitative analysis demonstrated that restoration-assisted segmentation reduced false positive regions, decreased over-segmentation, and lowered fragmentation of detected microstructures. Specifically, restored-image segmentation reduced the false-positive component ratio from 0.36 to 0.29 and decreased fragmentation metrics relative to models trained on degraded data.The results suggest that deep learning-based SEM restoration may provide advantages not fully captured by traditional image-quality metrics alone, particularly when evaluated within automated materials characterization workflows. This approach demonstrates the potential of AI-assisted SEM post-processing for improving robustness and reliability in microstructure segmentation tasks.

AIML-ThP-10 Enabling AI-Driven Materials Discovery Through Data Infrastructure, ***Akshay Talekar,*** UL Research Institutes

Advances in machine learning have expanded the role of AI in materials discovery, but model development is rarely the primary constraint in practice. Instead, progress is limited by fragmented data ecosystems, inconsistent metadata, and weak integration between computational and experimental workflows.

This talk frames materials discovery as a data-centric systems problem, where the ability to ingest, standardize, and operationalize heterogeneous data ultimately determines the effectiveness of downstream learning. Emphasis is placed on the role of data architecture, provenance, and interoperability in enabling reproducible and scalable experimentation.

More broadly, this perspective highlights the importance of tightly integrated data and learning pipelines that support continuous iteration under real-world constraints. Addressing these challenges is essential for transitioning AI from isolated modeling efforts to robust, production-scale capabilities within experimental science.

AIML-ThP-11 Statistical Analysis of Pressure-Growth Correlations in Temporal ALD and MLD toward the Identification of Process Deviations, *Andrew Ball, Joelle Scott, Jay Werner,* ***David Bergsman,*** University of Washington

In the development of many new vacuum deposition-based processes, such as in atomic layer deposition (ALD) and molecular layer deposition (MLD), process conditions are optimized through correlation with deposition outputs, such as film thickness and growth per cycle (GPC). Other data, such as reactant dose pressure and exposure, can also be used in process optimization, either quantitatively (e.g., by correlating growth per cycle with reactant exposure) or qualitatively (e.g., by identifying erroneous dose conditions or reactant depletion). However, while there are many robust tools informing process optimization, there remains a need for tools that can identify deviations within a deposition run.

In this work, we introduce a diagnostic approach for processing and analyzing reactor parameters in temporal ALD/MLD processes. By linking reactor pressure data (via LabVIEW JSON output) with a Python-based processing pipeline, we are able to correlate steady-state and maximum chamber pressure of a given step in the deposition process with the overall process growth-per-cycle (GPC). Through this correlation, we identify processing steps and pressures that most influence the GPC of the process, which can help identify areas for process improvement. False positives were filtered from the list of correlations using a perturbation stress test that involved repeatedly injecting 15% Gaussian noise across 1,000 iterations of a given step. To test this pipeline, we analyzed the pressure and GPC data from several processes in development in our lab as case studies. Results of these analyses suggest that this approach is able to identify subtle pressure drifts as well as processing steps that may be contributing to effects like CVD. This work provides a framework for cleaning data for potential use in interpretable machine learning models like Random Forest and Gradient Boosting, enabling autonomous process optimization with suitable, high-training data, while maintaining the transparency needed for physical reactor troubleshooting.

Advanced Microelectronic Materials and Devices Mini-Symposium
Room Ballroom A - Session AM+EM+TF-ThP
Advanced Microelectronic Materials and Devices Mini-Symposium Poster Session

AM+EM+TF-ThP-1 AlScN Ferroelectric Diode-based Non-volatile Memory on $TaSi_2$ for Harsh-Environment Computing, ***Nghi Pham,*** University of Pennsylvania, Viet Nam*; Dhiren Pradhan,* Agni Semiconductor*; Xindi Yang, Ravali Gudavalli, Deep Jariwala,* University of Pennsylvania

Electronic systems capable of operating in harsh environments—including space exploration (e.g., Venus and near-solar probes), aeronautics, oil and gas exploration, nuclear power plants, and heavy industrial processes—must withstand extreme temperatures and radiation. These applications demand in situ computing and sensing with stable performance under extreme conditions. However, no NVM technologies reliably function above 250 °C, creating a critical gap in high-temperature electronics. Despite well-established high-temperature logic with reliable operation > 800 °C, the absence of a compatible NVM technology hinders fully integrated computing for extreme environments. Ferroelectric diodes (FeDs) are promising candidates for selector-free, non-volatile memory (NVM) due to their nonlinear current–voltage behavior, potential multistate operation, and simple two-terminal architecture. For harsh-environment electronics, however, maintaining a high ON/OFF ratio and stable switching at elevated temperatures remains a major challenge, largely due to stronger internal fields and increased charge trapping.

In this work, we have successfully grown 45 nm of $Al_{0.68}Sc_{0.32}N$ on $TaSi_2$ despite the large lattice mismatch. $TaSi_2$ is a well-known high-temperature metal electrode and has been employed in NASA's Junction Field Effect Transistors (JFETs). The XRD omega scan of $Al_{0.64}Sc_{0.36}N$ reveals a full width at half maximum (FWHM) of 4.06°. Stacks with and without an AlO_x interlayer were compared to evaluate the role of interfacial engineering in leakage suppression, switching behavior, and ON/OFF ratio retention at elevated temperatures. The devices consisted of Ni top electrodes, a ~10

nm AlO_x interlayer (IL) dielectric, a ~45 nm AlScN ferroelectric layer, and $TaSi_2$ bottom electrodes.

Temperature-dependent DC-IV, AC-IV, and Positive-Up Negative-Down (PUND) measurements were performed up to 800 °C. For the 32% Sc AlScN device without an IL dielectric, the ON/OFF ratio remained measurable, decreasing from ~10 at 25 °C to 2.37 at 800 °C. By contrast, devices with an AlO_x IL dielectric exhibited substantially higher ON/OFF ratios, reaching values above 500 at room temperature and ~6 at 800 °C. These results highlight the role of AlO_x interfacial engineering in suppressing leakage and improving state distinguishability at elevated temperatures. High-temperature ferroelectric polarization switching, and other NVM characteristics such as read and write endurance, retention measurements of the ferrodiodes of $Al_{0.68}Sc_{0.32}N$ on $TaSi_2$ with 10 nm AlO_x IL dielectrics up to 900 °C are currently underway and will be presented at the meeting.

AM+EM+TF-ThP-2 Flexible Ag and Cu Pattern Films: A Comparative Study on Conductivity, Adhesion, and Mechanical Stability*, **Seonhee Jang**, Samuel Goutierrez, Kenneth Lathrum,* University of Louisiana

The integration of metallic nanoparticles (NPs) has revolutionized the fabrication of flexible electronic devices. Compared to their bulk counterparts, metallic NPs exhibit unique shape and size-dependent properties that make them indispensable to the electronics industry. However, achieving superior electrical conductivity requires specialized post-processing to remove the stabilizing agents and additives used during NP synthesis.

In this study, silver (Ag) and copper (Cu) NP inks were employed to fabricate conductive patterns via printing and sintering processes for flexible electronics applications. These inks were printed onto 0.1 mm thick flexible Kapton polyimide (PI) sheets. The Ag ink was formulated with a solid content of 42±2 wt%, a density of 1.6 g mL^{-1}, and a viscosity of 3.5-6.0 Pa S at 10 s^{-1}. The Cu NP ink featured a solid content of 88 wt%, a density of 3.9 g mL^{-1}, and a viscosity of 20-40 Pa S at 50 s^{-1}.

Metal NP patterns were printed using a single-nozzle printing system and subsequently dried and sintered under four distinct sintering conditions: thermal treatment only (TO), laser irradiation only (LO), thermal treatment followed by laser irradiation (TL), and laser irradiation followed by thermal treatment (LT). This allowed for a comprehensive comparison of single and dual sintering techniques on the physical, chemical, mechanical, and electrical properties of the metal patterns. Post-sintering evaluations include microstructure analysis, crystallography, chemical composition, electrical sheet resistance, and mechanical strength.

The results demonstrated that for Ag patterns, the LT condition yielded the best performance for flexible electronics, achieving the lowest sheet resistance (0.0031 Ω Sq^{-1}) and superior mechanical stability (R/R_0=1.75) due to enhanced grain growth and effective organic removal. For Cu patterns, the TO condition proved optimal; while the LT condition provided the lowest resistance (0,0117 Ω Sq^{-1}), the TO condition ensured more uniform grain growth and higher flexibility (R/R_0=10.58). Overall, Ag patterns outperformed Cu in both conductivity and adhesion, as Cu suffered from oxidation and brittleness associated with high hardness (37.18-55.36 N/mm^2). These findings suggest that optimizing sintering parameters such as laser intensity and thermal atmosphere can further enhance the overall properties of Cu. Moreover, the adoption of dual sintering methods can improve the performance of printed flexible electronic devices, and there are more scopes for continuing research related to this method.

AM+EM+TF-ThP-3 Study of Acoustoelectric Interactions in α-In_2Se_3 - $LiNbO_3$ Heterostructure for Efficient RF Communication System*, **Marzia Sultana**, Jackson Anderson,* University of Vermont

The growing global demand for energy is creating an urgent need for more efficient computation and communication technologies (Figure 1a) [1]. Despite vast improvements in computational efficiency, modern radio systems integrated on-chip still cannot simultaneously transmit and receive data (Figure 1b). Although circulators enable concurrent transmission and reception, conventional designs rely on magnetic fields, making them difficult to integrate with modern semiconductor technologies (Figure 1c) [2]. Acoustoelectric devices provide a promising magnet-free alternative for realizing compact and energy efficient circulators. In this work, we explore a novel heterostructure based on α-In_2Se_3 which is a two-dimensional ferroelectric semiconductor with moderate bandgap (1.39 eV) and carrier mobility up to 3392 cm2/(V*s) [3]. This study will be carried out in three main stages. The first stage focuses on simulating the acoustoelectric device gain to optimize heterostructure dimensions based on key material properties of α-In_2Se_3, such as carrier mobility and doping concentration. The second stage involves 2D material fabrication through mechanical exfoliation and characterization of exfoliated α-In_2Se_3 flakes to evaluate practically achievable device performance (Figure 2). In the final stage, the optimized structure will be integrated into a complete device design guided by simulation results. The simulation framework for the α-In_2Se_3–$LiNbO_3$ heterostructure was first validated against an existing InGaAs–AlScN design [4]. The proposed model exhibits higher gain in the low-frequency regime (Figure 3a). Additionally, the gain-to-power ratio (Figure 3b) indicates improved efficiency, attributed to the moderate carrier mobility of α-In_2Se_3. While higher mobility (InGaAs) can increase gain, it also leads to greater power dissipation, reducing overall efficiency. Figure 4 illustrates the impact of doping concentration on performance. Maximum gain is observed near a doping level of 10^{16} cm^{-3} (Figure 4a), whereas efficiency is higher at lower doping levels (Figure 4b). An optimal operating region is identified (Figure 4c), where both gain and efficiency are balanced. At 1 GHz, the device achieves a gain of 37.8 dB with a low power dissipation of only 0.02 mW. Mechanical exfoliation of α-In_2Se_3 using different adhesives initially produced poor-quality flakes, prompting investigation of process parameters such as substrate baking conditions. Increasing the baking temperature from 150°C to 200°C improved flake uniformity and size, and a Design of Experiments approach will be used to further optimize yield for device fabrication.

AM+EM+TF-ThP-4 Spatial Mapping of Spin Wave Dynamics in Shape-Optimized Magnetostatic Wave Cavity Filters*, **Kelsey Collins**,* Air Force Research Laboratory

Yttrium iron garnet (YIG) magnetostatic wave (MSW) radio frequency (RF) cavity filters offer wide frequency tunability, making them highly promising for sixth-generation (6G) communication systems. However, finite cavity dimensions generate severe spurious modes that degrade filter performance. While tailoring the transducing electrode shape can suppress these undesired modes and enhance the primary passband, the underlying wave dynamics remain poorly understood. This study utilizes micro-focused Brillouin light scattering (BLS) spectroscopy to spatially map and analyze the excited spin waves within the cavity. Spatial profiles reveal that conventional straight-line electrodes exhibit frequency-dependent mode propagation. Conversely, optimized half-cone electrodes maintain consistent spin wave propagation across the entire frequency range. These findings demonstrate that electrode shaping directly controls the RF passband by stabilizing constituent spin wave propagation, offering critical insights for designing high-performance, spur-free nonreciprocal devices.

AM+EM+TF-ThP-5 Nanoscale structural and chemical characterization of AlxTi1-xN wurtzite thin films.*, **Sai Saswat Tripathy**, Elizabeth Dickey,* Carnegie Mellon University*; Ian Mercer, Jon-Paul Maria,* Penn State University

Wurtzite ferroelectrics based on the composition $Al_{1-x}M_xN$, with M representing transition metals, have shown to possess large remnant polarization values, and higher thermal stability than conventional ferroelectrics like lead zirconate titanate (PZT) or barium titanate (BTO), and thus find potential applications in high operating temperature non-volatile memories. In this study, transmission electron microscopy (TEM) and scanning transmission electron microscopy-based energy-dispersive X-ray spectroscopy (STEM-EDS) were employed to investigate the structural and chemical characteristics of a stack comprising of a silicon substrate, titanium bottom electrode with a thin TiN layer, $Al_{0.92}Ti_{0.08}N$ thin film and tungsten top electrode. $Al_{1-x}Ti_xN$ based wurtzite thin films have previously been used for piezoelectric applications, and have potential ferroelectric applications, if polarization switching by the application of external electric field can be shown. Electron-transparent cross-section lamellae were prepared from the stack using focused ion beam (FIB) milling to enable site-specific TEM/STEM analysis. Bright-field (BF) and dark-field (DF) TEM images revealed a fiber-texture in the film with columnar grains aligned parallel to the growth direction. Zone-axis diffraction patterns (ZADPs) acquired from the film demonstrated wurtzite phase purity and c-axis oriented growth of the film. STEM-EDS revealed uniform distribution of Al, Ti and N throughout the film, further confirming wurtzite phase purity, which is essential for ferroelectric switchability.

AM+EM+TF-ThP-6 IGZO Thermal ALD application in 3D High Aspect Ratio (HAR) Features: Conformality and Elemental Uniformity Studies, ***Adarsh Rajashekhar**, Fei Zhou,* Sandisk Technologies*; Ritwik Bhatia, Ganesh Sundaram,* Veeco Instruments*; Senaka Kanakamedala,* Sandisk Technologies

Multi-component oxide IGZO ($In_xGa_yZn_zO_p$) has been proposed as the channel material enabling low-cost and scalable future 3D-DRAM technology [1], [2]. This application would necessitate uniform deposition in high pattern density, high aspect ratio (HAR) structures. However, benchmarking of conformality and compositional uniformity in HAR structures is lacking in literature. With this objective, IGZO ALD deposition has been studied within deep hole features with two different aspect ratios (7:1 and 90:1). As a first step, a baseline deposition recipe was developed on blanket substrates. TMIn, TMGa and DEZ precursors were chosen due to their relatively high vapor pressures and well understood ALD processes. An optimal 200˚C deposition temperature avoids decomposition of DEZ and TMIn above 250˚C, while overcoming low growth-rates of GaO_x below 200˚C. Precursors and Reactant (O_3) dose times were separately optimized to ensure growth saturation, with GaO_x growth typically needing ~20x the O_3 dose time to ensure complete reaction, as compared to InO_x, ZnO_x. Based on these optimizations, carbon content in the developed IGZO films were found to be below the detection limit of X-ray photoelectron spectroscopy (XPS). The initial blanket baseline recipe (not optimized for HAR depositions) comprising of In-O-Ga-O-Zn-O growth sub-cycles yielded 50% coverage (bottom/top sidewall) for a 7:1 HAR structure, and 25% coverage for the 90:1 case. Specifically, In (precursor with highest molecular weight and lowest vapor pressure) saw a 21% to 38% reduction in partial fraction from top to bottom, whereas was partially compensated by Ga and Zn partial fractions increase that ranged around -3% to 20% in the different structures. Continuous coverage and compositional uniformity improvements are planned, with longer dose times as one of the knobs (and with particular emphasis on the In component).

1. D. Ha et al, "Exploring Innovative IGZO-channel based DRAM Cell Architectures and Key Technologies for Sub-10nm Node," pp 1-4 IMW (2024)

2. M. Okajima et al, "Highly stackable Oxide-semiconductor Channel Transistor Technology for Future High-density and Low-power 3D DRAM," pp 1-4 IEDM (2025)

Atomic Scale Processing Mini-Symposium
Room Ballroom A - Session AP+EL+PS+TF-ThP

Atomic Scale Processing Mini-Symposium Poster Session

AP+EL+PS+TF-ThP-1 Design of Gas Flow Field for a Slip Flow ALD Processing Chamber, ***Kyung-Hoon Yoo,*** Korea Institute of Industrial Technology, Republic of Korea*; Geun-Soo Song,* The KUMYOUNG Inc., Republic of Korea*; Chun-Sik Kim,* TNG Co., Republic of Korea*; Jun-Young Hwang, Sang-Ho Lee, Jeong-Jin Kang, Shin-Ae Song, Kyung-Tae Kang,* Korea Institute of Industrial Technology, Republic of Korea*; Hyeong-Cheol Lee,* Hanyang University, Republic of Korea*; Kun-Hyung Lee,* SAMSUNG DISPLAY, Republic of Korea

As semiconductor feature sizes reach the nanometer scale, ALD processing equipment has become indispensable for atomic-layer control. However, conventional ALD processes face significant challenges regarding economic and environmental feasibility due to the excessive consumption of precursors and energy.[1,2] To address these issues, it is essential to establish sustainable manufacturing technologies through the development of high-efficiency ALD processing chambers. In the present study, we propose a slipflow based ALD chamber designed to optimize the process space and minimize resource waste. The nitrogen flow fields within the chamber were numerically investigated using Computational Fluid Dynamics (CFD) for process gap sizes of 1, 10, and 100 mm at 400 °C. Under an inlet static pressure of 1 Torr and a mass flow rate of $4.233x10^{-5}$kg/s, the Knudsen number (Kn) and flow Reynolds number (Re) were evaluated as 0.0137 and 0.822, respectively for the 10 mm gap. These values confirm that the flow resides within the slip flow regime, where rarefaction effects at the surface wall become significant. Accordingly, the steady-state compressible laminar flow field was simulated by solving the continuity, momentum, and energy equations.[3,4]

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AP+EL+PS+TF-ThP-2 Nucleation and Evolution of Dislocations and Extended Faults in Complex Perovskite Oxides, ***Rishi Raj**, K. Andre Mkhoyan,* University of Minnesota, USA

The stoichiometric flexibility of a perovskite oxide (ABO_3) results in several unique properties due to the presence of three elements in the crystal structure. This allows it to host a variety of defects across all dimensions. 1D primitive edge dislocations with varying terminations, screw dislocations as well as 2D structural faults like Ruddlesden-Popper, elastic distortions, and BO_3 octahedral tilts are commonly observed and studied. Even though structure and electronic properties of some of these defects have been reported, the nucleation and growth of such defects and dislocations is still unclear. Analytical STEM study of perovskite oxide thin films of $BaSnO_3$ and $SrSnO_3$ show the existence of two kinds of edge dislocations: single ([001]/(100)-type) and dissociated ([001]/(110)-type) edge dislocation each with two half planes missing. Six different types of such dislocations are possible and observed due to the terminations of the perovskite half planes. Similarly, 2D Ruddlesden-Popper faults are also observed to result from missing planes of atoms, suggesting a correlation with 1D dislocations. Apart from such conventional topological defects, complex perovskite oxides also showcase several line defects and dislocations with reconstructed cores. This suggests we can selectively populate the material with defects by altering the terminations of crystal half planes. Strain tuning during growth by swapping substrates or decorating the surface morphology can effectively allow termination control. This would allow certain defect and dislocation structures to be more favorable than others. By establishing this correlation between 1D and 2D faults, this work provides a potential pathway to transition from passive extended defect management to intentional, termination-controlled defect engineering.

AP+EL+PS+TF-ThP-3 Atomistic Study of the Effect of Moisture-Modified Amorphous SiO_2 Interfaces on Gas-Phase Clustering in LPCVD, ***Minseung Cha,*** Seoul National University, Republic of Korea

Particle formation is a critical issue in LPCVD processes because nanoscale contaminants can cause film defects, pattern failure, yield loss, and process instability. Although particle generation is often explained by precursor decomposition and homogeneous gas-phase reactions, the chemical state of quartz-glass components used in LPCVD equipment has not been sufficiently considered. In particular, amorphous SiO_2 surfaces are widely exposed in parts such as process tubes, chambers, boats, injectors, and nozzles, and these surfaces can be modified by moisture during air exposure.

In this study, we investigate the role of moisture-modified amorphous SiO_2 interfaces in gas-phase clustering using molecular dynamics and density functional theory calculations. Dry SiO_2, hydroxylated SiO_2 surface models are constructed to represent different surface states. H_2O adsorption and dissociative chemisorption are first examined to evaluate silanol formation. The interaction between reactive molecules or cluster precursor species and each SiO_2 surface is then analyzed in terms of adsorption stability, residence behavior, and desorption tendency.

We propose that hydroxylated SiO_2 surfaces can act as reactive boundaries rather than inert walls in LPCVD environments. Surface silanol groups may temporarily stabilize reactive species through hydrogen bonding and electrostatic interactions, increasing local molecular concentration near the interface. These stabilized species can subsequently return to the gas phase and enhance molecular aggregation, thereby increasing the probability of cluster and particle formation.

This study provides an atomistic interpretation of how the moisture exposure condition of quartz-glass parts can influence gas-phase clustering in LPCVD processes. The results suggest that controlling moisture exposure and the hydroxylation state of amorphous SiO_2 interfaces in components

such as nozzles, chambers, and boats may be important for particle suppression and process stability.

Keywords: LPCVD, amorphous SiO_2, H_2O vapor, hydroxylation, silanol, molecular dynamics, MD, density functional theory, DFT, gas-phase clustering, particle formation, quartz glass, semiconductor, process

AP+EL+PS+TF-ThP-4 Low Temperature Atomic Layer Deposition of ZnO for Optoelectronic Applications, ***Anil Yadav***, *Aditya Sadhanala,* Indian Institute of Science, India

This work demonstrates the ultra-low-temperature atomic layer deposition (ALD) of ZnO thin films at 50 °C and 70 °C using a 1 M diethylzinc (DEZ) solution in hexane and water as precursors. This was achieved in a custom-built ALD chamber with precise control over the process parameters. Despite the ultra-low deposition temperatures, the resulting ZnO films demonstrated excellent uniformity. This approach not only solves the problem of substrate compatibility by enabling ultra-low-temperature growth but also demonstrates the use of solvent-diluted pure precursors. The X-ray diffraction (XRD) patterns of as-deposited ZnO films deposited at 50 °C and 70 °C as a function of the number of ALD cycles from 50 to 250 were measured. As the ALD deposition cycles increased to 100, distinct diffraction peaks corresponding to (100), (002), and (101) planes emerged. When the deposition temperature increased from 50 °C to 70 °C, the (002) peak became more intense and sharper, indicating improved crystallinity.

To evaluate the electronic properties of ZnO thin films deposited at ultra-low temperatures of 50 °C and 70 °C, we integrated them as the active layer in field-effect transistors (FETs). The fabricated devices demonstrated exceptional electrical characteristics, exhibiting an I_{ON}/I_{OFF} ratio exceeding 10^8 with the saturation mobility of 0.85 cm^2/V.s. These results clearly confirm the applicability of solution-based precursors for ultra-low-temperature ALD depositions in electronic device applications.

AP+EL+PS+TF-ThP-5 Oxidation-Assisted SF_6 Remote Plasma Etching for Surface Roughness Reduction of TiN, ***Min Kyun Sohn***, *Subin Heo, Seong Hyun Lee, Sun Kyu Jung, Jeong Woo Park, Dongwoo Suh,* Electronics and Telecommunications Research Institute, Republic of Korea

Titanium nitride (TiN) is widely used as a conductive diffusion barrier and work-function metal in advanced semiconductor devices. As device dimensions continue to scale down, controlling not only the etch amount but also the post-etch surface morphology becomes increasingly important, because nanoscale roughness can directly affect electrical reliability, interface quality, and subsequent film deposition. In the present study, we investigate the effect of SF_6 remote plasma-based etching on the surface morphology of TiN thin films, with particular emphasis on the role of a pre-oxidation step.

Three TiN surface conditions were compared: as-deposited TiN, TiN exposed to SF_6 radicals only, and oxidized TiN followed by SF_6 radical exposure. The etch per cycle (EPC) increased from 0.16 Å/cycle for the SF_6-only process to 0.38 Å/cycle for the oxidation-assisted SF_6 radical process, indicating that surface oxidation enhanced the fluorine-radical-driven removal of TiN. Atomic force microscopy measurements showed that the as-deposited TiN exhibited an RMS roughness of 1.313 nm, which modestly decreased to 1.117 nm after direct SF_6 radical exposure. In contrast, when the TiN surface was oxidized prior to SF_6 radical exposure, the RMS roughness further decreased to 0.850 nm, corresponding to an approximately 35% reduction compared with the as-deposited TiN surface, demonstrating a clear surface-smoothing behavior.

This difference suggests that the oxidation step plays a critical role in modifying the TiN surface before fluorine-radical exposure. The smoothing behavior is attributed to the formation of a TiO_x or TiO_xN_y surface layer during oxidation, followed by its conversion into volatile TiF_x species during SF_6 radical exposure. The higher EPC and lower RMS roughness obtained after oxidation-assisted SF6 exposure suggest that the modified surface layer can be removed more efficiently and uniformly than the native TiN surface. This oxidation-assisted pathway provides a chemically controlled route for reducing TiN surface roughness without relying on ion-driven physical sputtering.

These results indicate that surface pre-oxidation can be an effective strategy for controlling the morphology of TiN during radical-based etching. The proposed oxidation-assisted SF_6 radical process offers a potential strategy for morphology-controlled TiN etching in nanoscale device integration.

AP+EL+PS+TF-ThP-6 Development of in-Situ Laser Diagnostics Measurements of CH_3 Radical Concentrations for Study of Thin Film Depositions Using Organo-Metallic Precursors, ***Mruthunjaya Uddi***, Advanced Cooling Technologies Inc.*; Prawal Agarwal, Devon Jensen,* ACT*; Anatoli Morozov,* Princeton University*; Arthur Dogariu,* Texas A&M University

Many environmentally friendly non-halogen precursors contain CH3 structure component. Plasma chemical vapor deposition of pure metallic thin films using these precursors is challenging and requires better understanding of the gas phase and surface reaction mechanisms. We present a novel, time and spatially resolved, in-situ femtosecond laser diagnostics method to measure CH3 radicals in a non-equilibrium plasma environment. The CH3 radicals are predissociated to CH2 and H radicals using a 275 nm femtosecond laser pulse, followed by a 205 nm probe beam to measure the H radical concentrations. A single femtosecond laser is used to generate the required 275 nm and 205 nm beams. Measuring and knowing the dissociation cross section of CH3 radical by 275 nm pump beam, allows the quantification of CH3 radical concentrations with spatial and time resolution.

AP+EL+PS+TF-ThP-7 Hybrid Electrospun ZnO Nanofiber and ALD ZnO Electron Transport Layers for Near-Infrared Organic Photodiodes, ***Anna Leonard***, *Neha Chaturvedi, Veena Misra,* North Carolina State University

Organic photodiodes (OPDs) require efficient electron transport layers (ETLs) to achieve charge-selective extraction while minimizing recombination and dark current impacts. In this work, hybrid ZnO ETLs consisting of electrospun ZnO nanofibers and atomic layer deposited (ALD) ZnO were investigated for integration into near-infrared OPDs with a PTB7-Th:IEICO-4F active layer. The inclusion of the electrospun ZnO nanofibers increases the interfacial area between the ETL and active layer and provides enhanced electron transport pathways while the ALD ZnO layer provides film continuity and assists in passivating traps to mitigate defect states introduced by the nanofibers.

Three ETL architectures were investigated: ZnO fibers beneath ALD ZnO, ZnO fibers above ALD ZnO, and ALD ZnO control devices. ZnO nanofibers were fabricated through electrospinning of a zinc acetate dihydrate/polyvinylpyrrolidone (PVP) solution followed by calcination to oxidize the fibers and remove excess PVP. Device performance was evaluated through dark current density vs. voltage (J_{Dark}-V) and external quantum efficiency (EQE) measurements. Devices utilizing hybrid nanofiber/ALD ZnO ETLs exhibited reduced initial dark current compared to control devices indicating suppression of leakage pathways and trap-assisted recombination. Enhanced EQE response was observed in devices with fibers deposited above the ALD ZnO layer, suggesting improved interface quality and charge extraction.

These results demonstrate that combining electrospun ZnO nanostructures with ALD ZnO provides a promising method to engineer ETLs for high-performance OPDs and other optoelectronic devices.

AP+EL+PS+TF-ThP-8 Site-Specific and Temperature-Dependent Hydration of Faceted Hematite, ***Asare Dua***, Illinois Institute of Technology*; Luke Pretzie,* Purdue University*; Ashley Bielinski,* Argonne National Laboratory*; Yue Li,* Argonne National Lab*; Valentine Novosad, Cong Liu, Alex Martinson,* Argonne National Laboratory*; Adam Hock,* Illinois Institute of Technology

Alpha hematite (α-Fe_2O_3) is an abundant metal oxide whose surfaces and interfaces control key processes in catalysis, sensing, and photoelectrochemistry. While the more stable α-Fe_2O_3 (001) surface is well studied, less stable facets such as (012) and (104) which are more relevant in the aforementioned applications due to higher surface activity remain least studied. Surface sites of α-Fe_2O_3 (012) and (104), as well as their distinct stability were identified through temperature-dependent hydration by combining in situ infrared reflection absorption spectroscopy (IRAS) with density functional theory (DFT) vibrational analysis. For α-Fe_2O_3 (012), we found sites that promoted the dissociative and molecular adsorption of D_2O. Dissociatively adsorbed D_2O were either terminal or bridging. In both cases the hydroxyls were either isolated or interacting with nearby species. Protons of bridging hydroxyls (μ3a-OD (isolated); μ3b-OD (interacting with nearby hydroxyls)) are bound to triply coordinated surface oxygens while terminal hydroxyls (μ1a-OD (interacting with nearby hydroxyls)) were bound to octahedral surface Fe atoms (Fe_{oct}^{3+}). Similar to dissociatively adsorbed D_2O, molecularly adsorbed D_2O was either isolated (D_2Oa) or interacting with nearby hydroxyls (D_2Ob). α-Fe_2O_3 (104) on the other hand exhibited an isolated doubly coordinated bridging hydroxyl (μ2a-OD) and an interacting bridging species (μ2b-OD) rather than triply coordinated bridging hydroxyls. This preference is backed by our DFT calculations which

shows triply coordinated bridging hydroxyls were highly unstable on α-Fe_2O_3 (104). Results from IRAS showed two isolated terminal hydroxyls, μ1a-OD and μ1b-OD, were present on the surface of α-Fe_2O_3 (104). This indicates two types of undercoordinated surface atoms existed with the first being undercoordinated tetrahedral Fe atoms (Fe_{tet}^{3+}) since they're the surface atoms of α-Fe_2O_3 (104), while the second is from the second layer of Fe atoms which have octahedral geometry. The undercoordination of Fe_{oct}^{3+} atoms however suggests oxygen vacancies (V_o) were present and some of these might migrate from surface to the second lattice of α-Fe_2O_3 (104). Our temperature dependent studies support this hypothesis since the population of μ1a-OD, μ1b-OD, and μ2a-OD increased with increasing temperature when under vacuum (0.8 torr). The distinct local environments of the sites on α-Fe_2O_3 (012) and α-Fe_2O_3 (104) and changes in properties with respect to temperature revealed through this work provide a fundamental tool that may be used to engineer the surface of alpha hematite through site- or facet-selective atomic layer deposition.

Applied Surface Science
Room Ballroom A - Session AS-ThP
Applied Surface Science Poster Session

AS-ThP-1 Scratching at the Surface of Leadership, ***Brian Strohmeier,*** Surface Science Solutions, LLC

In today's dynamic research and business environment, strong technical skills are essential, but insufficient, for sustained career growth. Many exceptional scientists find themselves promoted to first-level management roles because of their outstanding scientific achievements, usually without having any formal training in leading people. Although they are well-prepared in technical and scientific areas, the toughest challenges for new managers usually involve delicate interpersonal skills, such as active listening, conflict resolution, empathy, and emotional intelligence, rather than science itself. Such topics are rarely encountered in graduate-level education and almost never in undergraduate curricula. To thrive amid constant change, managers and technical leaders need to hone and adapt their leadership styles to optimize resource management for each situation, focusing on prioritizing, empowering, and motivating their teams. This poster presentation will highlight effective modern leadership skills and strategies that can enhance your personal long-term growth and boost your career success.

AS-ThP-3 Sample Preparation Checklists and Instrument Parameter Tables: Newly Published Aids to Reliable and Reproducible Surface Analysis Data, Paper Reviewing, and Information Reporting, ***Don Baer,*** Pacific Northwest National Laboratory*; Linda Dake,* retired

Several examinations of surface analysis information reported in the literature indicate a significant degree of flawed data analysis and a high degree of inadequate reporting regarding sample handling, instrument operation and analysis details. This poster provides information about two newly published "tools" intended to help address three issues:

- Researchers and others with surface analysis needs, but unfamiliar with the sample handling requirements often present "damaged" samples for analysis.
- Information about how a sample has been handled before and in preparation for surface analysis is often not provided, and may not be recorded, limiting the ability of others, looking at a data report or in a publication, to assess the reliability of the analyses.
- Many publications do not contain either adequate sample or instrument information to assess the data quality or to verify adequacy for use in databases or AI input

To assist those unfamiliar with collecting and preparing samples for surface analysis and to assist surface analysts in collecting data that should be recorded, two checklists based on new ISO standards have been published in the open literature. The first checklist is designed to guide a sample owner in selecting, handling and transporting a sample to a surface analyst. The second checklist is intended to assist a surface analyst in obtaining and reporting information regarding sample treatment, processing and mounting for surface analysis. These are based on ISO standards 20579 part 1: Documenting and reporting the handling of specimens prior to analysis and ISO 20579 part 2, Documenting and Reporting the Preparation and Mounting of Specimens for Analysis. In addition to the reporting requirements, which include information about the sample history and analysis objectives, there are normative annexes that provide information about sources of sample contamination, ways to minimize contamination and expected or generally required components of sample handling to extract useful surface information.

A new series of papers in Surface Science Spectra is being published to help analysts and authors report the relevant instrument information and provide readers with the information needed to assess the meaning and quality of XPS data. Included in these papers are instrument parameter tables which provide both the "fixed" instrument parameters and those that are operator selected and need to be called out in reports and journal articles.

The poster will show the checklists and examples from published parameter tables.

AS-ThP-4 Atmosphere-Controlled Surface Engineering of $CuRh_2O_4$ Nanofibers For Alkaline Water Oxidation, ***Namhee Kim,*** *Hyeon Gyeong Jeon, Myung Hwa Kim,* Ewha Womans University, Republic of Korea*; Dasol Jin,* Jeonbuk National University, Republic of Korea

Controlling the surface chemical states of metal oxide electrocatalysts is critical for optimizing catalytic performance, yet Cu-based oxides pose a particular challenge since Cu readily shifts its oxidation state depending on the synthesis atmosphere. In this work, Cu-Rh bimetallic oxide nanofibers were prepared by electrospinning followed by post-annealing under controlled O_2/He flow, where the O_2 concentration was systematically varied to examine its effect on surface composition and phase evolution. AR-XPS analysis revealed that insufficient oxidation leaves Cu and Rh incompletely oxidized, while excess oxygen promotes unwanted secondary phase formation. Only at the optimized O_2 concentration were Cu^{2+} and Rh^{3+} simultaneously stabilized on the surface, and single-phase $CuRh_2O_4$ formation was verified by XRD and Raman spectroscopy. The phase-pure sample demonstrated superior oxygen evolution reaction (OER) activity in 1 M NaOH, outperforming commercial Ir/C, along with stable performance over extended operation. These results highlight that annealing atmosphere engineering is a straightforward yet powerful route to controlling surface chemical states and achieving phase-pure Cu-based spinel oxide electrocatalysts. This work was supported by the National Research Foundation of Korea funded by the Ministry of Science and ICT and the Ministry of Education. (NRF-RS-2018-NR031064 and RS-2025-16063688).

AS-ThP-5 Surface Chemical Characteristics of Electrospun Multicomponent Rutile Oxide Nanofibers for pH-Universal Oxygen Evolution Reactions, ***HyeonGyeong Jeon,*** *Namhee Kim, Youngmi Lee, Myung Hwa Kim,* Ewha Womans University, Republic of Korea

Lattice-entropy modulation in multicomponent oxide systems has attracted increasing interest as a strategy for tuning surface chemical environments and interfacial electrocatalytic properties. In this study, rutile-type $(RuIrCrMnSn)O_2$ nanofibers were fabricated via electrospinning followed by thermal treatment. Electron microscopy and elemental mapping analyses confirmed the formation of continuous fibrous structures with relatively uniform distributions of Ru, Ir, Cr, Mn, and Sn species throughout the oxide framework. X-ray diffraction, SAED, and Raman analyses supported the formation of rutile-related multicomponent oxide structures with broadened structural features associated with multication incorporation. X-ray photoelectron spectroscopy revealed mixed oxidation states and defect-related oxygen species on the oxide surface, indicating chemically diverse surface environments within the multicomponent oxide structure. Among the prepared samples, the $(RuIrCrMnSn)O_2$ nanofibers calcined at 400 °C exhibited overpotentials of 199.7, 244.4, and 330.1 mV at 10 mA cm^{-2} under acidic, alkaline, and neutral electrolytes, respectively. The optimized sample also maintained stable operation for up to 35 h in acidic electrolyte. These results suggest that multicomponent rutile oxide nanofibers can provide chemically diverse electrocatalytic interfaces for pH-universal oxygen evolution reactions. This work was supported by the National Research Foundation of Korea funded by the Ministry of Science and ICT and the Ministry of Education. (NRF- RS-2025-16063688).

AS-ThP-6 Industrial Problem Solving with Low-Cost ToF-SIMS, *Nick Long, Torsten Henkel,* SAI, UK*;* ***Aidan Harrison****, Silverio Iacono,* SAI Americas

Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) is often perceived as a complex high-end research tool requiring extreme mass resolution and accuracy. However, lower cost ToF-SIMS systems with restricted mass resolution operating at high vacuum levels for increased sample throughput remain exceptionally powerful for troubleshooting the processing of materials in industrial environments. These instruments can provide actionable data for resolving production bottlenecks, including (but not limited to) those arising in the following application areas.

Resolving Adhesion Failures

Adhesion problems in industrial processes often stem from monolayer-level surface modifications that are invisible to bulk analysis techniques. Low-cost ToF-SIMS excels here by identifying functional group distributions at the interface. For instance, the technique can detect sub monolayer presence of mold release agents (such as silicones or stearates) which can negatively impact adhesion performance. Additionally, a detailed inspection of the mass spectra from such surface contaminants can distinguish any subtle molecular differences between them in order to identify likely sources.

Detecting and Identifying Industrial Cleaning Residues

In a production electronics environment, contamination issues which can affect the performance of assembled parts often involve residues left by cleaning processes. These residues will have distinct signatures or fragmentation patterns that can be measured by ToF-SIMS even without high-resolution mass separation, helping to trace the source of the issue back to a specific stage in the manufacturing line such as a contaminated wash bath.

Detecting and Identifying Corrosion under Painted Metal Surfaces

Filiform corrosion is an atmospheric corrosion affecting organic coated metals by producing “threadlike” residues beneath the coating. Scanning Kelvin Probes can detect problems beneath the coatings physically by measuring work functions but for absolute chemical identification of the surface corrosion products a Low-Cost ToF-SIMS can provide the necessary answers.

Optimizing LDPE Roll Packaging Efficiency

The efficiency of Low-Density Polyethylene (LDPE) roll packaging often depends on the controlled migration of additives, specifically slip agents such as erucamide. These additives must bloom to the surface in precise concentrations to reduce friction during high-speed packaging processes. Restricted mass resolution ToF-SIMS is highly effective at monitoring the surface coverage of these slip agents, helping to resolve any blocking issues in the packaging process.

AS-ThP-7 Analysis of Interfaces by Soft and Hard X-ray Photoemission*, Jia Lu, *Jennifer Mann, Sarah Zaccarine, Norb Biderman, Cesar Saucedo, Kateryna Artyushkova,* Physical Electronics USA

Recent developments of lab-based hard X-ray photoelectron spectrometers (HAXPES) have created new, accessible opportunities for routine analysis of technologically significant devices. A micro-focused, monochromatic Cr Kα X-ray source not only provides three times greater analysis depth in comparison to the traditional Al Kα X-ray source, but it also provides high sensitivity for small area analysis. Using a combination of soft and hard X-rays allows for the analysis of materials non-destructively for their in-depth compositional heterogeneities. For film thicknesses that require ion beam sputtering to reach buried interfaces and layers, Cr sources allow one to probe below the depth of ion beam damage.

This poster will showcase how combining soft and hard x-ray photoemission within a single laboratory instrument offers a robust, non-destructive solution for chemical state analysis across the surface to bulk depth range. By using the micro-focused, monochromatic Cr X-ray source with increased analysis depth, accurate bonding chemistry and stoichiometry ratio of Ti/Al flakes (less than 100µm in diameter) can be probed below the surface organic contaminations with high sensitivity. In combination with soft X-rays, hard X-rays provide improved insight of how the NiPt nanowire surface was affected by annealing and surface treatments. Using a combination of XPS and HAXPES, high accuracy was obtained for calculating the thin film layer thickness of carbon/HfO_2/SiO_2/Si substrate using *Strata*PHI. For depth profile analysis of tin oxide, Cr X-ray source shows lower degree of tin reduction in comparison to Al X-ray source, showcasing its capability to probe below the depth of ion beam damage.

AS-ThP-8 Ion Scattering Spectroscopy to Identify and Quantify Selective Internal and External Decorations of Pt Nanoparticles on Porous Carbon Supports*, Alessio Cosenza, *Ich Tran, Plamen Atanassov,* University of California Irvine

Determining whether metal nanoparticles are located on the external surface or within the internal pore network of porous supports remains a key challenge in applied surface analysis, catalyst design, and host–guest nanomaterials. This distinction is especially important for porous carbon-supported Pt catalysts, where nanoparticle locality affects accessibility, utilization, and stability. However, common characterization methods provide incomplete information. TEM and dark-field imaging give projected contrast through the specimen thickness, making internal and external nanoparticles difficult to distinguish. Secondary-electron imaging is more surface-sensitive, but remains qualitative and can be ambiguous for nanoparticles beneath nanometer-scale carbon shells. XPS provides surface and chemical sensitivity, but Pt beneath thin carbon shells can still contribute to the Pt 4f signal because of the finite information depth.

Here, we investigate ion scattering spectroscopy (ISS) as a direct surface-sensitive approach to distinguish externally exposed Pt nanoparticles from Pt shielded inside mesoporous carbon black supports. Pt nanoparticles with similar size distributions were synthesized either within the carbon shell/pore network or on the external carbon surface. Carbon supports with different shell thicknesses and graphitic structures were used to evaluate how nanoparticle confinement affects the ISS and XPS response.

For each matched internal/external Pt pair, the external-Pt catalyst was used as a local reference corresponding to fully externally accessible Pt. The Pt ISS signal of the internal-Pt catalyst was normalized by total Pt loading and compared with the corresponding external reference. This provides a semi-quantitative estimate of the fraction of Pt accessible to the outermost surface. The complementary XPS response was used to evaluate how much of the internal Pt population remains detectable through the carbon shell, providing an apparent Pt 4f visibility factor rather than a direct measure of external exposure.

The results show that ISS can resolve large differences in external Pt accessibility between nominally similar Pt/C catalysts and estimate the fraction of nanoparticles shielded within the pore/shell structure. In contrast, XPS and electron microscopy provide valuable complementary information but cannot alone quantify nanoparticle locality in these non-ideal porous systems. This work establishes ISS as a practical surface-analysis tool for evaluating nanoparticle placement in porous catalyst supports and suggests broader application to host–guest, core–shell, encapsulated catalyst, and carbon peapod-type nanostructures.

AS-ThP-9 Probing Energy Level Alignments in NFA Organic Solar Cells: Combined UPS and LEIPS Study on Blend Films*, Yongsup Park, *Seunggu Lee,* Kyung Hee University, Republic of Korea

Energy level alignment (ELA) in non-fullerene acceptor (NFA) organic photovoltaic (OPV) cells is crucial, as the offsets between HOMO and LUMO levels at the bulk heterojunction (BHJ) interface determine charge separation efficiency and significantly affect the open-circuit voltage (Voc). Traditionally, ELA has been measured using a combination of cyclic voltammetry (CV) and optical absorption (OA), despite their limited accuracy. More precise measurements can be obtained through UV photoemission spectroscopy (UPS) and low-energy inverse photoemission spectroscopy (LEIPS). However, most studies have focused on neat films, while ELA can differ significantly in blend films. In this study, we used UPS and LEIPS to measure the HOMO and LUMO levels for both neat and blend films of the donor-acceptor pairs (PM6:Y6 and PM6:L8-BO). The results reveal significantly different ELA in blend films compared to neat films, particularly when using conventional vacuum level alignment was applied to the neat films. These differences are discussed in the context of Voc estimation and the impact of the HOMO offset (ΔE_HOMO) on charge separation efficiency.

AS-ThP-10 Tuning Topography and Morphology of Mg2-MOF-74 Metal-Organic-Framework to Study Optimization of Carbon Capture Capabilities*, Corbyn Stosich, *Sean Lubner,* Boston University

In order to combat the climate crisis and keep global warming under the 1.5℃ threshold for human safety, it is imperative that our net carbon emissions reach not only zero, but be negative by 2050 [1], [2]. To accomplish negative emissions, carbon capture via direct air capture (DAC) and point capture are necessary and on the scale of gigatons per year [3]. This process is energetically exhaustive due to the thermal energy required to regenerate carbon capture materials, and these energy demands cannot be met by global energy production [2], [3].

Metal organic frameworks (MOFs) are a highly tunable class of materials that have demonstrated exciting abilities in adsorption of CO_2 for point capture and primarily DAC purposes. These materials have particularly high CO_2 capacity with incredibly fast kinetics. The tunable nanostructure inherent to MOFs allows for many ways to minimize the energy requirement of material regeneration.

In this work, we tweak synthesis environments of otherwise identical MOF materials (Mg_2-MOF-74) to study the resulting topography and morphology. This process is accomplished through heterogeneous crystallization on

different substrates with varying temperature and polarity environments. We then characterize the resulting crystals by running BET, SEM, and NMR to identify both surface and chemical variances. We aim to isolate variables such as crystal length and orientation, porosity, pore percent, and surface area. These factors influence the MOF's ability to capture CO_2 as capacity, kinetics, and selectivity are affected and measured by TGA and our house dynamic gas sorption system. By tuning the nanostructure of these materials, we aim to optimize these variables to alleviate the energy burden of sorbent regeneration.

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AS-ThP-11 XPS Analysis of Plasma Exposed TiB2 and ZrB2 Substrates, ***Harry Meyer**, Lauren Nuckols, Chad Parrish,* Oak Ridge National Laboratory

Deuterium and hydrogen plasma exposures were performed on ultra-high temperature ceramics TiB2 and ZrB2 using the PISCES-RF linear plasma device as early screening tests for first wall, plasma facing material applications. These ion plasma exposures were performed using 40 eV ion energies at 240, 525, and 800 ◦C sample temperatures and 90 eV ion energies at 240 ◦C sample temperatures to analyze TiB2 and ZrB2 sputtering and surface morphology evolution behavior. Post-plasma exposure chemistry characterization of the near surface (< 50 nm) region using x-ray photoelectron spectroscopy (XPS) shows transition metal enrichment, indicating boron preferential erosion, and resulting in reduced total sputtering yields compared to predicted assuming stoichiometric sputtering. Transition metal to boron fractions vary with plasma exposure temperature under the 40 eV ion energy exposure at different temperatures; metal enrichment is maximized at 800 ◦C and then minimized at 525 ◦C. Sputtering yield measurements of the 40 eV ion energy plasma exposed samples show that the samples with greater metal surface enrichment have lower sputtering yields, likely due to the rougher surfaces of the more metal-enriched samples leading to higher instances of prompt redeposition processes. XPS data was acquired on the as-exposed TiB2 and ZrB2 samples. Depth profiles were then done to track the amounts of T (or Zr) and B as a function of Ar-ion sputter depth. Data was finally acquired on the well sputtered sample surfaces. This abstract has been authored by UT-Battelle, LLC under Contract No. DE-AC05-00OR22725 with the U.S. Department of Energy.

AS-ThP-12 Thin-Film Characterization Using the Surface Analysis Toolbox: From Data to Answers, ***Jonathan Counsell**,* Kratos Analytical Limited, UK

Thin films play a critical role in semiconductor devices and coatings due to their unique physical and chemical properties. Accurate characterization of these films is essential for understanding their behaviour and optimizing their performance. The surface analysis toolbox, including techniques such XPS, HAXPES and both destructive and non-destructive methods.

In this study, we utilize the surface analysis toolbox to characterize metal oxide and nitride thin films focusing on the interfacial regions where different materials meet. We employ XPS to determine the chemical states of elements in the thin films, particularly focusing on interfacial oxidation states. HAXPES is used to complement XPS by providing information on the elemental composition and depth profiling of the thin films.

By integrating these surface analysis tools, we capture detailed information about the chemical interactions and electronic configurations at the interfaces. Our work aims to bridge the gap between raw data and meaningful interpretations, providing a comprehensive understanding of the thin-film characteristics. Through optimized sample preparation and advanced data analysis techniques, we offer insights into the fundamental properties of thin films, enabling the development of more reliable and efficient semiconductor technologies.

AS-ThP-13 Cryo-XPS of nanoparticles. Vitrification... where speed is everything!, ***Chris Moffitt**,* Kratos Analytical Inc.*; Liam Soomary,* kratos Analytical Inc, UK

Vitrification, a rapid cooling process that prevents ice formation, is crucial for preserving the structural integrity of nanoparticles during cryogenic applications. In this study, we employ Cryo-XPS (X-ray Photoelectron Spectroscopy) to investigate the surface chemistry and phase transformations of various nanoparticle types during the vitrification process. Our findings highlight the importance of ultrafast cooling rates in maintaining the desired physical and chemical properties of these materials. We discuss the challenges associated with achieving uniform vitrification across different nanoparticle sizes and compositions and propose strategies to optimize and improve experimental workflows during the vitrification process for enhanced material stability and performance. These insights are particularly relevant for applications in nanotechnology, biomedicine, and advanced materials science.

AS-ThP-14 Surface and Bulk Characterization of Organic Macrocyclic Coordination Compounds Using XPS and UPS Techniques, ***David Surman**,* Kratos Analytical Inc.

Organic semiconductors have gained attention due to their potential for flexible, lightweight, and low-cost electronic applications. These materials enable charge transport via delocalized electronic states, a characteristic of their pi-conjugated molecular structures. Their utility includes various organic electronic devices, such as Organic Thin-Film Transistors (OTFTs) and Organic Photovoltaics (OPVs). The selection and performance of these materials depend on properties such as charge carrier mobility, energy level alignment, and stability. Here we utilize a combination of experimental methods - XPS and XPS imaging, to probe the surface and bulk properties of both blanket and printed organic semiconductor structures. We will discuss the relevance of scattered electron backgrounds and background subtraction for analytical clues. Also, we will explore the effects of deposition processes and the evolution of electrical properties as a function of depth using Argon cluster etching ultra thin layers. UPS is also used in with profiling to give not just an elemental distribution but also the electronic properties of these molecules as a function of depth, determining the work function of these materials, a critical parameter in optimizing charge injection and transport. A methodological approach to surface characterization will also be discussed, providing insights into the interfacial properties that govern device performance.

AS-ThP-15 Automatically Determining the Cutoff of the Transfer Function in Reciprocal Space for the Fourier Denoising of X-ray Photoelectron Spectroscopy Data, ***Tyler B. Andersen**, Maxsym Gerashchenko, David E. Aspnes, Matthew R. Linford,* Brigham Young University

The Fourier denoising of X–ray photoelectron spectroscopy (XPS) data is valuable when optimal (low noise) XPS data cannot be collected. It should also prove to be important when preparing XPS data for analysis by artificial intelligence (AI). Because of its sigmoidal shape in reciprocal space, its adjustable position, and the shape of its Fourier transform in real space, the Gauss-Hermite transfer function is an excellent transfer function for denoising data. However, the position of this transfer function on a set of Fourier coefficients is determined manually by the user. In this work, we describe two algorithms for automating this positioning. It is believed that these algorithms will also work for other transfer functions, e.g, the brick wall filter function. In addition, these approaches should apply well to data from other techniques, for example, spectroscopic ellipsometry, low-energy electron scattering, and x-ray diffraction, among others.

AS-ThP-17 Heterointerface-Induced Charge Transfer Kinetics in Sputtered $MoTe_2$-MoS_2 Nanocomposite for High-Performance Ambient NO_2 Detection, *Sonika Kodan,* ***Ramesh Chandra**,* Indian Institute of Technology Roorkee, India

The present research reports a nanostructured $MoTe_2$-MoS_2 n-n heterojunction-based gas sensor developed on a silicon (Si) substrate, demonstrating room-temperature (RT, 30 °C) nitrogen dioxide (NO_2) sensing. A controlled and one-step magnetron co-sputtering approach is utilized to deposit $MoTe_2$-MoS_2 nanocomposite thin film on a Si substrate, producing a uniform, dense, and porous nanoscale morphology. Herein, surface analysis and structural characterization of the $MoTe_2$-MoS_2/Si sensor reveal a rough, and defect-rich morphology with abundant exposed edge sites, which significantly enhances the availability of active adsorption sites for effective gas sensing. The developed $MoTe_2$-MoS_2/Si heterostructured sensor delivers an exceptional sensor response of 74.4% with an ultrafast response/recovery time of 7.5/2 s towards 25 ppm NO_2 at RT. Additionally, the present sensor showcases highly reproducible and consistent behavior over a wide range of NO_2 concentrations (1-60 ppm), along with remarkable selectivity against common potential interfering gases (H_2S, NH_3, CO, H_2) and a low detection limit of 700 ppb. This study provides critical insights into NO_2 sensing induced by heterointerface band modulation and defect-assisted adsorption at the sensor's surface, thereby

providing a strong foundation for a reliable platform for high-performance NO_2 gas sensors based on the MoTe2-MoS2 heterostructure.

AS-ThP-18 ASSD Student Award Finalist Poster: Sen-Banerjee (SB) Number as a Unified Scaling Parameter for Deviant Density Enhancement in Nanofluids, ***Anusree Sen***, *Debjyoti Banerjee,* Texas A&M University

Nanofluids are attractive for modulating heat transfer (thermal management), energy storage (e.g., battery), transport, and radiation-shielding applications because adding nanoparticles can anomalously change the effective properties of a base fluid (neat solvent). In practice, measured property changes (e.g., density) do not match the classical two-phase mixture model predictions. This mismatch is usually tied to interfacial effects near the particle surface that standard models do not include.

In this study, we evaluate the Sen-Banerjee number (S_B) as a practical scaling parameter for interpreting and predicting these anomalous density deviations. The analysis leverages a three-phase model of a nanofluid: the nanoparticle, the surrounding bulk liquid, and a compressed interfacial liquid layer formed at the solid-liquid boundary (this is also termed as the "*nano-Fin effect*" or "*nFE*"). We tested the framework across three representative nanofluid families, molten-salt nanofluids, poly-alpha-olefin nanofluids, and casein oleo-nanofluids, while varying nanoparticle shape, nanoparticle mass fraction, and interfacial-layer thickness.

A clear pattern emerges when surplus density is plotted against the Sen-Banerjee number (S_B). Interestingly, results from different systems and particle geometries collapse toward a common trend. At low S_B, density enhancement is stronger and highly sensitive to small changes in concentration. At higher S_B, the response gradually approaches classical mixture-rule behavior (two-phase mixture rule). Among the systems studied, casein oleo-nanofluids show the strongest deviations, consistent with their density contrast between phases. Overall, SB offers a physically meaningful and scalable way to compare nanofluids and guide formulation choices for targeted applications.

KEYWORDS: Sen-Banerjee number; nanofluids; deviant density; interfacial compressed layer; nano-Fin effect; thermophysical properties; scaling analysis; density enhancement, anomalous property, nFE.

AS-ThP-20 A Priori designed NiAg Single-Atom Alloys for Selective Epoxidation Reactions, ***E. Charles H. Sykes***, Tufts University

Ethylene oxide, produced through the partial oxidation of ethylene, is one of the highest-volume chemicals manufactured globally—and also one of the most carbon-intensive. While silver (Ag) catalysts can achieve high selectivity (~90%) for ethylene oxide, this requires a combination of promoters such as chlorine (Cl), which increases selectivity by 25%, cesium (Cs), and rhenium (Re). The reaction must also be run at low conversions (<15%) to prevent complete combustion of ethylene to CO_2. In this work, we present a theory-guided investigation showing that the incorporation of small amounts of nickel (Ni) into Ag(111) surfaces lowers the activation barrier for O_2 dissociation and facilitates the spillover of atomic oxygen onto the Ag surface. Temperature-programmed desorption (TPD) experiments confirm the facile dissociation, spillover, and desorption of O_2 on NiAg(111). Remarkably, and in contrast to previous studies, Ni enables the formation of atomic oxygen on Ag(111) under near-ultra-high vacuum conditions without the need for oxygen atomizers or reactive species like NO_2 or O_3. Ambient pressure X-ray photoelectron spectroscopy (AP-XPS) further reveals that Ni not only promotes O_2 activation and spillover but also stabilizes nucleophilic oxygen species, which are typically associated with total combustion pathways. Guided by these findings, we synthesized and tested supported catalysts, demonstrating that NiAg single-atom alloy nanoparticles improve both conversion and ethylene oxide selectivity by 25%—achieved without the use of Cl, the ubiquitous industrial promoter.

Reference

1. A. Jalil, E. E. Happel, L. Cramer, A. Hunt, A. S. Hoffman, I. Waluyo, M. M. Montemore, P. Christopher, and E. C.H. Sykes Nickel promotes selective ethylene epoxidation on silver *Science* **387**, 869-873 (2025)

Biomaterial Interfaces
Room Ballroom A - Session BI-ThP
Biomaterial Interfaces Poster Session

BI-ThP-1 Interactions of KSCN with Phospholipid Monolayers Studied by Sum Frequency Generation and X-Ray Fluorescence, ***Sadia Afroz***, Pennsylvania State University*; Bastian Mueller, Emanuel Schneck,* TU Darmstadt, Germany*; Paul S. Cremer,* Pennsylvania State University

Thiocyanate (SCN^-) is a weakly hydrated anion that can interact relatively strongly with lipid membranes compared to other anions in the Hofmeister series. To date, the specific mechanisms governing this processes remain poorly characterized. To shed light on ion-lipid membrane interactions, we introduced KSCN into the subphase below 1,2-dilauroyl-sn-glycero-3-phosphocholine (DLPC) monolayers. This saturated lipid was chosen because it remains in the fluid phase at room temperature. Both the two-dimensional pressure of the monolayer and the salt concentration were varied. SFG was used to follow vibrational signals associated with the interfacial water structure, the lipid headgroups, the ordering of the alkyl chains, as well as the SCN^- anions. Such data are vital for characterizing the system, but the concentration of interfacial ions is not directly quantifiable. As such, we also employed total reflection X-ray fluorescence which can monitor the interfacial concentration of both K^+ and SCN^- concentrations. Details of these interactions as well as their implications for Hofmeister chemistry will be discussed.

BI-ThP-2 The Neurotoxin Vipoxin Induces Changes in Mechanical Properties of Breast Epithelial Cells, *William Linthicum,* Oxford Instruments*; Qi Wen,* ***Nancy Burnham***, Worcester Polytechnic Institute*; Svetla Petrova, Konstantin Balashev,* Sofia University, Bulgaria

The investigation of how drugs or toxins alter cell mechanics is gaining significant traction in biomedical science, driven by the dual objectives of elucidating their mechanisms of action and enhancing drug screening processes. In this study, Atomic Force Microscopy (AFM) was employed to examine and analyze the mechanical responses of cells exposed to the neurotoxin Vipoxin. This method enables the precise measurement of key mechanical parameters such as cell stiffness and viscoelasticity before and after toxin introduction in the cell culture. It was demonstrated that the cells' stiffness and viscosity decreased with increasing Vipoxin concentration. Additionally, Total Internal Reflection Fluorescence Microscopy (TIRFM) was utilized to monitor morphological changes in the cells over time. These morphological changes were quantitatively analyzed using fractal analysis of the acquired images. The observed changes in cell shapes implied the reorganization of the cell cytoskeleton, thus providing insight into the cell mechanics under the influence of Vipoxin.

BI-ThP-3 Sustainable Bioinspired Polymer–Mineral Composites for Adaptable Repair in Conservation Applications, ***Zoe Weber-Porter***, *Rishima Agnihotri, Ashwin Marichetty, Marco Rolandi,* UC Santa Cruz

Every year, tens of thousands of tons of plaster-based materials are used in restoration and conservation applications, many of which are derived from non-renewable sources and discarded at the end of their service life. Here, we introduce a biodegradable, bio-derived composite based on chitosan and calcium carbonate that is composed of simple, widely available constituents and designed for adaptable repair applications. By varying polymer molecular weight, concentration, and mineral content, the composite can be formulated to span injectable, paste-like, and putty-like behaviors, enabling accommodation of diverse structural filling and stabilization needs. We examine relationships between composition, flow behavior, and mechanical performance through rheological characterization of the wet composite and measurements of bulk density, porosity, and compressive strength in the hardened state. Rather than targeting a single optimized formulation, this work demonstrates a tunable material platform in which relationships between composition, flow behavior and mechanical performance guide selection of material behavior based on application requirements. Future applications of this approach include sustainable repair and conservation materials for exhibits, architectural restoration, and other contexts where adaptable handling, mechanical integrity, and biodegradability are desired.

BI-ThP-5 Pulsed Plasma Surface Functionalized Nanosilver for Gene Delivery, ***Ajinkya Trimukhe,*** University of Milan Bicocca, Italy*; Prasad Pofali,* Pravara Institute of Medical Sciences, India*; Amogh Vaidya,* University of Texas Southwestern Medical Center*; Uday Koli, Prajakta Dandekar, Rajendrasing Deshmukh, Ratnesh Jain,* Institute of Chemical Technology, India

The efficient intracellular delivery of nucleic acids remains limited by the lack of vectors that are both effective and biocompatible. In this study, we synthesized silver nanoparticles, that were surface-engineered using low-pressure pulsed RF plasma polymerization with acrylic acid in vapor phase to introduce carboxylic functionalities, followed by covalent coupling to chitosan oligosaccharide (COS) through EDC chemistry, yielding metallo-polymeric nanocarriers (MPNCs). Surface functionalization characterization confirmed successful functionalization: FTIR and XPS evidenced carboxylation and amide bond formation, while DLS showed an increase in hydrodynamic size from AgNPs to AgNPs/COOH (166.3±23.04 nm) and then to MPNCs with attached DNA (276.0±17.75 nm). Zeta potential shifted from negative values for AgNPs (-13.4±1.39 mV) to strongly positive values for MPNCs, supporting electrostatic complexation with plasmid DNA (27.0±1.1 mV). Gel retardation assays demonstrated stable nanoplex formation at a plasmid:MPNC ratio of 1:6, and the complexes remained stable across a broad pH range. Importantly, the MPNCs protected plasmid DNA against both DNase I degradation and sequence-specific restriction digestion. Cell viability assay demonstrated that the COS used to encapsulate the modified nanosilver using EDC (92.05±9.46% and 102.79±2.85%), was substantially less cytotoxic than bare AgNPs (0% and 0%), and AgNPs/COOH (0% and 0%) equivalent to Triton X-100 (positive control); MPNCs at 0.5 mg/ml (87.06±3.98% and 93.55±1.65%) maintained high viability in A549 and HeLa cells respectively. Cellular uptake studies (in-vitro) further showed that MPNC-bound plasmid-DNA was internalized efficiently, with GFP expression detected in A549 cells and quantified by flow cytometry, reaching about 10% transfection efficiency at 24 h. Overall, the work demonstrates that pulsed plasma surface functionalization, combined with COS conjugation, can transform silver nanoparticles into a stable, biocompatible, positively charged non-viral vector with meaningful gene delivery performance.

BI-ThP-6 UVC Surface Sterilization Comparative Study via a New, Rapid Handheld Bio-Sensor for Pathogens, InnovaBug™, using Macroscopic DNA/RNA Epi-Fluorescence On Calibrated *E.Coli* Cultures Vs Standard Plating, *Nicole Herbots,* Arizona State University Department of Physics/SiO2 Innovates LLC/InnovaBug LLC*; Archana Suresh, Adith Shankar,* SiO2 Innovates LLC/BacteroBug LLC/FungiBug LLC*; Ananya Suresh,* SiO2 Innovates LLC/BacteroBug LLC/InnovaBug LLC*; Manassa Suresh,* SiO2 Innovates LLC/BacteroBug LLC/FungiBug LLC*; **Viraj Amin**, Zaid Abu-Salah, Nachiket Rajinikhant,* University of Missouri-Kansas City School of Medicine/SiO2 Innovates LLC/InnovaBug LLC*; Cara Jacobs,* University of Missouri-Kansas City/SiO2 Innovates LLC/InnovaBug LLC*; Eric J. Culbertson,* SiO2 Innovates LLC/InnovaBug LLC*; Robert J. Culbertson,* Arizona State University Department of Physics

Anti-Microbial Resistance kills 50,000 patients/y in the US, 1.3 Mil /y globally. Meanwhile, since 2009, new pathogens, epidemics, pandemics and global outbreaks occur about every 2.5 years, not every 8-year as measured since the 1800s. H1N1 (2009), MERS (2012), Ebola (2014), Zika (2015), Covid-19 (2019), mpox (2022), Ebola-causing Bundibugyo virus disease (BVD) (2026) – occurred in the last 17 years.

Two key strategies to address such crisis are prevention and detection, in other words, sanitation and sterilization as prevention, especially of surfaces, and rapid triage of infected patients as detection.

Standard sterilization methods such as autoclaving at 121 °C under high water steam pressure and gamma irradiation are not usable in public and hospital spaces. But an - as of yet unestablished - sterilization method, UVC, potentially is.

In this work, a methodology for sterilization via UVC irradiation, is investigated on two different model bacteria to establish which combinations of UVC irradiation dose can meet sterilization criteria.

Sterilization criteria require reducing the probability for a single viable microorganism to remain, to less than 10^{-6}, which is also defined as a Sterility Assurance Level (SAL) of 6.

UVC irradiation can eradicate pathogens by breaking bonds in nucleic acid pairs in DNA/RNA and is used in disinfection (SAL = 3). The present study investigates 260-280 nm LEDs to sterilize surfaces beyond disinfection (SAL=3) using as model bacteria *Lactobacillus Acidophilus* and *E.Coli*. to achieve full sterilization, or SAL 6.

The LEDs deliver a power density of 80 ± 0.04 μW/cm^2, at a distance of 1 cm. For reproducibility and accuracy, six identical sets of 10 cultures are tested, three of which are used for control and three of which are irradiated.

*E. Coli*CFU counts were calibrated to yield 20 ± 5 × 10^{9}typical for microbial cultures reproducibility. After serial dilution, A and B are inoculated. The three control sets are compared to three sets irradiated for 180 second at 1 cm on one half of the plate, while the other half is shielded to remain unirradiated. This is to verify that absence or limits on bacterial growth in the UVC irradiated area is indeed due to irradiation, not failed culturing.

Irradiation for 180 s. yields a total of 144 ± 7 mJ/cm^{2}on a 4 cm^{2}square area, and an average kill rate of 99.9999% on surfaces, with reproducibility achieved over 9 different plates.

In conclusion, UVC LEDs can consistently achieve sterilization with a SAL of 6. However, the timeframe for final sterilization may not be immediate, as measured within minutes with a new sensor, InnovaBug™, instead of after 48 hours culturing.

BI-ThP-7 Physics–Driven Mechanisms Governing the Pharmacokinetics and Immune Fate of Gold Nanoparticles: The ADIE Framework Perspective, ***Bashiru Sodipo,*** Kaduna State University, Nigeria*; Hafsah Oyedokun,* Kaduna University, Nigeria

The clinical translation of gold nanoparticles (GNPs) in nanomedicine hinges on a mechanistic understanding of their pharmacokinetics (PK) at the nano–bio interface. Traditional ADME (Absorption, Distribution, Metabolism, Elimination) model is effective for small molecules and biodegradable polymers. But it fails to capture the unique behaviour of inorganic GNPs, which are non-biodegradable, and not subject to enzymatic metabolism. Also, the interactions of GNPs in-vivo are not random biochemical processes. This Perspective introduces the ADIE (Absorption, Distribution, Immune interaction, and Elimination) framework. Immune interaction replaces metabolism as the pivotal phase. The journey of GNPs in-vivo is governed by transport physics and interfacial energetics. Convection and diffusion dictate distribution of the GNPs. While the collision of the nanoparticles with blood biomolecules and protein corona (PC) formation is governed by stochastic Brownian motion. The PC dictates immune recognition through competitive adsorption and thermodynamic binding energies. Also, it determines opsonization and clearance pathways. The elimination of GNPs is mainly via renal elimination. This is governed by size-exclusion physics and stealth coating (surface chemistry) property of the inorganic nanoparticles. While hepatic sequestration results from immune recognition. ADIE model offers a predictive foundation for designing GNPs with optimized biodistribution and clearance. Also, it advances the rational development of nanomedicines by integrating principles of transport physics, interfacial thermodynamics, and immune interaction.

BI-ThP-8 Rapid Solidification of Blood Drops Into Homogeneous Thin Films via Hyper-Hydrophilic Coatings: Electrolytes and Blood Iron Comparative Analysis by EXAFS, XRF and RBS, *Nicole Herbots, Yash Pershad,* ***Thilina Balassoriya**, Nikhil Suresh, Wesley Peng, Saaketh Narayan, Rianna Rane, Harshini Thinakaran, Ashwin Suresh,* Arizona State University Department of Physics/SiO2 Innovates LLC/MicroDrop Diagnostics LLC*; Arjun Sekar,* Arizona State University Department of Physics/SiO2 Innovates LLC/MicroDrop Diagnostics*; Aarush Thinakaran, Arya Saravanan,* Arizona State University Department of Physics/SiO2 Innovates LLC/MicroDrop Diagnostics LLC*; Robert J. Culbertson,* Arizona State University Department of Physics

The most common, initial test to diagnose a plethora of conditions – especially in ERs- is to test electrolytes and blood iron quickly so that the most common causes conditions such dehydration, hyponatremia, anemia, de-nutrition, etc can be assessed .. In 2026, 4 to 10 milliliters (mL) of blood are the standard Blood Volume (BV) required per test, with 10 mL being the most commonly sampled BV.

Drawing 3 to 8 vials is the norm, for a total of 30 to 80 mL blood per test. In hospitals, such tests are conducted **daily**. Iron anemia occurs when 10% of BV has been removed. It takes only 5 to 10 days to cause 75% of patients to incur Hospital-Acquired Anemia (HAA) In infants, it is standard practice to replace their ***entire*** blood volumes by continuous transfusion every 10 days.

Reducing BV can improve healthcare practices and outcomes.

HemaDrop™ is a ***Hyper-Hydrophilic*** coating that can rapidly solidify microliters (μL) sized blood droplets in minutes.

Hyper-Hydrophilicity (HH) can flatten droplets into flat films by rapidly absorbing H_2O, transforming liquid drops into Homogeneous Thin Solid

Films (HTSF) without phase separation or segregation. Solidification via HH occurs no matter the temperature and relative humidity. By instantly flattening drops into thin liquid films with large areas of contact, HemaDrop™ does not rely on surface evaporation, unlike coagulation.

Inhibiting coagulation yields HTSF with smooth, glistening surfaces and uniform thickness unlike the rough surfaces and uneven thickness of conventional Dried Blood Spots (DBS). 0.05 mL or 50 µL of blood yields HTSF of uniform composition to ±10% over ~0.25 cm^2, or 5 mm diameter blood disks.

Rapid solidification of blood drops via HH allows for solid state analysis in minutes via hand-held X-ray Fluorescence (XRF) while the BV drawn is reduced to 0.1 mL

Three independent methods were used to test this proposition.

Rutherford Backscattering Spectrometry (RBS) is used to study lateral uniformity, absolute elemental composition. compositional depth profile, and comparison to DBS.

X-ray Fluorescence (XRF) measured relative elemental composition of the blood HTSF

Extended X-ray Absorption Fine Structures (EXAFS) was used to detect blood iron to p.p.b.. EXAFS spectra show consistent, reproducible detection iron in multiple HTSFs of the same blood.

Accuracy and reproducibility of Solid State Analysis of Blood HTSFs via RBS, XRF, and EXAFS were tested by measuring electrolytes (Na, K, Mg, Ca, Cl) and Fe from single 50- µL droplets. Relative error analysis for XRF, RBS and EXAFS measured on multiple HTSFs shows reproducibility within 10%, the medically accepted standard.

BI-ThP-9 Rapid Differential Detection & Triage of Bacterial, Viral & Fungal Infection Triage for Early Outbreak Containment via Differential Macroscopic DNA/RNA Epi-Fluorescence (DMEF) in a Small Fluid Volume Diagnostic (SFVD) handheld Device: MicrobeD™*, Nicole Herbots,* Arizona State University Department of Physics/SiO2 Innovates LLC/InnovaBug LLC*; **David Guo**,* Drexel University School of Medicine/SiO2 Innovates LLC/InnovaBug LLC/ViroBug LLC*; Arya Saravanan,* Arizona State University School of Health Sciences/SiO2 Innovates LLC/BacteroBug LLC/MicrobeD LLC*; Nithish Prakash,* University of Pennsylvania School of Medicine/SiO2 Innovates LLC/InnovaBug LLC/ViroBug LLC/MicrobeD LLC/*; Manassa Suresh,* SiO2 Innovates LLC/InnovaBug LLC/MicrobeD LLC*; Jonathan Guo,* SiO2 Innovates LLC/InnovaBug LLC/ViroBug LL/MicrobeD LLC*; Nila Kathivaran,* Arizona State University Department of Physics/SiO2 Innovates LLC/BacteroBug LLC/MicrobeD LLC*; Sudharshini (Sudhi) Ram,* Arizona State University Department of Physics/InnovaBug LLC/ViroBug LLC/MicrobeD LLC/AID-TRIAGE LLC*; Ananya Suresh,* Arizona State University Department of Physics/SIO2 Innovates LLC/BacteroBug™/MicrobeD LLC*; Archana Suresh,* Arizona State University Department of Physics/SiO2 Innovates LLC/BacteroBug LLC/MicrobeD LLC*; Adith Shankar,* Arizona State University Department of Physics/SiO2 Innovates LLC/innovaBug LLC/MicrobeD LLC*; Esther Guo,* Arizona State University Department of Physics/SiO2 Innovates LLC/Innovabug LLC/ViroBug LLC/MicrobeD LLC*; Sriram Rajesh, Edawrd Kelemen,* Arizona State University Department of Physics/SiO2 Innovates LLC/InnovaBug LLC/BacteroBug LLC/MicrobeD LLC

In the years 2000-2026, **ten** viraloutbreaks have arisen, **four from new viruses**: West Nile (2003), **SARS-Cov-1 (2002-04),H1N1/Swine flu (2009-10), MERS-CoV (2012)**, Zaire Ebola virus (2013-2016), Zika (2015-2016), **COVID-19 (2019-21),**mpox (2022), Ebola-causing Bundibugyo Virus (BVD) (4/24/2026-), Andes Hantavirus, (5/9/2026-), thus one outbreak per 2.6 years, in contrast to an average of 1 per 8.5 years between 1800 and 2000.

Current diagnostics for viral infections use polymerase chain reaction (PCR) and virus-specific antigens. Covid-19 PCR swabs yield 40 % False Negatives (FN), 50% False Positives (FP) in the first 7 days of infection and need 3 days and advanced lab equipment for results. Covid-19 Rapid Antigen tests yield 66% FN and 40% FP in asymptomatic individuals.

Rapid, reliable detection of viruses is needed early in outbreaks until virus-specific tests are available. Two months into the 2026 Ebola BVD outbreak, **no** BVD tests exist. OTC COVID-19 became widely available only on Dec. 15, 2020, 12 months on.

Here, a new approach for detection and triage, *Differential Macroscopic DNA/RNA epi-fluorescence (DMEF),* uses test strips inserted a single hand-held, 'Small Fluid Volume Diagnostic' (SFVD) device, MicrobeD™*, akin to a blood glucose meter, but designed as an accessory to attached to a Smartphone camera. Test strips - called InnovaBug™*, with design subcategories specified as BacteroBug™*for bacteria , ViroBug™* for viruses, and FungiBug™ for fungi, are optimized to detect and differentiate in minutes viral infections and loads from bacterial ones, use pairs of 0.015 mL drops, and aim for an accuracy ≤ 10% for FN and FP, 10% being the medical gold standard.

Strips combine DMEF from different dyes.

Micro-filters integrated to the strips impregnate blood serum, urine, sputum, etc .. with safe DNA/RNA fluorophores.

The strips are inserted into MicrobeD™, where the smartphone camera captures irradiances: $I_B$of LEDs inducing fluorescence, and fluorescence irradiances, $I_F$from DNA and RNA. Net $I_F$are analyzed via an AI App, AID-TRIAGE™*, which normalizes $I_{F\ with} I_B$, as a $R_{F/B}$ratio. AID-TRAIGE™ matches $R_{F/B}$to pathogen type and load via calibration tables from plating and assays databases. Sensitivity spans $10^5$to 10^9CFUs/mL, test duration ~ 5 -20 min. DMEF was collected on 500 InnovaBug™ strips, in 4 labs disseminated in Phoenix Metro, via 12 studies over 2 years with 4 MicrobeD™ prototypes. Manual analysis and AID-Triage™ established proof-of-concept, accuracy & reproducibility of DMEF to detect and differentiate pathogen types and loads via*in vitro*diagnostic device, MicrobeD™, InnovaBug™* test strips and the AID-Triage™ App.

* Patents Pending (2026)

BI-ThP-10 Decoding Antifouling Failure: How Primary Microfouling Communities Compromise Biocide Release*, **Kailey Richard**,* National Research Council Research Associateship Program at US Naval Research Laboratory*; Kenan Fears,* Naval Research Laboratory

For decades, copper-based marine coatings have been the primary defense against biofouling. However, their failure, suspected to be caused by microbial copper tolerance, is a growing concern. Primary colonizers, like bacteria and diatoms, can develop resistance, forming biofilms that may slow biocide release and accelerate macrofouling. This study investigates the role of key fouling species in this process, with a focus on diatoms. To achieve this, we exposed *Navicula incerta* and the green alga *Enteromorpha* sp. to copper biocides, copper (II) ions and copper (II) pyrithione, to assess their level of tolerance, their influence on the biocides chemical state, and their impact on copper release rates. Furthermore, this study investigates the interactions between bacterial and diatom communities, by establishing bacterial biofilms on coatings prior to the introduction of diatoms to observe the effects on subsequent diatom adhesion and growth.

Advances in Battery Engineering, Interface Design, and Characterization Mini-Symposium
Room Ballroom A - Session BT+AS+CA+TF-ThP
Advances in Battery Engineering, Interface Design, and Characterization Mini-Symposium Poster Session

BT+AS+CA+TF-ThP-1 Orientated Deposition of Li2S for Fast-Charging Lithium-Sulfur Batteries*, Jeong-Hoon Yu, **Jong-Sung Yu**,* DGIST, Republic of Korea

Precipitation/dissolution of insulating Li_2S has long been recognized as the rate-determining step in lithium–sulfur (Li–S) batteries, which dramatically undermines sulfur utilization at elevated charging rates. Herein, we present an orientated Li_2S deposition strategy to achieve extreme fast charging (XFC, ≤15 min) through synergistic control of porosity, electronic conductivity, and anchoring sites of electrode substrate. Via magnesiothermic reduction of a zeolitic imidazolate framework (ZIF), a nitrogen-doped and hierarchical porous carbon with highly graphitic phase was developed. This design effectively reduces interfacial resistance and ensures efficient sequestration of polysulfides during deposition, leading to (110)-preferred growth of Li_2S nanocrystalline between (002)-dominated graphitic layers. Our approach directs an alternative Li_2S deposition pathway to the commonly reported lateral growth and 3D thickening growth mode, ameliorating the electrode passivation. Therefore, a Li–S cell capable of charging/discharging at 5C (12 min) while maintaining excellent cycling stability (82% capacity retention) for 1000 cycles is demonstrated. Even under high S loading (8.3 mg cm^{-2}) and low electrolyte/sulfur ratio (3.8 µL mg^{-1}), the sulfur cathode still delivers a high areal capacity of >7 mAh cm^{-2} for 80 cycles.

BT+AS+CA+TF-ThP-2 High Voltage Li-ion Battery Cathodes: Surface Fluorination and Transition Metal Doping of Lithium Cobalt Oxide (LCO), ***Falak Sher***, *Carlos Yescas, Timothy Spila, Arghya Patra, Ben Zahiri, Paul Braun,* University of Illinois at Urbana-Champaign, USA

Lithium cobalt oxide cathode (LCO) is extensively used as a cathode material in lithium-ion batteries for portable electronics. It is among the highest-performing cathode materials because of its structural stability, long cycle life, and high volumetric density at a cut-off voltage of 4.2 V (vs. Li/Li^+). Significant energy density increases would be provided by lifting the cut-off voltage from 4.2 V to 4.6 V (vs. Li/Li^+), increasing the specific capacity from 140 mhA/g to 200 mAh/g. However, at high-voltages, the cathode material undergoes severe challenges such as unstable cathode-electrolyte interface (CEI), undesirable permanent phase transformations, and oxygen loss which limit energy density and cycle life. To improve the high-voltage stability and electrochemical performance of LCO, we demonstrate plasma-assisted surface modification and fluorine, and transition metal doping. Incorporation of fluorine, in combination with transition elemental doping, protects the surface by reconstructing the layered structure of LCO into a short-range disordered rocksalt structure. Once protected, the LCO can be cycled to higher voltages, resulting in enhanced energy density and cycle-life. Time-of-Flight Secondary Ion Mass Spectroscopy (ToF-SIMS) analysis of both untreated and plasma engineered LCO confirms fluorination of the surface of plasma treated LCO. X-ray Fluorescence (XRF) and ToF-SIMS analyses of the plasma modified and pristine LCO show the incorporation of transition metals in the surface. High resolution STEM indicates that the surface is reconstructed from a layered LCO structure to a local disordered rocksalt structure. SEM images of the pristine and plasma treated LCO before and after cycling clearly show the increased stability of the plasma-treated material. surface modifications. At higher cycling voltages (4.6 V vs Li/Li^+) plasma modified LCO cathodes show significantly improved electrochemical results including longer cycle life, higher capacity retention, and higher energy density.

BT+AS+CA+TF-ThP-3 Development and Characterization of Sputtered Thin-Film Solid Electrolyte for Microbattery Applications, ***Ananya Bansal***, *Ramesh Chandra,* Indian Institute of Technology Roorkee, India

Thin-film solid electrolytes are gaining significant attention for next-generation microbatteries due to their high safety, compact size, and compatibility lab on chip electronic devices. In this work, thin-film solid electrolyte was fabricated using RF magnetron sputtering, a scalable technique that enables precise control over film thickness, composition, and uniformity. The deposited films were characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM), and X-ray photoelectron spectroscopy (XPS) to investigate their structural, surface, and chemical properties. Electrochemical impedance spectroscopy (EIS) was employed to evaluate the ionic conductivity, activation energy, and interfacial behavior of the thin films. The influence of sputtering parameters on the microstructure and electrochemical performance of the electrolyte films is discussed. The results demonstrate that sputtered thin-film solid electrolytes exhibit good film uniformity, dense morphology, and high ionic transport conductivity (~10^3 S/cm) suitable for microbattery integration. This study highlights the potential of sputtering-based thin-film electrolytes for the development of compact, reliable, and high-performance all-solid-state microbatteries for wearable electronics, IoT devices, and miniaturized energy storage systems.

BT+AS+CA+TF-ThP-4 Fabrication and Characterization of the Thin Film Solid State Li and Na Ion Batteries, ***SATILMIS BUDAK***, *Zhigang Xiao, Mebougna Drabo, Aschalew Kassu, Richard Lagle, Jamar Dozier, Kendall Montgomery, Kelvin Perkins,* Alabama A&M University

In this project, thin films of $LiCoO_2$ (cathode), LiPON (solid electrolyte), Sn (anode), and a multilayer stack combining these materials were deposited on silicon and silicondioxide substrates using electron-beam evaporation. Samples were annealed at 50°C, 100°C, and 150°C, with unannealed films serving as a baseline. Electrical properties were observed using a Van der Pauw measurement system to obtain resistivity, mobility, carrier density, Hall coefficient, and sheet resistance, and were complemented by current–voltage (I–V) characterization for each material and for the multilayer stack. Further analysis involved Seebeck analysis and Scanning Electron Microscopy/Energy-Dispersive X-ray Spectroscopy (SEM/EDS) to observe sample thermoelectric properties and microstructure. Similar studies are being under study for Na ion batteries. Finding will be shared during the meeting.

Chemical Analysis and Imaging at Interfaces
Room Ballroom A - Session CA-ThP
Chemical Analysis and Imaging at Interfaces Poster Session

CA-ThP-1 Synthesis and Characterization of Bayerite sub-Micrometer Particles, ***Mackenzie Savage***, *Xiao-Ying Yu,* Oak Ridge National Laboratory

The Hanford Site in Washington state houses the largest collection of nuclear waste in the United States, including 56 million gallons of mixed waste that must be processed for vitrification by the Department of Energy (DOE). However, the waste contains many insoluble micro- and nanoparticles that have unpredictable rheology due to their complex chemistry and are difficult to model. Aluminum hydroxides and oxyhydroxides such as bayerite make up a significant portion of these particles, and they must be filtered out before vitrification, as excess amounts can degrade the quality of the glass. Supply chain issues and a lack of information on their aqueous behavior has led to this study of aluminum (oxy)hydroxide nanoparticles. This research synthesizes bayerite micro- and nanoparticles using a hydrothermal synthesis process, namely by titrating and heating an aluminum hydroxide gel precursor solution. The resultant crystal structure of the largest particles was confirmed via powder x-ray diffraction, and elemental analysis confirmed that the particles were composed of bayerite. Scanning electron microscopy showed that particle sizes ranged from 70 nm needles to 4 µm particles in a bimodal distribution depending on the crystallization interval, with particles plateauing in size after about 48 h. Future work is needed to refine synthesis methods to reduce impurities and to obtain images of smaller particles at higher resolutions. Raman and Fourier Transform Infrared (FTIR) spectroscopy are also expected to confirm crystal structure of smaller particles. In situ characterization of particles in solution is necessary to observe the aqueous behavior of bayerite nanoparticles and how their rheology at varying pH might affect processing of Hanford waste.

CA-ThP-2 Enhanced Nanoprojectile Secondary Ion Mass Spectrometry (NP-SIMS): Correlation Among Spatially Resolved Secondary Ions, ***Pierre Hirchenhahn***, *Stanislav Verkhoturov,* Texas A&M University*; Michael J. Eller,* University of Mississippi*; Emile A. Schweikert,* Texas A&M University

Nanoprojectile secondary ion mass spectrometry (NP-SIMS) consists in bombarding an analyte with a heavy projectile in an event-by-event fashion. Each impact is resolved in space and time. Thus, the secondary ions (SIs) from each impact can be mass analyzed and recorded as individual mass spectra. The crater size is in the range of 10-15 nm wide and depth. These dimensions enable molecular analysis with unparalleled lateral resolution. Yet more information can still be extracted from the SI, by considering their anisotropic distribution. The eject have distinct spatial distributions set by their axial and radial energies. These parameters in turn reflect the molecular environment, the formation-ejection mode and metastable decay. They can be accessed with the temporally and spatially correlated detection of SIs. We demonstrate spatially resolved SI analysis on a homogeneous surface of Tris(8-hydroxyquinolinato)aluminium (Alq_3) sublimated on a silicon substrate. The NP-SIMS measurement was performed on a custom-made system equipped with a fullerene effusion source accelerated at 50 keV coupled to a linear time-of-flight mass analyzer with a 64 anodes detector. We identify analyte-specific moieties, SIs synthesized by impact chemistry by their distinct spatial distributions. The latter can be crucial for enhanced accurate identification of SIs in surfaces of unknown composition.

CA-ThP-3 Studying Neutron Irradiation Effects on Lithium Aluminate Pellets Using Tof-Sims, ***Xiao-Ying Yu***, *Jiyoung Son,* Oak Ridge National Laboratory*; Tanguy Terlier,* Rice University*; Gabriel Parker,* Oak Ridge National Laboratory*; David Senor,* Pacific Northwest National Laboratory

We studied tritium breeding lithium aluminate pellets in the Tritium-Producing Burnable Absorber Rod.The selected irradiated pellets have three different thickness, namely standard, thin, and thick wall thickness, which relates to their tritium producing and retention capacities.Irradiated materials were reduced to small sizes using scanning electron microscopy (SEM) – focused ion beam (FIB).Light isotopes, such as deuterium, tritium, and lithium, are detected using highly sensitive time-of-flight secondary ion mass spectrometry (ToF-SIMS).We show that the standard and thin thickness pellets are better in retaining tritium than the thick pellet in tritium production.The thinner wall pellet retains more tritium than the standard or thick ones.Isotope exchange reactions take place and tritiated hydrocarbons exist in all pellets.As the first study of irradiated pellets using ToF-SIMS, this work provides a new way to determine isotopic abundance

of irradiated materials, improving understanding of tritium breeding in fission and fusion reactors.

CA-ThP-4 In-Plasma XPS: A New Operando Metrology For Process Development and Control, ***Andrei Kolmakov***, NIST

Modern near-ambient-pressure X-ray photoelectron spectroscopy (NAP or AP-XPS) instruments now cover the pressure range typical of standard plasma applications, expanding the capabilities of XPS into plasma environments. We recently demonstrated that XPS spectra can be successfully collected in these conditions, extending the application of XPS to plasma-surface interactions [1]. We highlighted the influence of plasma chamber wall reactions on sample surface chemistry and showed that plasma-XPS can capture plasma chemistry in the gas phase [2]. Plasma-induced charging and damage of wafers is a well-known challenge in semiconductor fabrication [3]. We apply plasma-XPS to model poorly conducting samples and observe anomalous XPS binding energy shifts due to sample charging during plasma exposure. We propose mechanisms that explain these shifts. Additionally, we observed plasma-induced binding-energy shifts and peak splitting in the XPS spectra of the plasma gas phase, which were related to the local plasma potential and its time alterations [4]. Overall, plasma-XPS metrology offers an opportunity to record real-time surface chemistry on plasma-exposed surfaces, along with wafer charge and plasma diagnostics, and has significant potential to advance semiconductor process development and control, as well as defect-mitigation strategies.

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CA-ThP-5 A High-Throughput Multimodal Workflow for Characterizing Soil Mineral–Organic Interfaces with XPS, FTIR, SEM/EDS and ToF-SIMS, ***Vaithiyalingam Shutthanandan***, *Ajay Karakoti,* Pacific Northwest National Laboratory*; Catherine Pettinger,* University of Wisconsin-Madison*; Kavin Thangaraj,* Washington State University*; Odeta Qafoku, Mark Engelhard, Bhuvana Modachur Sivakumar, Zihua Zhu, Ravi Kukkadapu,* Pacific Northwest National Laboratory*; Erica Majumder,* University of Wisconsin - Madison

Understanding how soil carbon is stabilized as mineral–associated organic matter (MAOM) at the molecular scale is critical for more accurately representing soil processes in Earth system models. In particular, quantifying the chemistry and spatial organization of organic matter (OM) at mineral interfaces including ion–binding mechanisms, the distribution and density of reactive sites, and the arrangement of functional groups which provides key insight into the persistence, transformation, and loss of soil carbon. To address these questions, we developed a high–throughput, multimodal imaging and spectroscopy workflow that characterizes mineral–organic interfaces in terms of their elemental composition, molecular structure, and micro– to nanoscale topology. This approach integrates X–ray photoelectron spectroscopy (XPS), Fourier–transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), and energy–dispersive X–ray spectroscopy (EDS), yielding complementary information on bonding environments, functional group chemistry, surface morphology, and mineral composition. We implemented a custom high–throughput sample preparation method based on a dot–blot style deposition system, enabling rapid and reproducible preparation of many small soil aliquots or mineral–OM extracts on a single substrate. This configuration allows all four analytical techniques to probe the same set of spots, ensuring direct comparability of chemical and structural measurements across methods. With this platform, we can analyze approximately 50 samples per day, supporting systematic, large–scale characterization of MAOM across environmental gradients. In this study, samples are drawn from the MONet project, providing a broad and spatially diverse soil inventory for establishing quantitative relationships between mineral surface properties, organic matter chemistry, and carbon stabilization.

CA-ThP-6 Influence of Surface Preparation on Au/P-Type Hgcdte Interfaces Investigated by Xps Depth Profiling, ***Alexandra Colas--Reuillon***, *Clément Lobre, Eugénie Martinez, Steven Bel, Marc Veillerot, Sarah Petit, Olivier Gravrand,* CEA-Leti, France

P-type metal contacts on semiconductors remain a major technological challenge, particularly in Mercury Cadmium Telluride ($Hg_{1-x}Cd_xTe$, MCT), a reference material for cooled infrared detectors [1]. In the context of the SWaP-C (Size, Weight, Power, and Cost) approach, current developments aim to increase the operating temperature of infrared devices. However, higher temperatures are associated with anomalous pixel responses and increased noise levels, partly attributed to non-ideal Schottky-type behavior at the metal/p-type MCT interface.

Among the different strategies proposed to improve contact quality, surface preparation prior to metallization plays a critical role through the reduction of interface defects, passivation of dangling bonds, and control of interfacial oxides. Despite previous XPS studies, the mechanisms governing contact formation remain insufficiently understood. In this work, we investigate the influence of surface preparation on metal/MCT interfacial reactivity using X-ray Photoelectron Spectroscopy (XPS) combined with gentle Ar^+ sputter depth profiling.

Gold thin-film contacts (~10 nm) were deposited on arsenic-doped p-type $Hg_{1-x}Cd_xTe$ (x = 0.29) with a carrier concentration of ~10^{18} cm^{-3}. Two surface preparation routes were compared prior to metallization: (i) a deoxidized surface obtained by dry plasma treatment followed by wet chemical etching, and (ii) a deliberately oxidized surface prepared by plasma treatment only. Depth profiles were acquired by XPS (Al Kα source, Quantes, ULVAC-PH) combined with low-energy Ar^+ sputtering. Quantification was corrected using sputter sensitivity factors determined from a non-metallized reference MCT sample.

The measurements revealed strong preferential sputtering effects following the sequence Hg >> Te > Cd, attributed to the fragility of Hg–Te bonds. After correction, the Au/MCT interface formed on the intentionally oxidized surface appeared significantly sharper than that obtained on the deoxidized surface. Surface deoxidation promotes Au diffusion into the MCT as well as reciprocal interdiffusion processes. In contrast, the plasma-grown oxide layer, richer in HgO and CdTeO species than the native oxide formed after air exposure, likely stabilizes the surface and acts as a barrier against Au interdiffusion during deposition.

Such diffusion phenomena may strongly affect the electrical quality of the contacts through the formation of interfacial defects, local stoichiometry changes, and Au-induced doping effects.

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CA-ThP-7 Multi-modal analysis of NIST standard Iron Ore for establishment of the LIOS database, ***Gabriel Parker***, *Mackenzie Savage,* Oak Ridge National Laboratory, USA*; Michael Mulholland,* Idaho National Laboratory*; Xiao-Ying Yu,* Oak Ridge National Laboratory, USA

Abstract: The US Department of Energy (DOE) recently announced $155 million to advance American industrial innovation toward enhancing the capabilities of US national laboratories to develop technologies which will improve technological innovation, reduce costs, and increase prosperity for American workers and consumers. The DOE Office of Critical Minerals and Energy Innovation (CMEI) invested in new programs to address critical industrial challenges in areas such as energy intensive industry, cross sector technologies, data center collaboratives, and national library for iron ore and scrap. This library for iron ore and scrap (LIOS) project focuses on the iron ore and steel scrap to develop a national resource center and to deliver advanced characterization of iron ore and steel scrap samples of shared or donated by users for boosting American industrial innovations. The ORNL team’s efforts are to develop analytical methods using X-ray diffractometry (XRD), inductive coupled plasma mass spectrometry (ICP-MS), and scanning electron microscopy (SEM) with energy dispersive x-ray spectroscopy (EDS) and electron backscatter detection (EBSD) to provide detailed characterization of the natural and processed/recycled feedstocks. In the first step, several iron ore reference materials available from National Institute of Standards (NIST) will be used to establish the analytical benchmarking for XRD, ICP-MS, and SEM/EBSD. Additionally, time-of-flight secondary ion mass spectrometry and atom probe tomography will be used as complementary techniques to verify composition and microstructures at the nanoscale. Our results provide the necessary baseline measurement to

build the foundation for a resource library, which will provide important technical information for industrial needs.

Keywords: iron ore, SEM/EBSD, ICP-MS, XRD, ToF-SIMS, chemical imaging

CA-ThP-8 Exploring Radiolytic Chemistry of Tin Oxide Photoresists for Extreme Ultra-Violet (EUV) Photolithography Using Plasma-XPS, ***Trey Diulus,*** NIST-Gaithersburg*; Priyanka Ketkar, Conan Weiland, Cherno Jaye,* NIST*; J. Anibal Boscoboinik, Ashley Head,* Brookhaven National Laboratory*; Andrei Kolmakov, Daniel Sunday, R. Joseph Kline,* NIST-Gaithersburg

Recent developments in semiconductor nanomanufacturing towards next generation extreme ultraviolet (EUV) lithography now allows for fabrication of leading edge microchips with even smaller features. EUV lithography utilizes higher photon energy than the previous industry standard, which allows for patterning with higher resolution. This is compromised by low photoabsorption cross-sections for elements commonly found in conventional polymer-based photoresists. As a result, tin oxide organometallic nanoclusters are being optimized as photoresist materials, as Sn has a cross section 30x higher than carbon. Unfortunately, this transition to metal oxides yields a different radiation mechanism that results in a solubility contrast compared to their polymer counterparts, while further contrasting in post exposure processing. To identify chemical changes upon EUV exposure, we prepared spin coated thin films of a well-known Sn_{12} dodecamer cluster and treated the films with flood exposures for a range of EUV dosages to correlate changes in solubility with structural changes in the resist, including loss of ligands and cross-linking between clusters. In addition to EUV exposure, we also exposed samples to O_2 and H_2 plasmas using an AC-driven cold cathode 22 kHz plasma to simulate basic post exposure etch processing. Recently, Plasma-XPS has been developed where x-ray photoelectron spectroscopy (XPS) can be collected during exposure to plasma, allowing for studies of chemical changes in operando. We additionally utilize x-ray absorption spectroscopy (XAS) to examine the electronic structure of the elemental components ex situ, after EUV and/or plasma exposure. XPS before and after EUV irradiation shows a decrease in C 1s intensity along with an increase in the O 1s corresponding to the metal oxide, which is expected as butyl ligands are cleaved and the clusters cross-link. Comparing the C and O K-edges for the unexposed versus EUV exposed samples display a clear change suggestive of an increase in carbonyl chemistry. Furthermore, exposure to H_2 plasma seems to further pattern the film, likely due to UV emission from the hydrogen Lyman series lines. Overall, we provide a more detailed understanding of the radiation induced chemistry that we anticipate will allow for the design of more efficient EUV photoresists and can lead to advances in EUV lithography.

CA-ThP-10 ToF-SIMS Analysis of Surface Deposited Reaction Species in Selectively Passivized MXene Catalysts, ***Tobias Misicko,*** *Gabriel Parker,* Oak Ridge National Laboratory, USA*; Yang Xiao,* Louisiana Tech University*; Xiao-Ying Yu,* Oak Ridge National Laboratory, USA

Heterogeneous catalysis is controlled by the chemistry of the outermost atomic layers of catalyst surfaces and interfaces, where active metals, promoters, supports, and adsorbed reactants interact to form the catalytic system. A key deactivation pathway is coking, leading to deposition of carbonaceous species onto active surfaces, which causes a progressive loss of catalytic activity over time. Selective passivation of heterogeneous catalysts, the intentional neutralization of unselective and unproductive sites[1], has been applied to platinum catalysts using MXene.MXene is a class of two-dimensional (2D) metal carbides with the empirical formula of $M_{n+1}X_nT_x$, where M is an early transition metal, X is a carbon or nitrogen, and T is a surface functional group (such as F^- or OH^-). In prior work,[2,3] platinum was deposited onto Mo_2TiC_2 MXene via incipient wetness impregnation to yield a 0.5 wt.% Pt/Mo_2TiC_2 nanolayer catalyst. This catalyst demonstrated excellent activity, with turnover frequencies (TOFs) of 0.4–1.2 s^{-1} for the conversion of methane[2] and ethane[3]. It also exhibited high selectivity, >98% toward C_2 products in non-oxidative coupling of methane (NOCM) and >95% toward ethylene in catalytic dehydrogenation of ethane, along with robust stability, showing no loss of activity over 72 h and 24 h time-on-stream (TOS) for NOCM and ethane dehydrogenation, respectively. This stability is attributed to the catalyst's strong coke resistance. Following kinetic performance evaluation, time-of-flight secondary ion mass spectrometry (ToF-SIMS) measurements were conducted to probe surface-deposited species formed during the catalytic conversion of short-chain alkanes. Surface spectral analysis, depth profiling, and mass spectral imaging were performed to elucidate the identities and spatial distribution of carbonaceous species on the 0.5 wt.% Pt/Mo_2TiC_2 surface. Surface spectral analysis revealed the presence of many hydrocarbon species, including known coke precursors such as tropylium (C_7H_7).

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CA-ThP-11 Multimodal Raman and Luminescence Techniques for Defect Characterization in Wide Band Gap Semiconductors., ***Praveena Manimunda,*** HORIBA

Wide band gap semiconductors such as SiC, Ga_2O_3, and GaN, are essential for next–generation power electronics, optoelectronics, and quantum technologies, yet their performance is strongly influenced by strain and crystallographic defects introduced during growth and processing. In this work, we demonstrate how Raman spectroscopy, Photoluminescence (PL), Time–Resolved PL (TRPL), and Cathodoluminescence (CL) provide a comprehensive, non–destructive characterization platform for evaluating these materials with high spatial and spectral resolution. Case studies on 4H–SiC and SnO_2 doped Ga_2O_3 nanowires illustrate how this multimodal approach enables the identification of defect–related optical signatures and microstructural non–uniformities that impact material quality and device reliability. Raman spectroscopy reveals crystal quality and strain distributions, while PL and TRPL provide insight into impurity levels, recombination dynamics, and defect–related transitions. CL further correlates luminescence features with microstructural variations at the microscale. Together, these results highlight how integrated optical and electron–beam characterization supports optimization of epitaxial growth, improves device yield, and accelerates materials development across high–performance wide band gap semiconductor technologies.

Spectroscopic Ellipsometry
Room Ballroom A - Session EL-ThP
Spectroscopic Ellipsometry Poster Session

EL-ThP-1 Optical Properties of Metal Thin Films Measured by Spectroscopic Ellipsometry, ***Kathryn Brown,*** *Suresh Chaulagain, Prabin Dulal, Mohammed Alaani, Ambalanath Shan, Nikolas Podraza,* University of Toledo

As the race for higher and higher efficiency photovoltaic (PV) cells accelerates, device simulation has gone from a niche theoretical tool to an absolute necessity. In order to make these simulations as accurate as possible, it is vital to have well understood optical properties for each layer in the device. One such layer which is often overlooked is the metal back contact.

This work investigated the optical properties of three common back contact materials, namely Copper, Silver, and Gold. Thin films of each metal were deposited on fused silica glass. All three films studied were of a nominal thickness such that they appear functionally infinite to the instrument. Samples were measured by variable angle spectroscopic ellipsometry (VASE) in the range from 0.031-5.87 eV and at three separate angles of incidence, 50°, 60°, and 70°. Data from two separate instruments were combined to achieve this range. The resulting data were analyzed using the Sellmeier method to create Kramers–Kronig consistent parameterized models for each material. Properties interpreted from these results include complex refractive index ($\varepsilon = \varepsilon_1 + i\varepsilon_2$) and surface roughness.

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EL-ThP-2 Engineering the Optimal Filter: Nonlinear Noise-Reducing Filters in Spectroscopy, ***David Aspnes,*** North Carolina State University*; Long Le,* Vietnam Academy of Science and Technology, Viet Nam*; Young Kim,* Kyung Hee University, Republic of Korea

In previous work, we assessed linear filters used in spectroscopy, which operate by attenuation. Here, we assess nonlinear filters, which operate by replacement. By eliminating apodization errors, these nominally outperform linear filters but require some level of modeling. In direct (spectral) space (DS) this takes the form of replacing all or part of the data with least-squares-fit model lineshapes. In reciprocal- (Fourier-) space (RS), the equivalent is least-squares-fitting model coefficients to the low-order coefficients dominated by information, then replacing the higher-order data coefficients dominated by noise. The RS approach is new, and required appropriate mathematical functions to be developed. This generalizes RS filtering, because the only previous approach, the corrected-maximum-

entropy (CME) method, can be applied only to spectra that are positive-definite and have no dispersion character. In RS filtering the option also exists to retain some of the low-order data coefficients, an advantage for complicated spectra.

Using false-data calculations, we rank filters in order of performance. If a model is known to represent a spectrum accurately, the best filters are DS lineshape-fitting and its RS counterpart. The next best are the partial-replacement RS noted above, and, in situations where it can be applied, the CME. As expected, apodization errors relegate linear filters to last place, although they have the advantages of simplicity and not requiring modeling.

Finally, our calculations show unequivocally that the fundamental limit of any filter, linear or nonlinear, to extract information from spectra is the inability to separate information from low-order noise. Examples are provided.

EL-ThP-3 Optical Properties of CrN Measured by Spectroscopic Ellipsometry, ***Farihatun Jannat Lima***, *Alexander Bordovalos, Suresh Chaulagain, Ambalanath Shan, Nikolas Podraza,* University of Toledo*; Dilara Sen, Olivia Fairlamb, Frank Peiris,* Kenyon College*; Duc V. Dinh, Xiang Lü, Oliver Brandt,* Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Germany

Chromium nitride (CrN), a transition-metal nitride, has attracted attention in the field of electronics and energy as resistive coatings due to its excellent mechanical characteristics. It also has intriguing electronic, magnetic, and thermoelectric properties. In this work, an epitaxial (111) oriented CrN film deposited on Al2O3 (0001) is measured by spectroscopic ellipsometry over a spectral range from 0.031 to 5.877 eV to extract complex optical properties and bandgap energy using a rotating compensator Fourier transform infrared (IR) ellipsometer (FTIR-VASE, J.A. Woollam Co.) and a single rotating compensator multichannel ellipsometer (J.A. Woollam Co. M-2000) from the near IR to ultraviolet. Divided spectral range analysis is performed to determine structural parameters and thicknesses and initial sets of optical properties described by physically realistic models in the respective spectral ranges. The weakly absorbing photon energy range from 0.3 to 0.734 eV is initially ignored to prevent model-dependent bias in the vicinity of the bandgap. From the structural model, it is determined that CrN surface is optically less dense than the bulk of the thin film. Numerical inversion is performed over the full measured spectral range to determine the complex dielectric function ($\varepsilon = \varepsilon1 + i\varepsilon2$) spectra of CrN. The numerically inverted ε spectra in the full measured range is parametrized using a Kramers-Kronig consistent model. Three transverse optical (TO) phonon modes are observed at 387 cm-1, 403 cm-1 and 1048 cm-1. Three corresponding longitudinal optical (LO) phonon modes are identified from the loss function ($-1/\varepsilon$) at 596 cm-1, 622 cm-1 and 871 cm-1. The absorption coefficient (α) is determined from numerically inverted spectra in ε. Tauc plots of $(\alpha hv)2$ and $(\alpha hv)1/2$ as functions of photon energy reveal a direct gap energy of 0.815 eV and an indirect gap energy of 0.56 eV.

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EL-ThP-4 Optical and Structural Properties of Sbxsey Thin Film Co-Evaporated via Elemental Sources, ***Bishal Shrestha***, *Mohammed Razooqi Alaani, Madan Mainali, Alisha Adhikari, Balaji Ramanujam, Prabin Dulal, Venkanna Kanneboina, Ambalanath Shan, Nikolas Jacob Podraza,* University of Toledo

Antimony selenide (Sb_2Se_3) is low cost, highly stable, low toxicity, high radiation tolerant, and earth abundant semiconductor with established applications in photodetectors, batteries, and memory device technologies. In recent years, it has emerged as a promising photovoltaic absorber owing to its high visible light absorption coefficient (>10^5 cm^{-1}), quasi one-dimensional structure favoring charge transfer, and an optimal band gap (1.1 – 1.3 eV). Although the current record power conversion efficiency for a single-junction Sb_2Se_3 solar cell stands at 10.57% with a theoretical limit of ~32%, further performance gains are primarily limited by the persistent challenge of achieving high-quality, phase-pure, and stoichiometric Sb_2Se_3 thin films. Owing to substantial disparity in vapor pressures between Sb and Se during deposition, conventional chemical and physical deposition techniques requiring precursor Sb_2Se_3compounds result in thin films with compositional deviations, secondary phases, and elevated defect densities, requiring additional treatments to lower the degree of imperfections. Hence, for photovoltaic device applications, an ideal fabrication and characterization technique must be developed to obtain optimized films with the appropriate optical, structural, morphological, and compositional properties. With this motive, our approach employs thermal co-evaporation of elemental Sb and Se sources, enabling improved stoichiometric control of Sb_xSe_y thin films through independent regulation of source temperatures. For material characterization, particular emphasis is placed on in-situ and ex-situ spectroscopic ellipsometry analysis to investigate evolution of optical response and structural parameters in the as-deposited to post-deposition annealed states of the films. Our study of complex dielectric function spectra over an extended spectral range from 0.03 eV (mid-infrared) to 5.87 eV (ultraviolet) is the first documented experimentally derived data for this material. These comprehensive optical data will serve as valuable resource for device simulation across broad spectral range to explore material's further potential, whereas the optical/structural parametric expression developed here can be applied to investigate similar materials regardless of fabrication technique. Scanning electron microscopy, energy dispersive spectroscopy, and x-ray diffraction measurements are used to compare the morphological, compositional, and crystallographic characteristics of the as-deposited and annealed thin films.

Public Affairs release approval #_____.

EL-ThP-5 Composition-Dependent Optical Properties of Silver-Aluminum Alloy: An Ellipsometric Approach, *Jonas Sikah,* ***Will Cusak***, *Alexander Kozen, Matthew White,* University of Vermont

Semitransparent metal thin films have been widely used in optoelectronics because of their excellent optical and electrical properties. Among such, silver (Ag) is commonly employed due to its excellent conductivity and low optical losses in the visible range. In addition, introducing a minor fraction of Al into Ag facilitates the formation of smooth thin films by decreasing the percolation threshold of pure Ag. However, the optical properties of these Ag-Al alloy films fails to represent the weighted average of optical properties of their independent metal counterparts. Therefore, we present a detail ellipsometric investigation of the optical properties of Ag-Al alloy thin films deposited on glass substrates using vacuum thermal evaporation. The alloy compositions were tailored by adjusting deposition rates to achieve Ag volume fractions ranging 100% to 0% while Al volume fractions ranging from 0% to 100%.The film thicknesses of all compositions of Ag-Al alloys were kept at 100 nm. Scanning electron microscope (SEM) images confirmed the smooth film formation when Al content is higher in the alloy film. Energy-dispersive X-ray spectroscopy confirmed the compositional variation, with atomic percentages tracking the intended volume fraction. Spectroscopic ellipsometry was conducted at room temperature across 200 – 1000 nm at incident angles of 500, 550, and 600. The complex refraction index (*n*) and dielectric function (*k*) were extracted using model-based fitting employing Bruggeman effective medium approximations.Within the UV–Visible spectral range, increasing the Ag concentration resulted in a reduction of *n* values, while a progressive increase in Al content led to an enhancement of *n* in Ag–Al alloy thin films. At near-IR to IR region, films with higher Ag content exhibited higher *n* values while increasing Al content systematically reduced the *n* values exhibiting a trend typical of metallic films due to the decreasing contribution of free electrons response. The *k* values followed a constant trend thoughtout the UV-Visible-IR range with a lower *k* values with higher Ag content and higher *k* values with lower Ag content in the Ag-Al alloy. These findings demonstrate the tunablity of optical behavior linked to alloy compositions which can be applied to plethora of optoelectronic devices accordingly.

EL-ThP-6 iCVD Parameters with Structural and Dielectric Properties of Hydrophobic and Hydrophilic Polymer Thin Films: A Multi-Sample Spectroscopic Ellipsometry Analysis, ***Parvez Amin Khan***, *Hamidreza Mohajeri, Ufuk Kilic,* University of Nebraska - Lincoln*; Mathias Schubert,* University of Nebraska-Lincoln*; Siamak Nejati,* University of Nebraska - Lincoln

Unlike the conventional Chemical Vapor Deposition (CVD) process, initiated CVD (iCVD) offers a unique, solvent-free pathway for synthesizing conformal polymeric thin films. Their tailored chemical functionality such as hydrophilicity, hydrophobicity, and lipophobicity polymer thin films have been utilized in several technological applications including photocatalytic applications, sensors, organic LED, and solar cells. In this study, we provide a comprehensive investigation on the wettability characteristics of iCVD grown Polytetrafluoroethylene (PTFE) and poly glycidyl methacrylate (pGMA) thin films. We focused on their hydrophobic and hydrophilic performances and correlated them to their optical and material properties. The pGMA and PTFE thin film samples were fabricated at 350°C on silicon wafer with a deposition rate of 7.89 nm/min and 8.26 nm/min respectively. The relationship between deposition parameters (filament temperature, monomer flow rates) and material and structural properties of fabricated thin films (thickness, roughness, surface energy) were identified using

spectroscopic ellipsometry techniques, X-ray photoelectron spectroscopy and the wettability characteristics of fabricated thin films were extracted from contact angle (CA) measurements. Moreover, Multi-Sample Approach based spectroscopic ellipsometry data analysis provides the dielectric function of the fabricated films across the near-infrared (0.72 eV) to vacuum ultraviolet (6.4 eV) spectral range. Cauchy dispersion model with Urbach absorption tail is employed for extracting parametrized optical properties of thin films. We found that while the optical properties remain identical for different thickness of the fabricated polymers, we observed an increase in the roughness from 21.97nm to 38.04nm with the increase in thickness from 29.32nm to 123.86nm of the thin films. For PTFE, the increase in roughness also results in enhanced hydrophobic characteristics as we observed 18% increase in the CA of drop cast DI water with increase in the thin film thickness. For pGMA, we also increase the thickness from 95nm to 118nm, however the roughness layer thickness was not changing. From the CA measurements, we found that unlike pTFE, pGMA exhibit hydrophilic characteristics and the increase thickness did not change wettability due to the surface morphology remain unchanged and the constant surface energy profile of this polymer kind. This finding shows the importance of surface profile in wettability characteristics of thin films which are critical in the advancement of surface engineering pathways.

EL-ThP-7 Optical Properties of Boro-aluminosilicate Glass using Spectroscopic Ellipsometry from 0.079 to 5.89 eV, ***Eva Mulloy***, *Prabin Dulal, Suresh Chaulagain, Emily Amonette, Alex Bordovalos, Ambalanath Shan, Nikolas Podraza,* University of Toledo

Boro-aluminosilicate glass has high mechanical strength and chemical durability and is used widely in a variety of applications, including liquid crystal display substrates, glass fibers, thermal shock-resistant glass containers, and radioactive waste glasses. A commercially available boro-aluminosilicate glass is optically characterized by reflection mode spectroscopic ellipsometry and unpolarized transmittance over the infrared (IR) through the ultraviolet (UV) spectral range. Ellipsometric spectra (N, C, S) are collected using a near IR to UV rotating compensator spectroscopic ellipsometer from 0.73 to 5.89 eV (M-2000FI, J. A. Woollam Co.) and one further extended in the IR from 0.032 to 0.73 eV (IR-VASE, J. A. Woollam Co.) each at 50°, 60°, and 70° angles of incidence. A continuous parameterization of complex dielectric function ($\varepsilon = \varepsilon_1 + i\varepsilon_2$) spectra is developed from 0.079 to 5.8 eV. The parameterization of ε for this glass consists of a constant additive term to ε_1 (ε_∞), a Sellmeier expression, and Gaussian oscillators. A transfer-matrix-based numerical inversion of unpolarized transmittance spectra provides enhanced sensitivity to weak absorption from the UV to the near IR region. Parameters defining absorption features in numerically inverted ε_2 are fixed, and parameters only impacting ε_1 are fit to produce a final parametric model. From ε, distinct infrared vibrational modes can be linked to specific bonding configurations, while the onset of ultraviolet absorption arises from electronic transitions and defect states within the glass network. Sensitivity to relatively strong features at 1379, 1040, 745, and 332 cm $^{-1}$ is obtained from ellipsometry, and transmission can resolve weaker features at 1782, 2710, and 3541 cm^{-1}.

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EL-ThP-8 Birefringence of GdScO3 using Transmission Spectroscopic Ellipsometry, ***Prabin Dulal***, *Balaji Ramanujam, Nikolas Podraza, Ambalanath Shan,* University of Toledo

Gadolinium scandate ($GdScO_3$) is an emerging material with potential applications in advanced electronics and photonics primarily due to its interesting electronic, magnetic, and optical properties. It crystallizes as a perovskite-type oxide with an orthorhombic crystal structure, exhibiting a high dielectric constant, thermal stability, and large band gap energy. This study investigates the optical properties of a commercially available single crystal, double-sided polished $GdScO_3$ sample with a (110) Miller index surface plane orientation. The birefringence of the sample was derived using Mueller matrix spectroscopic ellipsometry (SE) over a spectral range of 280 nm to 1650 nm.

A full set of Mueller matrix data were obtained using an ellipsometer in straight-through mode with the sample at normal incidence. The fast axis of the biaxial sample was aligned with respect to the transmission axis of the polarizer in the generation arm of the ellipsometer. The measured matrix elements show no discernible dichroic effects, and the off-diagonal elements are virtually zero, implying that the sample exhibits properties of an ideal compensator. The measured lower right block Mueller matrix element data, composed of pure sinusoidal functions of retardance, shows oscillatory behavior with respect to spectra, consistent with a compensator with high retardance due to the thick (~ 0.54 mm) sample being evaluated. The lower right matrix elements also show a steady attenuation in the oscillatory data, beginning around 600 nm and approaching zero around 350 nm. Since there is no significant absorption in this region, we attribute this to depolarization resulting from incoherence due to the interaction of multiple beams within the thick sample with the finite bandwidths of the ellipsometer's source and detector.

To determine birefringence, the measured lower right Mueller matrix elements, for a spectral range greater than 400 nm, were first deconvolved from polarization-dependent attenuation. Next, because the order of the retardance is undetermined due to the relative thickness of the sample, there is ambiguity over the true retardance value determined from the deconvolved matrix elements. To address this, a model-based approach in which an extended Cauchy model with four fit parameters was employed to model the birefringence. Fit parameters were generated using the Monte Carlo approach, and the Levenberg-Marquardt algorithm was used to fit the relevant matrix element data to experimental data while minimizing mean squared error between datasets.

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Electronic Materials and Photonics
Room Ballroom A - Session EM-ThP
Electronic Materials and Photonics Poster Session

EM-ThP-1 A Comparison between Nbmotaw Refractory High-Entropy Alloy (HEA) Thin Films Fabricated by Sputtering from a Single Pre-Alloyed Target and from Individual Elemental Targets (Co-Sputtering), ***Nafisa Tabassum,*** Old Dominion University

NbMoTaW refractory high-entropy alloy thin films were deposited using two separate sputtering paths: a single pre-alloyed equimolar composite target and individual Nb, Mo, Ta, and W elemental targets. While previous studies examined NbMoTaW films deposited from composite targets, the influence of deposition path on the microstructure and mechanical behavior remains insufficiently understood. In order to produce the same or similar equimolar compositions of the NbMoTaW films sputtered from the composite target, the sputtering power has to be tuned for each individual target. The sputtering pressure was varied between 0.2 and 1.25 Pa. Both deposition paths produced near-equiatomic NbMoTaW films with stable BCC structure. FESEM, XRD and nanoindentation results showed similar pressure-dependent trends in grain size, crystallite size, dislocation density, lattice constant, microstrain, and hardness. The results indicate that sputtering pressure and film thickness dominate the microstructural and mechanical behavior, while deposition path mainly suggests processing flexibility.

Overall, this study shows that comparable NbMoTaW films can be produced by either path when composition is controlled. Composite-target sputtering offers simplicity and reproducibility, whereas individual-target co-sputtering provides compositional flexibility and cost-effective alloy design capability.

EM-ThP-2 Localized Dielectric Breakdown in Monoclinic HfO_2 MOS Capacitors on Non-Epitaxial 4H-SiC, *Melissa Mederos Vidal, Rodrigo Reigota César, Audrey Roberto Silva, Jacilene M. Medeiros, Renato Massaroto Beraldo, Marcos Vinicius Puydinger dos Santos,* ***José Alexandre Diniz,*** University of Campinas (UNICAMP), Brazil

A RF-sputtered HfO_2 thin film deposited on N_2+O_2 plasma-passivated non-epitaxial 4H-SiC substrate was investigated aiming to understand the dielectric breakdown behavior of MOS capacitors and its correlation with interface quality and defect-assisted transport mechanisms. The use of substrates without epilayers enables the evaluation of electrical limitations associated with bulk and interface defects, which are often less evident in optimized epitaxial structures.

Raman and FTIR analyses confirmed the formation of predominantly monoclinic HfO_2 and revealed the presence of an ultrathin interfacial oxide layer induced by plasma passivation (Fig. 1). Raman spectra showed characteristic monoclinic HfO_2 modes at ~526, 582, and 640 cm^{-1}, while FTIR measurements identified Hf–O vibrational bands together with Si–O–Si stretching modes associated with interfacial SiO_2 formation. These results indicate the formation of a chemically stable dielectric film and suggest that plasma treatment modifies the HfO_2/SiC interface.

Current–voltage measurements revealed high leakage current and a progressive current increase before dielectric failure (Fig. 2). The pre-

breakdown region exhibited behavior consistent with trap-assisted conduction and trap-controlled space-charge-limited transport, suggesting the participation of defects located within the dielectric and at the HfO_2/SiC interface. Dielectric breakdown occurred at ~17 V (electric field of ~3 MV/cm). Although this value is lower than those typically reported for optimized epitaxial HfO_2/SiC systems, the devices maintained stable electrical behavior prior to catastrophic failure, without abrupt fluctuations associated with premature localized conduction paths.

Post-breakdown SEM and FIB analyses revealed highly localized dielectric failure confined to the probe contact region (Fig. 3). The damaged region exhibited severe morphological deformation, with local fusion of Al, HfO_2, and SiC caused by intense current flow during breakdown. In contrast, adjacent regions remained structurally preserved, maintaining a distinguishable dielectric layer and interface with the SiC substrate. These observations indicate that breakdown was dominated by localized electrical overstress rather than dielectric delamination or structural inhomogeneity.

The results provide insight into defect-assisted transport and localized dielectric breakdown mechanisms in HfO_2-based MOS capacitors fabricated on non-epitaxial 4H-SiC substrates. Furthermore, the preserved and smooth dielectric/SiC interface observed after breakdown suggests that the N_2+O_2 plasma passivation contributed to interface stabilization in the investigated structures.

EM-ThP-3 Expert-Feedback-Driven Autonomous Experimentation for Nanoscale Discovery, ***Yongtao Liu,*** Oak Ridge National Laboratory

Autonomous experimentation and self-driving laboratories are transforming scientific discovery through adaptive exploration (e.g., using Bayesian Optimization (BO)). However, most BO workflows rely on predefined scalar descriptors to guide experiment selection, limiting their ability to capture complex phenomena that resist simple scalar representation. Here, I will show our development of deep kernel pairwise learning (DKPL), an expert-feedback-driven framework that integrates human scientific intuition directly into autonomous experimentation. Rather than relying on explicit scalar objectives, our approach learns a latent utility function from expert evaluations of experimental outcomes to guide autonomous microscopy experiments. We further apply this approach to autonomous scanning probe microscopy studies of ferroelectric thin films and complex ferroelectric domain-wall structures in lead zirconate titanate and erbium manganite systems, where multidimensional polarization configurations cannot be adequately represented by conventional scalar metrics. DKPL autonomously identifies physically meaningful domain structures, prioritizes high-information measurement regions, and discovers complex domain-wall phenomena without requiring explicit physical parameterization. The results establish DKPL as a new framework for expert-guided autonomous experimentation capable of identifying complex nanoscale phenomena without explicit scalar parameterization.Acknowledgments: This research was supported by the Center for Nanophase Materials Sciences (CNMS), which is a US Department of Energy, Office of Science User Facility at Oak Ridge National Laboratory.

EM-ThP-4 Cycling–Driven Non–Monotonic TER Dynamics in HZO Ferroelectric Tunnel Junctions: Competing Wake–Up, Fatigue, and Memory–Window Collapse Mechanisms, ***Alexander Blevins,*** *Sanghyun Lee,* University of Kentucky*; M. David Henry, Samantha Jaszewski,* Sandia National Laboratories, USA

Ferroelectric tunnel junctions (FTJs) based on hafnium zirconium oxide (HZO) stacks show a promising platform for next-generation in-memory computing. The asymmetric Ta/HZO/TaN electrode stack is particularly attractive because the two metals exhibit different oxygen affinities. However, Ta readily scavenges oxygen and forms sub–stoichiometric TaOx under electrical stress, whereas TaN remains chemically stable and functions as an diffusion barrier. This provides an accessible asymmetric interface for investigating cycling-induced evolution. Ultrathin HZO films < 10nm, demonstrate remanent polarization (Pr) values of 8–30 μC/cm^2 and facilitate tunneling-based ON/OFF resistance modulation, with ON/OFF ratios ranging from 5 to 30. However, the device-level mechanisms responsible for the non-monotonic tunnel electroresistance (TER) trajectory- including initial wake-up enhancement, subsequent fatigue, and memory-window collapse- continue to be significant challenges for existing predictive models.

In this work, Ta/HZO(6nm)/TaN FTJ devices were fabricated and subjected to comprehensive materials and device characterization, and all parameters were calibrated to experimentally extracted structural, interfacial, and polarization data to conduct the empirical and theoretical interpretation and modeling. The calibrated material and device model implemented in Sentaurus TCAD simulation reproduces the characteristic wake–up behavior emerging within 10^2- 10^4cycles, as well as the progressive fatigue that drives memory–window collapse under extended cycling, which agrees with experimental measurements. The resulting predictive model delineates degradation trajectories that align with endurance regimes from our experimental data from HZO-based devices.

We introduced the Two–regime saturating–exponential/power–law non–monotonic model with cycle–dependent Pr, which captures the experimentally observed wake–up and fatigue behavior in HZO FTJs. In the wake–up regime, oxygen vacancies redistribute from interfaces into the HZO bulk, progressively depinning ferroelectric domains and increasing switchable polarization. With continued cycling, a fatigue regime emerges in which irreversible trap generation at the reactive Ta/HZO interface due to cumulative TaOx formation, which creates an asymmetric depolarizing field. This field destabilizes polarization and precipitates memory–window collapse. Interface trap densities are modeled independently to capture the disparate electrochemical behaviors of Ta and TaN. Cumulatively, our study quantitatively separates polarization– and trap–driven TER contributions and pinpoints the crossover cycle where the dominant mechanism shifts.

EM-ThP-5 Workfunction and Interface Guided Electrode Alloying for High TER and performance Metal-Ferroelectric-Metal HZO-based Tunneling Junction devices, ***Chowdhury Haque,*** *Sanghyun Lee, Alexander Blevins,* University of Kentucky*; M. David Henry, Samantha Jaszewski,* Sandia National Laboratories, USA

Metal–ferroelectric–metal (MFM) tunnel junctions based on HfZrO(HZO) have emerged as leading candidates for next–generation non–volatile memory and neuromorphic computing, yet the coupled dependence of tunneling electroresistance (TER), current density, and polarization retention on electrode work–function asymmetry remains poorly constrained by existing design frameworks. To address this gap, we present a comprehensive TCAD investigation that establishes stability–aware design rules for HZO ferroelectric tunnel junctions (FTJs) by treating electrode work functions as continuous, tunable variables and validating the model against experimental Ta/HZO/TaN and Ti/HZO/TiN devices.

After fabricating and calibrating devices, we conducted a systematic non–symmetric sweep of top and bottom electrodes' workfunction from 3.8-5.2 eV for varying HZO thickness (5-10 nm) through modeling and Sentaurus TCAD simulation in this study. Furthermore, we mapped target MFM electrodes based on workfuction and interface layers between electrodes and HZO. Each parameter point employed two solve sequences: a WRITE → READ (+/- 0.2V) sequence to extract on- (Jon) and off-current (Joff) and TER, and a 1 μs zero–bias hold to quantify polarization decay and compute the depolarization field (Edep). The model was calibrated against measured Ta/HZO/TaN and Ti/HZO/TiN stacks, reproducing Ta/HZO/TaN metrics (TER ~ <10 at 0.2-0.3 V and Jon < 1 x 10^{-3} A/cm^2, coercive voltage (Vc) < 1.0 V). For metrics for Ti/HZO/TiN devices, we used metrics (TER ~ 16 and on-current (Jon) ~ 1.2 x 10^{-2} A/cm^2, coercive voltage (Vc) < 0.9 V), validating the chosen band–offset and ferroelectric parameters.

Our result indicates that ferroelectric polarization is required to meet dual stability constraints for stable polarization only when the net internal field (built–in field from electrode work–function asymmetry and the depolarization field from incomplete screening) remains below the coercive field. Since these contributions can add or subtract depending on polarization direction, both programmed and erased states are required to hold simultaneously to ensure reliable retention Ebi +Edep < Ec for programmed state and Ebi +Edep > -Ecfor erased state). Based on Pareto analysis, a narrow window where high TER and high on-current coexist can be achieved when built-in fields remain below the coercive threshold. Finally, we mapped optimal target work-function offsets with and without interlayers, offering a CMOS-compatible route to high-performance, retention-robust FTJs suitable for memory and neuromorphic applications.

EM-ThP-6 ErAs/Semiconductor Nanocomposites for 1550nm and 780nm pumped Multicolor Terahertz Emitters, ***Angelique Gordon,*** *Shreya Shrestha, Mohammad Tomal Hossain, Matthew Doty, Lars Gundlach, Xi Wang, Benjamin Jungfleisch, Joshua Zide,* University of Delaware

We present our latest results on ErAs/III-V semiconductor materials optimized for photoconductive devices operating at 1.55 μm and multicolor terahertz emitters. Terahertz (THz) technology remains a significant engineering challenge known as the "Terahertz Gap." This study addresses the need for advanced material synthesis designed to provide the performance and stability required for robust THz applications. Photoconductive switches (PCS) are key components for THz pulse

generation and detection, but face challenges under 1.55 µm excitation. ErAs:InGaAs and other nanocomposites have been explored for this purpose, but their high electron concentration, driven by the Fermi level residing in the conduction band, limits dark resistivity. To overcome these limitations, we have recently demonstrated a pentanary digital alloy ErAs:[$(InGaBiAs)_x(InAlBiAs)_{1-x}$)] with incorporated nanoparticles as a suitable PCS material for telecom-wavelength usage. Molecular Beam Epitaxy (MBE) is chosen as the synthesis pathway for this alloy due to its unparalleled control over material composition. The incorporation of bismuth results in the formation of dilute bismuthides, a class of highly mismatched alloys. MBE enables the simultaneous management of strict growth constraints required for high quality bismuthides including substrate latticing matching, low growth temperatures (280°C), bismuth/arsenic ratio, and V/III stoichiometric growth. The freedom offered by the InGaAlBiAs short-period superlattice enables tunable bandgap engineering—aluminum raises the conduction band edge while bismuth, through valance band anti-crossing, maintains a bandgap suitable for 1.55 µm excitation. Introducing self-assembled ErAs nanoparticles produces sub-picosecond carrier lifetimes ensuring high temporal resolution while simultaneously pinning the Fermi level within the bandgap. The digital alloy approach combined with ErAs nanoparticles achieves both low carrier concentration, high dark resistivity, and stable electronic properties, enhancing the performance of THz photoconductive devices at 1.55 µm. Finally, we demonstrate our progress on the implementation of this digital alloy alongside a secondary film, ErAs:InAlAs, for multicolor THz emission. The development of Cl-ICP processes for the etching of ErAs/III-V nanocomposites provides access to the fabrication of mesa structures and the independent biasing of these dual films by orthogonal antennas. Inspired by Hybrid Terahertz emitters, this device allows for simultaneous operation at two distinct wavelengths, facilitating control over emerging THz functionalities such as elliptical polarization and advanced pulse control.

EM-ThP-7 Influence of Fluorine-Containing Surface Ligands on the Optoelectronic Behavior of NiO Thin Films, ***Sanuthmi Dunuwila***, *Chaiwarut Santiwipharat,* University of Delaware*; Zonglun Li, Alexander A. Shestopalov,* University of Rochester*; Ujjwal K. Das, Andrew V. Teplyakov,* University of Delaware

Nickel oxide (NiO) is a transparent conductive oxide (TCO) widely used in electrochromic devices, photodetectors, gas sensors, dye-sensitized solar cells, and perovskite solar cells as a hole transport layer. NiO possesses a wide bandgap of 3.6–4.0 eV and functions as a p-type semiconductor, where Ni3+ species contribute to hole transport. In addition, NiO exhibits excellent chemical and thermal stability along with antiferromagnetic, electronic, and optoelectronic properties. However, using NiO as an inorganic hole transport layer (HTL) causes some challenges, such as an energy level mismatch between NiO and perovskite layers, which results in increased charge transfer barriers. Furthermore, defects at the NiO perovskite interface act as recombination centers for electron–hole pairs, reducing carrier lifetime. One successful approach found to be is surface modification of NiO with organic ligands.

In this work, gas-phase surface modification of NiO thin films using hexafluoroacetylacetone (hfacH) and acetylacetone (acacH) was investigated under vacuum conditions. The objective of this study is to understand the chemical reactivity of fluorinated and non-fluorinated β-diketones on the NiO surface and correlate these interactions with changes in the electronic and optical properties of the films. Surface treatment with acetylacetone resulted in enhanced electrical conductivity over the investigated temperature range, while hexafluoroacetylacetone treatment improved the optical transparency. Both ligands also increased the work function of NiO, indicating their potential for tuning and improving energy level alignment in optoelectronic applications.

X-ray photoelectron spectroscopy (XPS) and time-of-flight secondary ion mass spectrometry (ToF-SIMS) were employed to investigate surface and interface chemical reactivity of NiO following ligand exposure. Ultraviolet photoelectron spectroscopy (UPS), conductivity measurements, and optical transmittance characterization were used to evaluate modifications in the electronic structure and optical behavior of the films before and after surface modification. These findings demonstrate that β-diketone surface functionalization provides an effective route for tuning the optoelectronic properties of NiO for next-generation optoelectronic and photovoltaic applications.

EM-ThP-8 Ultraviolet-C (UVC) Irradiation as Post-Treatment for Property Modification of Hydrogenated Amorphous Carbon (a-C:H) Thin Films, ***Kenneth Lathrum***, *Jhonatan Gil Romero, Seonhee Jang,* University of Louisiana

Amorphous carbon thin films exhibit a wide range of properties, such as chemical inertness, high hardness, and tunable optical properties. They are utilized in many different devices such as micro-supercapacitors, batteries, solar cells, sensors, semiconductor devices, and nanomembranes. A key challenge in the successful development of these applications lies in the precision tuning of synthesis and modification parameters to achieve desired material properties.

In this study, hydrogenated amorphous carbon (a-C:H) thin films were prepared by plasma-enhanced chemical vapor deposition (PECVD) of a cyclohexane precursor and subjected to ultraviolet-C (UVC) irradiation with a wavelength of 255nm to tune the film's properties. The intensity of the irradiation light varied from 2.2 to 16.5 mW/cm^2. This wide range of irradiance of UVC light effectively altered the physical, chemical, and optical properties of a-C:H thin films.

The surface of a-C:H transformed from hydrophobic to hydrophilic under UVC irradiation. The surface became more hydrophilic with increased UV light intensity, reaching a minimum contact angle of 75.09° at the high intensity irradiation of 16.5 mW/cm^2. Atomic force microscopy (AFM) data showed a change in surface roughness under UVC irradiation. The surface roughness was reduced with increased UV intensity. The surface became the smoothest with a roughness of 0.202 nm when exposed to UVC irradiation at 16.5 mW/cm^2.

Fourier-transform infrared (FTIR) spectra exhibited a prominent absorption band between 3000–2800 cm^{-1}, corresponding to variousv CH_x stretching modes. Deconvolution of this band reveals three primary components: sp^3 CH_3 asymmetric stretching (v_{as} sp^3 CH_3), sp^3 CH_2 asymmetric stretching (v_{as} sp^3 CH_2), and sp^3 CH_2 symmetric stretching (vs sp3 CH2). Additionally, low-intensity features observed at 1750–1500 cm^{-1} are associated with C=C and C=O bonding. Following UVC irradiation, the FTIR spectral features shifted significantly. As the UV intensity increased, there was a decrease in the v CH_x stretching modes and the appearance of C=O groups due to dehydrogenation and surface oxidation. Optical data indicated that UVC irradiation increased transparency and decreased density of the a-C:H films. The refractive index and extinction coefficient both decreased with an increase in UVC irradiance, reaching a minimum of 1.535 and 0.003, respectively, at 16.5 mW/cm^2. In contrast, the optical band gap broadened under UVC irradiance, reaching a maximum of 5.23 eV at the highest intensity of 16.5 mW/cm^2. The findings suggest that UVC post-treatment is a versatile tool for tuning the density, wettability, and optical constants of a-C:H films.

EM-ThP-9 Effect of Ge Incorporation on Ti/Al-Based Ohmic Contacts for N-Polar GaN HEMTs on SiC, ***Alejandro Perez***, University of Illinois - Chicago

N-polar GaN high-electron-mobility transistors are promising for next-generation high-frequency and high-power electronics, but reproducible low-resistance ohmic contacts remain a key processing challenge. In this work, we investigate ohmic contact optimization for N-polar GaN HEMT structures grown on SiC using transfer length method structures with different pad widths and contact spacings. Traditional Ti/Al/Ni/Au metal stacks were compared with Ge-containing contact schemes to evaluate the effect of Ge incorporation on contact resistance, sheet resistance, and transfer length. Additional process variations, including different Ti/Al ratios and annealing conditions, were examined to understand their influence on contact formation and electrical reproducibility. Extracted TLM parameters were compared across 50, 100, and 200 µm pad geometries to assess consistency between layouts. These results provide practical feedback for improving ohmic contact recipes for N-polar GaN devices and support continued development of reliable wide-bandgap semiconductor fabrication processes.

EM-ThP-10 Plasma–Enhanced ALD of Ferroelectric $Al_{1-x}Sc_xN$ Under Ultrahigh–Purity Conditions, ***Gilbert B. Rayner Jr.***, *Noel O'Toole, Nathaniel Nelson,* Kurt J. Lesker Company*; Bangzhi Liu,* The Pennsylvania State University*; Jeffrey Shallenberger,* The pennsylvania State University*; Gregory Muha, Piush Behera, Suraj Cheema,* Massachusetts Institute of Technology*; Blaine Johs,* Film Sense*; Nastazia Moshirfatemi,* General Technical Services, LLC*; Daniel Drury, Brendan M. Hanrahan,* Army Research Directorate, DEVCOM Army Research Laboratory*; Glen R. Fox,* Fox Materials Consulting, LLC*; Nicholas A. Strnad,* Army Research Directorate, DEVCOM Army Research Laboratory

Wurtzite aluminum–scandium nitride ($Al_{1-x}Sc_xN$) thin films are emerging materials for next–generation electronic and sensing technologies, yet achieving precise composition control and uniform deposition on complex three–dimensional structures remains a significant challenge. In this work, we report the ultrahigh–purity plasma–enhanced atomic layer deposition (PEALD) of $Al_{1-x}Sc_xN$ using a supercycle approach that alternates AlN and ScN constituent processes. The process employs trimethylaluminum (TMA), bis(ethylcyclopentadienyl)scandium chloride [$ClSc(EtCp)_2$], and N_2–H_2 plasma as co–reactants at substrate temperatures between 215 and 300 °C.

A 60.3 nm–thick $Al_{0.83}Sc_{0.17}N$ film deposited at 300 °C on a {111}-oriented Pt bottom electrode on Si (100) exhibits clear ferroelectric switching behavior. The film shows switched polarization values ($2P_r$) of 163 μC cm^{-2} and 139 μC cm^{-2} under negative and positive pulsing, coercive fields as low as of ±3.3 MV cm^{-1}, and a dielectric constant of 12.8–13.8 at 100 kHz under ±10 V.

Structural characterization reveals that films grown on {111} Pt are fully c–axis (0001) oriented, demonstrating high crystalline quality even along the sidewalls of three–dimensional features. When deposited on single–crystal GaN, $Al_{0.83}Sc_{0.17}N$ exhibits strong in–plane and out–of–plane ordering consistent with epitaxial growth. Deposition over narrow trench structures further confirms uniform, conformal coating. Collectively, these results show that PEALD enables high–quality $Al_{1-x}Sc_xN$ films suitable for advanced three–dimensional electronic and sensing applications.

Advances in EUV Lithography
Room Ballroom A - Session EUV-ThP
Advances in EUV Lithography Poster Session

EUV-ThP-1 Multilayer Graphite Pellicles with Engineered SiNx Capping for High-Power Extreme Ultraviolet Lithography, *Hye-Young Kim, Sung Kyu Jang, Jihun Kim, Jong-Hyun Choi,* ***Hyun-Mi Kim****, Seul-Gi Kim, Hyeongkeun Kim,* Korea Electronics Technology Institute, Republic of Korea

To withstand the severe thermal and chemical environments of next-generation extreme ultraviolet lithography (EUVL), this study demonstrates a high-performance multilayer pellicle comprising a low-temperature directly synthesized graphite core and a dense silicon nitride (SiNx) protective layer optimized via plasma-sequence-engineered atomic layer deposition (PSE-ALD).

First, to overcome the non-uniformity and transfer damage inherent in conventional CVD, a low-temperature (500 °C) metal-induced crystallization of amorphous carbon (MICA) process was developed using a nickel (Ni) catalyst. Nucleation and crystallization occur predominantly at the Ni/amorphous carbon (a-C) interface, where the lateral growth rate significantly exceeds vertical growth. By optimizing the a-C to Ni thickness ratio to 45 nm: 30 nm (~1:1 atomic ratio), uniform graphite films free of residual metal clusters were directly synthesized on 8-inch wafers without a transfer step. Freestanding 15-nm-thick graphite membranes fabricated by backside etching exhibited an outstanding EUV transmittance of 91.56% and a high thermal emissivity of 0.37, satisfying industrial criteria for high-power EUV operation.

Second, to shield the inert graphite from harsh hydrogen radicals (H*) in EUV scanners and KOH solutions during membrane fabrication, PSE-ALD was introduced using HCDS (Si_2Cl_6) and NH_3 plasma, followed by a sequential N_2 plasma step. Real-time mass spectrometry verified that the sequential N_2 plasma effectively extracts volatile HCl by-products, facilitating dense cross-linking and eliminating chlorine and hydrogen impurities. Under a mild plasma power of 50 W, the NH_3-N_2 sequence yielded a stoichiometric, oxygen-free SiNx ultra-thin film (5 nm) with a high mass density of 3.07g/cm^3.

Third, permutation tests confirmed that film mass density is the primary factor governing wet-etching resistance. The optimized SiNx capping layer exhibited a pinhole-free structure and an extremely low etch rate of 0.17 nm/h in a 30 wt% KOH solution for 16 hours. Finally, the capped graphite pellicle was evaluated under a 250 W H_2 plasma for 5 minutes. While the pristine graphite suffered severe degradation and a thickness loss over 5 nm, the SiNx-capped graphite showed negligible change. This integrated strategy offers a robust framework for carbon-based multilayer pellicles in next-generation high-power EUVL systems.

EUV-ThP-2 Understanding the Initial Deposition and Etching of Tin in an Extreme Ultraviolet (EUV) Source, ***Nathan Bartlett****, Jameson Crouse, Andrew Herschberg, Emily Greene, Jaime Robertson, Lucia Suarez Heredero, Marisol Velapatino, Karl Vu,* University of Illinois at Urbana-Champaign*; Niels Braaksma, Sergio Ferraris,* ASML*; David Ruzic,* University of Illinois at Urbana-Champaign

Tin laser produced plasmas (LPPs) are used to generate 13.5 nm light in state-of-the-art extreme ultraviolet (EUV) lithography tools. Inside these tools, hydrogen gas is used as a buffer gas to decelerate ions from the LPP and is photoionized in the process creating a steady background hydrogen plasma. This plasma etches away tin as it accumulates on the wall of the EUV source forming the volatile compound stannane. The interaction of hydrogen plasma species and tin lead to complex morphologies. In this work, we study the initial growth of tin thin films in a relevant hydrogen plasma environment. Tin is deposited using a high temperature thermal evaporation source and a hydrogen plasma is generated using an RF power supply. Thin films are measured using a scanning electron microscope and resistivity probes. The plasma is measured using optical emission spectroscopy, Langmuir probes, and radical probes. Impurity gasses, such as water, are also injected into the experiment to determine the effect on tin growth and etching. Water is expected to affect surface reactions which in turn increases the concentration of hydrogen radicals in the plasma. These results are used to validate both plasma models as well as tin thin film growth models.

EUV-ThP-3 Development of Mass Limited Targets for Enabling Fundamental Studies of Next Generation of EUV Lithography, ***Ajay Karakoti****, Peipei Wang, Mathew Polek, Tyler Ray, Sivanandan Harilal,* Pacific Northwest National Laboratory

Extreme ultraviolet (EUV) lithography at 13.5 nm is a cornerstone of advanced semiconductor manufacturing, where continued device scaling depends on improvements in source brightness, spectral purity, and optics lifetime. The ANGEL (Accelerating Next-Generation EUV Lithography) project, led by Pacific Northwest National Laboratory, targets significant improvements in the conversion efficiency of EUV sources based on low-density Sn targets by carrying out fundamental experimental studies and modeling to understand and control the underlying plasma physics.

Studies of laser produced plasma from bulk Sn sources emit substantial particulate, ionic, and neutral debris, with high-velocity ions and neutrals capable of damaging nearby collection optics. In addition, fully dense Sn plasmas produce a broad recombination continuum that limits spectral purity in the in-band region around 13.5 nm. Mass-limited, low-density targets, in which Sn is dispersed as a dilute dopant within a low-Z foam matrix, offer a route to mitigate both issues. Incorporating Sn as an impurity in a low-Z host reduces the average plasma ionization state and recombination continuum, narrowing the unresolved transition array (UTA) around 13.5 nm, while simultaneously limiting the total Sn inventory available to generate debris. Low-density foam targets further provide a well-defined geometry and density prior to laser illumination, enabling reproducible laser–plasma interactions.

This poster presents the fabrication and comparative characterization of Sn-doped mass-limited foam targets synthesized from two distinct low-Z matrices. It compares the performance of resorcinol-formaldehyde (RF) aerogels, a well-established foam chemistry for laser-plasma targets, and nanocrystalline cellulose (NCC) foams, an emerging bio-derived alternative. We compare the (i) ease and reproducibility of synthesis, (ii) morphology, Surface area and pore-size distribution, and (iii) spatial uniformity of Sn dispersion as characterized by different in-situ and ex-situ tools. Finally, we correlate these structural and compositional metrics with EUV emission characteristics, comparing the spectral profiles of doped RF and NCC foam targets against bulk Sn references to assess their suitability as mass-limited targets for spectrally clean, low-debris EUV generation.

EUV-ThP-5 High Purity Component Cleaning for EUV: Current Challenges in the Process Chain, ***Michael Flaemmich****,* VACOM USA

Unlike classic component cleaning, high purity cleaning for EUV Lithography is not about cleaning off large amounts of production residue (e.g. several gallons of oil per batch or several pounds of chips). Rather, high purity cleaning for EUVL focuses on removing even the slightest residual

contamination (particulate, organic, and inorganic) and then keeping the cleaned surfaces clean and preserving them. As a consequence, the creation of high purity surfaces for EUVL is not only the task of the process step cleaning. This induces some familiar and some new challenges for cleaning technology and the entire process chain, which will be highlighted in the talk.

Furthermore, we will introduce our approach to transfer our high purity parts cleaning concepts for EUVL cleaning from Europe to the US. VACOM recently opened a parts cleaning facility in Lewistown, Montana. We will give some insights into the machines, processes and the current challenges in the high purity process chain for EUVL component cleaning.

Besides EUVL, industries requiring high-purity cleaning and ultra-clean parts are those where microscopic contamination causes component failure, product spoilage, or safety hazards, primarily semiconductor manufacturing, aerospace/defense, pharmaceuticals, and medical device production. These sectors necessitate specialized cleaning techniques to remove contaminants - such as particulate matter, lubricants, and ions - from surfaces, often requiring ISO-certified cleanroom environments.

EUV-ThP-6 Investigation of Cold Spitted Sn Particle Transport in a Hydrogen Plasma*, **Jaime Robertson**,* University of Illinois at Urbana-Champaign

In Extreme Ultraviolet (EUV) lithography, defectivity in printed wafers is a significant concern due to yield loss. Defects hinder the performance of semiconductors, dependent on its size and location. Defectivity, in relation to this work, arises from the migration of particles and the subsequent contamination that occurs when these particles stick to sensitive components. This includes the reticle, which holds the pattern to be printed on the wafer. Sn particles are a significant contributor to reticle defectivity, resulting in substantial downtime for EUV machines at customer fabs. Sn defectivity arises from the complex interaction mechanisms of Sn particles with EUV-induced plasma. Each of these pathways contributes to the overall presence and movement of Sn particles within the system, potentially leading to contamination of sensitive components. These mechanisms need to be investigated in detail to tackle Sn defectivity and ensure high uptime for EUV machines, as understanding each process can inform the development of targeted mitigation strategies. Therefore, the studies described here investigate the interactions between hydrogen plasma, similar to the EUV scanner environment, and Sn found in certain regions within the EUV scanner. Three known plasma material interactions occur with Sn, which result in mass migration. These include ion etching, chemical etching, and electrostatic particle lift-off. Although these methods have been studied to varying degrees, modeling of the EUV scanner has shown that these mass migration processes cannot contribute to particles reaching the reticle. Therefore, the aim has been to determine whether other methods of mass migration occur, which result in particles found on the reticle. Specifically, cold spitting has been proposed as a potential mechanism for particle migration to the reticle. Cold spitting refers to the ejection of solid particles due to a buildup of hydrogen gas beneath the surface. Once the pressure of hydrogen bubbles formed is sufficiently high, the bubble bursts, ejecting nano-particles away from the surface. The difficulty in independently studying cold spitting has been in separating the migration mechanisms to ensure that the particles analyzed were formed by cold spitting. We present a method which allows for cold spit Sn particles to be collected on an adjacent surface while preventing particles formed through other mechanisms from being captured. Therefore, proving that cold spitting occurs for Sn. From the initial findings, the rate of ejections from a $1cm2$ sheet of Sn was approximated. The resulting flux was *5.1*101±1Sn particlescm2s.*

EUV-ThP-7 Open-Use, Synchrotron-Based EUV Exposure/Characterization System at LLS*, Ali Parastesh, Anthony Engler, **Phillip Sprunger**,* Louisiana State University

A designated synchrotron-based EUV exposure/characterization system has been commissioned at the Louisiana Light Source, or LLS (LSU's Center for Advanced Microstructures and Devices). Using both a toroidal mirror and a Si/Mo multilayer spherical mirror, the system delivers focused EUV light (~2% bandpass centered at the required 13.5 nm wavelength) to the sample holder, with a simulated FWHM spot size of ~1.2 × 0.5 mm at ~3 W/cm^2. In addition to a low-energy external electron gun, an in situ quadrupole mass spectrometer and a hemispherical electron analyzer (with an X-ray source) enable operando characterization of photoresists during EUV exposure. The goal is to elucidate key aspects of the physics and chemistry of EUV exposure mechanisms and to better develop photoresists with enhanced performance (higher sensitivity, lower line edge roughness, and higher resolution) than those currently used in high-volume chip manufacturing. The beamline is an open-use EUV exposure/characterization facility for both academic and industrial users.

Initial studies on polyaldehyde-based resists capable of thermally driven, dry development are underway. Specifically, we have studied the effects on thin-film poly(phenyl glyoxal)s (PPG). Employing 100eV electrons, soft-X-ray XANES of the O- and C-edges reveals details of carbonyl elimination and the conversion of the pristine PPG backbone to a degraded state capable of developing the latent image. These results are supported by EPR, consistent with a Norrish mechanism of photodegradation.

EUV-ThP-8 Development and Performance of a University-Scale EUV Lithography Source*, **Dren Qerimi**,* University of Illinois

To expand our lab's capabilities in EUV photoresist research, we developed an in-house EUV light source that provides lithography exposures at a cost feasible for a university setting. The system uses an Nd:YAG laser to produce plasma on a tin target, which generates EUV radiation without relying on the extremely expensive infrastructure found in commercial systems. A 150 nm zirconium transmission filter isolates the EUV wavelengths and allows direct exposure of the photoresist. The exposure dose is monitored in real time using an EUV-sensitive photodiode, and we have confirmed the accuracy of these measurements through successful exposures and development of EUV photoresists. Using this setup, we have demonstrated a clear contrast curve with exposure times typically under 120 seconds, showing that the system can reliably deliver controlled and repeatable EUV doses. During optimization, we adjusted the laser power, the focusing conditions, the chamber pressure, and the movement of the target to stabilize the dose and improve EUV output. Debris from the plasma remains one of the primary challenges, so we are continuing to refine the target handling and filtering approach to extend the lifetime of internal components. Even with ongoing improvements, the system already provides consistent and tunable EUV exposure that supports photoresist testing and development. Compared to commercial EUV lithography platforms that cost several million dollars, this tool offers a practical and flexible option for research. It enables the study of new photoresist materials, dose response behavior, and exposure strategies without depending on limited industrial access. Current work includes blanket exposure testing and efforts to lower the required dose for full development. In this way, the system provides a meaningful bridge that allows academic research groups to work directly in the EUV regime.

EUV-ThP-9 A Computational Molecular Framework to Investigate EUV Lithography Photoresist Sensitivity: Poly(Pthaladyhede) and Poly(Methyl Methacrylate) Degradation Study*, **Amrutha Raghu**,* Louisiana State University*; Tianyi Wang,* Lousiana State University*; Revati Kumar,* Louisiana State University

High-volume EUV lithography at sub-7 nm nodes is constrained less by optics than by photoresist performance. The resolution-LER-sensitivity tradeoff tightens with every technology node, and stochastic failures from photon shot noise set hard limits on what current resist platforms can deliver. Chemically amplified resists compound the problem by introducing chemical inhomogeneity that worsens stochastic acid generation and diffusion at the length scales that matter for sub-10 nm features. Single-component depolymerizable resists such as poly(phthalaldehyde) (PPA) avoid acid diffusion entirely, and cyclic PPA (c-PPA) achieves spontaneous dry development at doses competitive with CARs. Two questions have remained open: why does cyclic topology outperform linear PPA in EUV sensitivity, and what drives dose-dependent crosslinking at higher doses? We address both using reactive molecular dynamics with the ReaxFF force field. The framework simulates the aftermath of EUV-induced ionization through the Primary Knock-on Atom (PKA) method: backbone carbon atoms are randomly selected across a 40-chain, 20-mer simulation box and assigned velocities equivalent to 10 eV secondary electron momentum, then the system evolves chemically in an NVE ensemble. The same protocol is applied to PMMA, a well-established EUV photoresist with extensively characterized experimental behavior, making it an ideal validation system. Together, PPA and PMMA allow us to connect repeat unit structure and polymer topology to the full spectrum of EUV-induced chemistry and establish molecular design principles for next-generation photoresist platforms. PKA recoil redistributes charge across the simulation system, generating active sites whose charges deviate significantly from equilibrium. For PPA, c-PPA shows 3.6 times more active sites than l-PPA, and active site locations correlate directly with bond breaks, indicating elevated bond stress from energetic neighboring atoms. The origin is thermodynamic: the ring blocks angular relaxation that linear chains use to

absorb the perturbation, forcing energy into bonds instead. Bond angle distributions, angle strain, conformational entropy, and radius of gyration all support this picture. For PMMA, PKA simulations show backbone bonds undergo higher scission than side-chain linkages, consistent with experimental EUV chemistry of methyl methacrylate polymers. This is traceable to the higher concentration of active sites on the backbone relative to side-chain carbons. Active site distribution and bond stress together explain the emergent EUV chemistry in both systems and provide a structural basis for rational photoresist design.

Materials and Innovations for Fusion Energy
Room Ballroom A - Session FUS-ThP

Materials and Innovations for Fusion Energy Poster Session

FUS-ThP-1 Experiment Setup of a Testbed Facility to Characterize Tritium Storage Materials, ***Simon Niemes***, *David Beisiegel, Nicolas Bekris, Noah Ellenbogen, Robin Größle, Ralph Lietzow, Immanuel Müller, Florian Priester,* Karlsruhe Institute of Technology (KIT), Germany*; Tim Teichmann,* Kyoto Fusioneering (KF), Germany

A key requirement for the transportation, storage and processing of tritium is the availability of storage devices compatible with tritium. Metal hydride storage bed, usually based on depleted uranium, are commonly used due to the low equilibrium pressure at room temperature and the efficient tritium release at temperatures above 400°C. However, the use of uranium requires a dedicated licencing and additional safety measures due to the pyrophoric nature of the storage material. Therefore, research efforts into alternative materials like ZrCo based alloys are required. At the Tritium Laboratory Karlsruhe (TLK), a new dedicated setup is currently being commissioned to assess the storage properties with high accuracy and using an inventory of up to 3 grams of tritium. This setup will be able to perform thermodynamic and kinetic measurements as well as investigations of disproportionation and regeneration behaviour for different getter bed materials

This contribution gives an overview of the working principles and status of the experiment and the considerations for the use with tritium.

FUS-ThP-3 Development of a Method for Hydrogen Species Analysis in Fusion Breeder Materials Using ICP-MS, ***Clemence Mont***, UKAEA, UK

The UK Atomic Energy Authority is investigating breeder material technologies through the LIBRTI (Lithium Breeding Tritium Innovation) programme to support tritium production for Fusion Energy. Tritium is a scarce resource around the world and one of the key fuels for Fusion with deuterium. The Fusion sector must develop breeding technologies to transform lithium into tritium using the neutrons generated during the fusion of deuterium and tritium. This will create a tritium fuel cycle where tritium is created as it is used for the fusion reaction.

The LIBRTI programme is investigating different breeder materials such as FLiBe, LiPb and liquid lithium among others. A facility will be built in the coming years on the Culham Campus in Oxfordshire, UK, to test the materials in a large-scale mock-up experiment. Within the LIBRTI programme, a project called CLIO is looking at developing an analytical method to determine the concentration of tritium in the breeder materials using ICP-MS (Inductively Coupled Plasma – Mass Spectrometry). Developing analytical techniques for tritium accountancy is a priority to ensure process control, safety, environmental protection and security around a fusion power plant.

The CLIO project is split into 4 phases. The first 1 started in June 2026, and its aim was to develop a method for hydrogen and deuterium analysis as surrogate to tritium. Hydrogen is famously difficult to analyse with an ICP due to its high ionisation energy, the development of a novel method would allow the instrument to be used in the Fusion sector. Phase 2, started in October 2026, introduces breeder materials as a sample. The detection of hydrogen might suffer from matrix effect coming from the different type of materials, assessing each of them is important to ensure accuracy of the results. Phase 3 starting in January 2027 will look at simplifying the sampling technique by adding the Laser Ablation – LIBS (Laser Induced Breakdown Spectrometry) system to the ICP-MS. While using the ICP-MS on its own necessitates the dissolution of the sample, the LA-LIBS add-on will allow surface analysis. The LA-LIBS-ICP-MS will be able to do bulk and surface analysis. The final phase planned later in 2027 will introduce tritium to the system. This step will ensure that the system can analyse all hydrogen isotopes and that it can be used in the LIBRTI programme as a tritium detection system.

Results from the method development carried out in phase 1 as well as preliminary data from phase 2 are presented in the poster.

FUS-ThP-4 the Actively Pumped Open-Surface Lithium LOop (APOLLO) – a Liquid Lithium Plasma Facing Component Technology Testbed, ***Brady Moore***, University of Illinois Urbana-Champaign*; Daniel O'Dea,* University of Illinois at Urbana Champaign*; Zachary Nordan, David Ruzic,* University of Illinois at Urbana-Champaign

Liquid lithium is being explored as a plasma-facing component (PFC) for fusion devices, particularly in the divertor region. Compared with traditional solid materials like tungsten, a flowing liquid surface can better recover from extreme heat fluxes during transient events, continually renew itself, and is impervious to neutron damage. Lithium also has a low atomic number leading to a higher tolerable concentration in the plasma core. Additionally, lithium readily reacts with hydrogen isotopes leading to a low-recycling boundary that can improve plasma performance and flatten plasma temperature profiles. However, this same property creates a key challenge: lithium can retain radioactive tritium which has strictly monitored inventories. Future fusion reactors will aim to minimize total tritium inventory and therefore effective tritium separation from liquid lithium is critical.

The University of Illinois Urbana–Champaign (UIUC), in partnership with Tokamak Energy Ltd., has developed the Actively Pumped Open-Surface Lithium Loop (APOLLO) to develop technologies required for implementing liquid lithium PFCs. APOLLO features a circulating liquid lithium loop, a free-surface lithium plasma-facing component operating under a magnetic field, a hydrogen/deuterium plasma source or electron beam heating system, and an in-line distillation column for the removal of hydrogenic species. The PFC employs a computationally optimized distributor that ensures uniform delivery of lithium from an inlet pipe across a 7.5 cm-wide, additively manufactured refractory metal mesh within an open-surface flow channel. Lithium traverses the mesh at average surface velocities up to 10 cm/s, with mass flow rates reaching 12 g/s, while simultaneously interacting with an electron cyclotron resonance (ECR) hydrogen/deuterium plasma. Plasma properties have been characterized in-situ using an array of 16 Langmuir probes, a retarding field energy analyzer (RFEA), and actinometric spectroscopy. After plasma exposure, the lithium is directed to the inductively heated Hydrogen Distillation Experiment (HyDE), where it is thermally processed at temperatures up to 700 °C to remove hydrogenic species and other impurities before being recirculated through the loop.

In this work, hydrogen uptake in flowing liquid lithium exposed to an ECR plasma, as measured by a novel resistive impurity probe, is investigated as a function of lithium flow rate and plasma operating conditions. The efficiency of hydrogen thermal extraction is also quantified using a resistive impurity probe and thermal desorption analysis.

FUS-ThP-7 An Analysis of Radiation Tolerance of Parylene Coatings for Nuclear Energy Applications, ***Steven Larson***, *Alex Mings, Joshua Young, Ronald Goeke,* Sandia National Laboratories

Steven R Larson, Alex Mings, Josh Young, Ron GoekeSandia National Laboratories

Parylene is a chemical vapor deposited (CVD) polymer coating widely used in the electronics industry due to its excellent chemical resistance and dielectric properties. Recently, Parylene has also attracted interest as a protective coating for components in nuclear reactor systems, where materials are often exposed to highly corrosive environments, elevated temperatures, and high radiation. Despite this interest, relatively little is known about how the different Parylene polymers response to ionizing radiation. Additionally, the extent to which radiation tolerance varies among the different types of parylene remains largely unexplored. While some data exists for parylene C, D, and N very little data has been published on the different parylene F polymers (VT-4 and AF-4) due to their difficulty in precursor fabrication. This talk will present efforts to determine the physical, chemical, optical, and electronic changes that occur in Parylene C, D, N, VT-4, and AF-4 following exposure to lifetime-relevant gamma and neutron irradiation. We will discuss the differences between the various parylene polymers and how to cost optimize for extremely expensive precursors. Sandia National Laboratories is managed and operated by NTESS under DOE NNSA contract DE-NA0003525 SAND2026-21514A

FUS-ThP-8 Torion USA Multi-Gram Tritium User Facility, ***Cody Fagan***, *Mike Koch,* Torion USA*; C.R. Shmayda,* Torion Plasma, Canada*; Walter Shmayda,* Tritium Solutions

The opening of the Torion USA multi-gram tritium facility marks a milestone in advancing fusion fuel cycle (FFC) science, engineering, and workforce development in the US. Designed as a flexible, user-oriented platform for experiments, prototyping, and applied training, the facility establishes a new private capability for hands-on engagement with FFC technologies at scales relevant to fusion demonstration systems.

The facility is equipped with a suite of state-of-the-art systems supporting tritium processing, accountancy, isotope separation, permeation, materials compatibility testing, and detritiation. Multiple modular glovebox systems and experimental stations are available to support tritium process equipment incorporating high technology readiness level (TRL) components. These systems are intended to demonstrate integrated FFC operations while also providing a place for deploying and validation of our next-generation technologies that are relevant to Fusion Pilot Plants (FPPs). By enabling both operations and technology advancemet, the user-facility is designed to accelerate innovation in FFC technologies while reducing barriers to access for emerging fusion companies and research partners to test developed concepts with tritium.

A central mission of the facility is the development of a highly trained fusion workforce capable of safely operating our advanced tritium systems. The laboratory will host immersive training programs that combine classroom instruction with direct hands-on operational experience using our glovebox systems and experimental stations. Participants will gain practical experience in tritium radiological safety, regulatory compliance, process control and maintenance of systems, and experimental methods essential for future fusion energy deployment. These programs are intended to cultivate the next generation of fusion scientists, engineers, operators, and safety professionals at a time of rapidly increasing demand across the fusion energy ecosystem.

FUS-ThP-9 Investigating Gaseous Impurity Production in a Baked UHV System, ***Gabriel Wilber***, Tritium Solutions, Inc.*; E. Koukina, K. McCormack, A. Knaian,* Acceleron Fusion*; W.T. Shmayda,* Tritium Solutions, Inc.

Muon-catalyzed fusion offers a unique alternative energy source. In this approach muons are injected into a high-pressure gas target containing a deuterium-tritium mixture. When a muon attaches itselves to a DT molecule, the probability for the DT molecule to fuse increases significantly. This event generates energy, creates a 4He atom, and releases the muon to attach itself to another DT molecule over its 2.2 μs mean lifetime. However, if the muon interacts with a gaseous impurity, it can no longer participate in catalyzing fusion reactions. This paper investigates on the type and quantity of impurities produced when D2 is injected into a heated 316-stainless steel ultrahigh vacuum system.

Light Source Enabled Science
Room Ballroom A - Session LS-ThP
Light Source Enabled Science Poster Session

LS-ThP-1 Ultrafast Science at the NSF-NeXUS Facility, ***Seth Shields***, *John Beetar,* Ohio State University*; Conner Dykstra,* ohio state University*; Joohyung Park,* ohio State University*; TJ Ronningen,* ohio state University*; Robert Baker, Lou DiMauro, Jay Gupta, Roland Kawakami, Claudia Turro,* Ohio State University

The National Science Foundation (NSF) National eXtreme Ultrafast Science Facility (NeXUS) is a new open access user facility that provides access to extreme light to researchers around the world. The facility contains a mix of optical and analytical capabilities that allow for the study of chemical and material properties on the time scale of femtoseconds to attoseconds and on the length scale of angstroms. A customized high power, high repetition rate (800 W @ 100 kHz) Yb-doped fiber laser and pulse compression scheme from Active Fiber Systems GmbH is used to produce extreme ultraviolet light (XUV) through high harmonic generation. The XUV light is conditioned through three beamlines, which provide tailored light to a variety of end stations, three of which support materials analysis: X-ray absorption/reflection spectroscopy (XAS/XRS), Angle Resolved Photoemission Spectroscopy (ARPES), and Scanning Tunneling Microscopy (STM).

This poster will present the preliminary results and progress during the commissioning and inaugural user experiments at NeXUS.

LS-ThP-2 Operando Study of CO_2 Adsorption on PtGa (111) Surface, ***Subin Jang***, Gwangju Institute of Science and Technology, Republic of Korea*; Minsik Seo,* Nanyang Technological University, Singapore*; Hyunsuk Shin,* Samsung Electronics, Korea (Democratic People's Republic of)*; Dongwoo Kim,* KBSI, Republic of Korea*; Kyungmin Kim,* Gwangju Institute of Science and Technology, Republic of Korea*; Hojoon Lim,* Myongji University, Republic of Korea*; Jongkeun Jung,* Korea Institute of Science and Technology, Republic of Korea*; Dong Junf,* Korea Advanced Institute of Science and Technology (KAIST), Republic of Korea*; Sung Yoo,* Korea Institute of Science and Technology, Republic of Korea*; Jeongjin Kim,* Pohang Accelerator Laboratory, Republic of Korea*; Lenart Dudy,* Synchrotron SOLEIL, France*; Jean-Jacques Gallet, Fabrice Bournel,* Sorbonne Université, France*; Bongjin Simon Mun,* Gwangju Institute of Science and Technology, Republic of Korea

Managing the surplus of CO_2 in Earth's atmosphere has become a critical global issue as it drives global warming and climate change. Consequently, many efforts are devoted not only on reducing CO_2 waste, but also on efficient conversion of CO_2 into valuable products. In this study, a PtGa (111) single–crystal alloy is used as a model catalyst to investigate surface chemical states under CO_2 using ambient–pressure X–ray photoelectron spectroscopy (AP–XPS). At 2×10^{-2} mbar CO_2 and room temperature, surface species assigned to carboxylate (CO_2^-) and carbonate (CO_3^{2-}) appear, indicating a clear pressure threshold for CO_2 adsorption on PtGa. When the surface temperature is raised under 0.2 mbar CO_2, the carboxylate signal disappears, while CO and carbonate intensify together with formation of GaO_x. During this process, only Ga is oxidized and Pt remains metallic, highlighting the key role of interfacial gallium oxide adjacent to Pt sites.

LS-ThP-3 Investigation Into Polymer Charge Localization with Soft X-Ray Absorption Spectroscopy, ***Jonathan Thurston***, University of Colorado at Boulder*; Shuya Li,* National Laboratory of the Rockies*; Qi Sun,* University of Arizona*; Dennis Nordlund,* Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory*; Luis Kitsu Iglesias, Collin Sindt,* University of Colorado at Boulder*; Santosh Kumar, David Grinter,* Diamond Light Source, UK*; Hong Li,* University of Arizona*; Ann Greenaway, Elisa Miller,* National Laboratory of the Rockies*; Michael Toney,* University of Colorado

Semiconducting polymers have sparked interest in electrochemical processes such as catalysis and energy storage due to their strong charge transport properties and ionic conductivity. Despite the importance of polymer-electrolyte interactions in device performance, there is a lack of understanding of the fundamental interphasial interactions that occur between the polymer and electrolyte. In this study, we use near-edge X-ray absorption fine structure spectroscopy (NEXAFS) and vibrational spectroscopy to study the local atomic electronic and chemical structure of a pi-conjugated redox active polymer. We use N2200, a well-studied polymer due to its high crystallinity, conductivity, and charge carrier mobility which has monomeric units consisting of an naphthalene diimide (NDI) with alkyl sidechains coupled with a bithiophene unit.

N2200 has two redox events correlating to the formation of polarons (-1 charge) and bipolarons (-2 charge) during charging that are accompanied by the absorption of counter-cations from the surrounding electrolyte for charge neutralization. We will introduce and discuss an *ex-situ* study in which carbon and oxygen NEXAFS is measured at different points in the polymer charging process and compare to an *operando* study in which the polymer charge is held potentiostatically while measuring NEXAFS. Using simulations, we assign electron excitation events to experimental NEXAFS spectra, identify polaron localization, and discuss how polymer-electrolyte interfacial interactions dictate charge transfer. Our results show how the charge localizes on the polymer and how elemental environments of the polymer change as a function of charge. This work addresses the impact of polymer choice as electrode materials on device performance and operation.

LS-ThP-4 Bridging Concept and Application: An LLM-Assisted Machine Learning Software Pipeline for Automated ARPES Analysis at MAESTRO, ***Sandy Adhitia Ekahana***, Carnegie Mellon University*; Hendrik Santoso Sugiarto,* Calvin Institute of Technology, Indonesia*; Chris Jozwiak, Aaron Bostwick, Eli Rotenberg,* ALS-LBNL*; Jyoti Katoch,* Carnegie Mellon University

Recent advancements in angle-resolved photoemission spectroscopy (ARPES) have enabled spatially resolved measurement, vastly increasing the dimensionality and complexity of the resulting multidimensional hyperspectral data. Processing this data creates a bottleneck, driving the need for automated techniques to label and map similar dispersion cuts

spatially [1]. While self-supervised learning combined with k-means clustering can successfully automate these tasks [1], incorporating spatially-aware representations via graph convolution significantly enhances the transfer learning capabilities and classification accuracy for spatially resolved ARPES data [2]. However, translating these proven machine learning methodologies into practical, user-friendly software at experimental facilities like the MAESTRO beamline remains a critical challeng. This poster presents a fully functional Python application deployed for the MAESTRO beamline, transforming these advanced machine learning models [1, 2] into an accessible tool for general facility users. The software was developed from scratch using a Large Language Model (LLM)-assisted prompt-based generation approach, colloquially known as "vibe coding," utilizing Gemini-Pro. By leveraging a deep conceptual understanding of the analytical workflow and offloading the syntax generation to the AI, the application development was structured through deliberate, step-by-step prompting. The interface and underlying logic were built sequentially, one tab at a time. This methodological approach resulted in a highly modular architecture where the codebase is segmented into easily digestible chunks. This poster demonstrates both the underlying machine learning pipeline for ARPES data reduction [1, 2] and a modern, AI-assisted paradigm for rapidly prototyping and deploying robust scientific software.

[1] Ekahana, S. A., et. al. (2023). *Machine Learning: Science and Technology*, 4(3), 035021.

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LS-ThP-5 Soft X-rays, Hard Questions: Identifying Band Character in Quantum Materials with ARPES*, **Jessica McChensey**, Fanny Rodolakis,* Argonne National Laboratory, USA

We highlight the Intermediate Energy X-ray (IEX) beamline 29-ID at the Advanced Photon Source (APS), optimized for SX-ARPES with variable polarization, a near–magic-angle geometry that minimizes broadening and footprint, sub-10 K six-axis cryogenic manipulation, and integrated x-ray absorption (total/partial electron yield) alongside photoemission. The APS Upgrade extends the accessible photon-energy range to hv ≈ 184–2000 eV with increased flux, strengthening opportunities for bulk and buried-interface studies. I'll present several examples illustrating how the photon-energy dependence and polarization can be used to disentangle band character. For instance, in the heavy-fermion compound Ce2RhIn8, SX-ARPES suppresses problematic surface contributions and yields near-constant-kz momentum cuts, clarifying bulk Fermi-surface signatures in the low-temperature hybridized regime while revealing strong matrix-element effects that motivate matrix-element-aware modeling. In addition, circular dichroism SX-ARPES can be used to investigate the topology of the band structure. In the nodal-line semimetal ZrSiS, circular dichroism SX-ARPES reveals ~30% dichroism for both Dirac bands near the Fermi level and deeper valence states, with sign reversals across crystallographic mirror planes.

LS-ThP-6 Palladium Nanofoams as a Framework for Hydrogen Storage*, **Alisson Steffli Thill**,* Universidade Federal do Rio Grande do Sul, Brazil*; Slavomir Nemsak,* Advanced Light Source, Lawrence Berkeley National Laboratory*; Fabiano Bernardi,* Universidade Federal do Rio Grande do Sul, Brazil

Hydrogen has gained major attention as a renewable fuel, but efficient storage methods remain a challenge [1,2]. Metallic and oxide nanostructures have been explored to enhance hydrogen adsorption [3]. In a previous work of our group [4], it was demonstrated the possibility of synthesizing NiO nanofoams, which showed promising hydrogen storage performance under mild conditions compared to literature results. In part, this great performance is explained by the existence of the quasi-molecular bonding regime for the hydrogen adsorption process in NiO nanofoams. The quasi-molecular bonding of hydrogen with solid materials is the key factor for reaching the ultimate goal for hydrogen storage applications [5]. Considering the high hydrogen affinity of Pd and the promising adsorption results of NiO nanofoams, the development of Pd nanofoams has great conditions to display an even higher hydrogen storage performance.

In this work, the synthesis method was extended to produce Pd nanofoams using five phytantriol/water template phases. Therefore, five different Pd nanofoam samples were obtained. The samples were characterized by SEM, TEM, XRD, SAXS, AP-XPS, and AP-GIXS. Hydrogen adsorption measurements were also performed in order to obtain the hydrogen adsorption performance of all samples. Furthermore, DFT calculations were performed to determine the binding energy of hydrogen molecules in Pd structures.

For all samples, SEM and TEM images revealed Pd nanofoams composed of interconnected nanoparticles with diameters in the tens of nanometers range, forming channels of about 50-100 nm. The samples also contained isolated nanoparticles with diameters around 4 nm. XRD showed tunable fractions of metallic Pd and PdO. AP-XPS measurements before hydrogen exposure indicated an almost fully oxidized PdO surface, which rapidly reduced upon hydrogen exposure. Analysis of the AP-XPS data during hydrogen exposure showed that hydrogen interaction and Pd-H bond formation depend on the sample. These results can be correlated with theoretical calculations and sample morphology to explain the hydrogen adsorption performance.

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LS-ThP-7 Strain and Electronic Correlations in Metal-Insulator Transition of $CaVO_3$ Thin Films*, **Amitayush Jha Thakur**,* Argonne National Laboratory, India

The metal-to-insulator transition (MIT), which can occur as a function of temperature, pressure, doping, or applied bias, is a paradigmatic example of the dramatic consequences of strong electron correlations in solids and holds promise for new applications in the emerging field of Mottronics. $CaVO_3$ is metallic in bulk form and in thick films, but undergoes a pronounced MIT when the film thickness is reduced below 20 unit cells (u.c.). Unlike the MIT reported in ultrathin $SrVO_3$, this transition cannot be explained solely by dimensional crossover in thin films. Instead, the MIT in $CaVO_3$ appears to be mediated by a complex interplay of epitaxial strain, surface crystal-field splitting, and possible structural and magnetic transitions. Preliminary low-temperature measurements at 30 K on a limited set of samples reveal the electronic evolution of thin films across the MIT; however, systematic measurements across the full thickness and temperature range are still lacking. Here, we present a study of the electronic and structural properties of $CaVO_3$ thin films across this phase space using angle-resolved photoemission spectroscopy (ARPES), X-ray photoelectron spectroscopy (XPS), X-ray absorption spectroscopy (XAS), and X-ray diffraction (XRD). These measurements allow us to investigate the drivers of the MIT and clarify the complex interplay between strain and electronic structure in this correlated oxide system.

LS-ThP-8 A NEXAFS Reference Library for Metal Compounds*, Matthijs A. van Spronsen, David C. Grinter, Pilar Ferrer, **Georg Held**,* Diamond Light Source, UK

Near edge X-ray Absorption Fine Structure (NEXAFS) spectroscopy is an ideal tool to study materials under *in situ* and operando conditions. It gives quantifiable and element specific information on the oxidation state. As X-ray absorption can be measured in a variety of ways (transmission, electron and fluorescence yield), it can be more easily adapted to difficult experimental configurations than XPS. Typical NEXAFS analysis comprises comparing the experimental spectra to those of reference materials of know oxidation state and/or chemical structure. This procedure can be extended to linear combinations fitting of the spectra of interest. However, everything hinges on the availability of a set of reference compounds that capture the relevant chemistry. Currently, many hours of beamtime are used to measure the same readily available references by different user groups. This is ineffective use of beamtime and oftentimes the set of references does not include more exotic, potentially unstable, compounds. These are, however, critical for understanding materials under operating conditions because the *in situ* formed structure can be very different from the stable, well-known compounds.

At Diamond Light Source, we are in the process of building a comprehensive library of reference materials. The focus thus far has been on Co, Ni, and Ti compounds, and a total of 30 compounds have been measured including $Ni(OH)_2$, $LiNiO_2$, NiO, NiO_2, Ni_3S_2, CoO, Co_3O_4, $LiCoO_2$, $Co(OH)_2$, CoCO, and various Co and Ni metalorganics. These reference samples will be published in a public repository (GitHub) in an open access

data format and viewable with an on-line data plotter. Furthermore, these will also be integrated in the control software used at Diamond (GDA).

Multifunctional and Hybrid Microsystems
Room Ballroom A - Session MC-ThP
Multifunctional and Hybrid Microsystems Poster Session

MC-ThP-1 Integrated Magnetic Bio-MEMS for High-Speed, Trajectory-Based Microparticle Classification in Laminate Microfluidic Channels, *Muhammad Tahir,* ***Umer Hassan,*** Rutgers, The State University of New Jersey

Microfluidic diagnostics increasingly depend on microsystems that combine sample handling, physical actuation, optical readout, and data analysis within one workflow. We present a magnetically actuated bio-MEMS platform that uses particle motion, rather than fluorescence or impedance, as the primary signal for distinguishing magnetically responsive microparticles in flow. The approach integrates a laminate polymer microchannel, an external permanent magnet, high-speed brightfield imaging, and automated video analysis, making it relevant to multifunctional microsystems where sensing, actuation, and signal processing are co-designed.

The device was constructed from three laser-cut polymer layers to form a transparent channel with a 35 mm length, 150 µm width, and 87 µm height. Nonmagnetic polystyrene beads and magnetic beads, both approximately 5–5.9 µm in diameter, were used as model negative and positive particle populations. Samples were introduced at 5 µL/min, producing an estimated particle velocity of 6.4 mm/s. Motion was recorded at 3,030 frames/s with 324 µs exposure over a field of view of approximately 600 µm × 162 µm. A computer-vision pipeline converted the image sequence into particle centroids, reconstructed paths, and extracted trajectory slope as a compact metric of magnetically induced lateral displacement. COMSOL Multiphysics modeling guided the microsystem geometry before testing. Simulations examined magnet-channel spacing from 0–10 mm, magnet width from 3.175–9 mm, and channel widths from 250–750 µm. The model showed that smaller magnet-channel separation, larger magnet width, and narrower channels improved deflection within the imaging window; for example, mean simulated slope decreased from 0.151 to 0.005 when the magnet was moved from the channel edge to 10 mm away.

Later, experimental data confirmed that trajectory-derived signatures can separate the two particle groups. Using a slope threshold of 0.03, 240 of 393 magnetic particles were classified as deflected, compared with 53 of 347 control particles. This corresponded to 61% deflection for the magnetic population and 15.2% apparent deflection for controls. Mean trajectory slope shifted from -0.01 ± 0.059 for control beads to 0.039 ± 0.062 for magnetic beads, demonstrating measurable motion contrast between populations. This work demonstrates an integrated fluidic-actuation-imaging-analysis platform for magnetic microparticle classification. With improved tracking and antibody-labeled cell validation, the system could support compact bio-MEMS workflows for cell phenotyping, surface-marker-linked magnetic response, and low-cost diagnostic microsystems.

MC-ThP-2 Internal Friction, Creep, and Mechanical Behavior of Zr-Based Metallic Glass Thin Films for MEMS/NEMS Applications, *KAI-AN YANG, Yan-Wei Chang,* National Chung Hsing University, Taiwan*; Hsiang-Yu Hsieh, Chen-Jia Wang,* National Chung Hsing University, Taiwan*; Tra Anh Khoa Nguyen,* ***Ming-Tzer Lin,*** National Chung Hsing University, Taiwan

Zr-based metallic glass alloys exhibit high hardness, wear and corrosion resistance, ductility, high strain toughness, and low Young's modulus, making them attractive candidates for MEMS and NEMS devices. Yet, research on the internal friction characteristics, creep behavior, and fracture mechanisms of metallic glass thin films remains limited, and the fundamental processes of internal friction and shear band slip within their amorphous structure are not fully understood. In this study, Zr-Cu-Ti metallic glass thin films are employed to investigate anelastic mechanical behavior, creep resistance, and fracture response across a broad temperature range from room temperature to elevated conditions. Internal friction measurements and bulge tests are conducted to quantify energy dissipation, structural relaxation, and crack propagation resistance. In addition, Zr-Cu-Ti metallic glass thin films are also examined before and after annealing to investigate the effects of phase transformation from amorphous to crystalline states. Preliminary results indicate that annealing-induced crystallization alters internal friction and mechanical performance, establishing correlations between atomic-scale structural evolution and macroscopic reliability. These findings provide new insights into the reliability of metallic glass thin films, enabling their integration into MEMS/NEMS devices where durability, adaptability, and long-term stability are critical. This work directly supports the MEMS and NEMS area of interest by advancing knowledge of thin-film mechanical behavior under structural transformation.

MC-ThP-3 Influence of the Structural Regions of a Si_3N_4 Membrane Window on the CMOS Image Sensor Signal, ***Kamil Baranowski,*** *Michał Krysztof, Michał Zychla,* Wroclaw University of Science and Technology, Poland*; Rupert Schreiner, Matthias Hausladen,* Ostbayerische Technische Hochschule (OTH) Regensburg, Germany*; Mathias Bartl,* Ostbayerische Technische Hochschule (OTH) Regensbur, Germany*; Alexandr Knápek,* Institute of Scientific Instruments of the Czech Academy of Sciences, Czechia

1. Introduction

A CMOS sensor coated with a copper layer can be used to detect an electron beam [1]. Incoming electrons are decelerated within the layer, generating Bremsstrahlung X-rays, which the sensor records and converts into a beam's image. The target application is the detection of an electron beam in a gaseous environment [2]. A silicon nitride (Si_3N_4) membrane separates the vacuum environment of the electron-optical column from the gaseous environment of the sensor, maintaining the pressure difference while allowing electron transmission. Here we examine how the membrane and supporting silicon chip influences the CMOS signal, aiming to isolate its contribution from effects caused by other factors, such as gas composition.

2. Experiment

To assess this, the CMOS signal intensity was mapped along a line scanning the membrane (Fig. 1). The CMOS matrix was mounted inside a JEOL JSM-100 SEM, which served as both the electron source and the vacuum chamber. The sample stage was moved along a predefined scanning path, directing the 10 keV electron beam at successive regions of the membrane window. Three regions are distinguished
(Fig. 1): A - full silicon substrate, ~350 µm thick; B - sloped pyramid wall formed during KOH etching; C - Si_3N_4 membrane, 100 nm thick. Signal intensities are reported relative to region C, taken as 100%. The recorded signal reflects the combined effect of electron scattering, energy loss, and Bremsstrahlung yield in the copper layer, rather than a simple beam transmission ratio.

3. Conclusion

The experiment quantified how the Si_3N_4 membrane and surrounding substrate geometry contribute to the CMOS signal. In region A no signal above the noise floor was detected (0%), confirming that the 350 µm silicon substrate fully absorbs the beam and X-rays that can be generated in it. In region B the signal increases as the silicon thickness decreases, indicating that the KOH-etched pyramid walls also contribute to the detected signal. In region C the signal reaches its maximum (100%). These results show that the etched window geometry significantly influences the signal and must be accounted for when separating membrane-related contributions from gas-related effects in future measurements at elevated pressure.

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Magnetic Interfaces and Nanostructures
Room Ballroom A - Session MI-ThP
Magnetic Interfaces and Nanostructures Poster Session

MI-ThP-1 Wilson Loop as a Tool to Investigate Chirality-Induced Spin Selectivity: Role of Vibrations and Multiple Channels, ***Leonardo Celada***, *D. K. Andrea Phan Huu, Alessandro Chiesa, Paolo Santini, Luca Griguolo, Stefano Carretta,* Università degli studi di Parma, Italy

Chirality-induced spin selectivity (CISS) has been observed in a wide range of chiral molecular systems, yet the minimal microscopic ingredients required for spin polarization remain debated [1]. Here we introduce the Wilson loop as a general theoretical criterion to identify when spin polarization can emerge in model Hamiltonians relevant to CISS.

Using open tight-binding models with spin-orbit coupling, we show that the Wilson loop provides a gauge-invariant characterization of spin-dependent interference and recovers the known absence of CISS in single-channel purely electronic models, where a local spin gauge transformation removes all spin dependence. By contrast, non-trivial Wilson loops arise in systems with multiple transport channels, providing a direct symmetry-based criterion for finite spin polarization, consistent with previous theoretical studies of CISS mechanisms [2].

We then extend this framework to electron-vibration models and show that vibronic pathways can generate non-trivial Wilson loops even in nominally single-channel systems. In particular, Peierls-type coupling creates spin-dependent interference in vibronic space and enables CISS, whereas Holstein coupling preserves a trivial Wilson loop and cannot induce spin polarization. This establishes a distinction between vibrational mechanisms proposed in the literature [3].

Beyond reproducing known results, the Wilson-loop formulation provides a unifying path-based picture connecting gauge structure, interference, and spin selectivity across electronic and vibronic mechanisms. The framework can be generalized to arbitrary molecular architectures and offers a tool to identify necessary conditions for CISS in transport and electron-transfer settings, including systems where spin selectivity has recently been observed experimentally [4].

This project is supported by the Horizon Europe program through the ERC-Synergy CASTLE project (proj. n.101071533).

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MI-ThP-2 Experimental Insights into Spin-Driven Correlated Phase Transitions in CrN, ***Khan Alam***, Department Of Physics, Kfupm, Saudi Arabia*; Arthur Smith,* Department of Physics

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Abstract

Chromium nitride (CrN) is an important transition metal nitride that serves as a model system for studying correlated structural, electronic, and magnetic phase transitions. The coupling among these transitions makes CrN a compelling example of a correlated material in which magnetic spin ordering plays a central role in driving the observed transformations. Upon cooling, CrN undergoes a first-order transition involving antiferromagnetic spin ordering, along with structural and electronic transitions. These structural, electronic, and magnetic transitions are not independent but strongly intertwined, offering insight into the mechanisms of magnetostructural coupling in correlated electron systems.

Our experimental investigations of these coupled transitions in CrN include neutron diffraction, reflection high-energy electron diffraction, variable-temperature x-ray diffraction, electronic transport measurements, and scanning tunneling microscopy, we probe the evolution of structural symmetry, magnetic spin order, and electronic states across the transition. The results elucidate how spin ordering triggers and stabilizes the structural and electronic phase transitions, highlighting the cooperative nature of these coupled phenomena. These findings not only deepen our understanding of CrN but also shed light on the broader class of correlated transition metal nitrides that exhibit intertwined spin-lattice-charge interactions.

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MI-ThP-3 Utilizing MOKE Magnetometry to Observe Properties of Magnetic Thin Films, ***Ivan Gray***, *Seth Woodwyk, Femi Akinrinola, Raj Bhandari, Jeremy Fanelli, Mikel Holcomb,* West Virginia University

In the study of thin film materials, magnetometry can be a powerful tool for understanding the magnetic properties and interactions of materials, though most widely available magnetometers are designed for bulk materials, so surface level probing at a focused point can be difficult. The magneto-optical Kerr effect (MOKE), however, offers a surface-sensitive alternative to bulk magnetometry techniques. MOKE is a magneto-optic phenomenon that results from interactions between light and the magnetization of a material. A magnetized material will experience differing refractive indices for left and right-circularly polarized light due to the off-diagonal tensorial elements of the dielectric constant of the material. As light reflects from this material, the two circularly polarized components are reflected with varying amplitudes and phase shifts, resulting in a changed polarization state of the reflected light. This is described by both the Kerr rotation, the angle in which the original polarization is rotated, and the Kerr ellipticity, describing the resulting elliptical polarization. Changes in these properties can be observed over a range of applied fields, showing the magnetic hysteresis of the material, noted as Kerr magnetometry. We are using this method to explore the mechanisms behind spontaneous magnetization reversal (SMR) in single layer thin films of $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) grown on $SrTiO_3$ (STO). SMR is more commonly seen in multilayer systems, while it has only been reported in a few single layer systems. In SMR, competing magnetic interactions under a cooling or applied field can result in the net magnetization reversing direction relative to the field. In particular, LSMO exhibits SMR both at low applied magnetic fields and near room temperature, allowing for potential real-world applications. Understanding how the mechanisms driving SMR in LSMO work will inform the design of future devices that exploit SMR under practical operating conditions.

MI-ThP-4 Early-Stage Experimental Training in Magnetism: A Hands-On Freshman Research Course as a Gateway to Advanced Magnetic Materials, ***Mikel Holcomb***, West Virginia University*; Femi Akinrinola,* West Virginia University, USA*; Robbyn Trappen, Seth Woodwyk, Ivan Gray, Tap Raj Bhandari, Jeremy Fanelli, Dorian Davis, Nethmi Kankanamge, John Stewart,* West Virginia University

The development of advanced magnetic materials and low-dimensional magnetic systems relies critically on a skilled experimental workforce capable of integrating measurement and data interpretation at early stages of training. I describe a hands-on freshman-level research course designed to introduce students to experimental magnetism through direct engagement with measurement techniques and a variety of magnetic systems. In this course, students perform studies on magnetic materials, with an emphasis on data acquisition and physical interpretation. Projects are structured to connect fundamental concepts—such as magnetic anisotropy, hysteresis and types of magnetism—to experimental observables, providing an entry point into phenomena central to modern magnetism research. Students develop experimental intuition through open-ended investigations that reflect the uncertainty and exploratory nature of contemporary research, with each project structured as a potentially extensible research direction. I will discuss course design, representative experiments, and evidence for improved student readiness for research in physics and materials science. This model suggests a pathway for broadening participation and accelerating training in areas aligned with emerging challenges in magnetic interfaces and nanostructures. This work is supported by NSF DUE 2417349.

Manufacturing Science & Technology
Room Ballroom A - Session MS-ThP
Manufacturing Science & Technology Poster Session

MS-ThP-1 Landing-Pad Geometry Engineering for Contact-Access Margin in Scaled Semiconductor Manufacturing, ***Dong Kyun Lim***, Department of Semiconductor and Display Engineering, Sungkyunkwan University (SKKU), Suwon, Republic of Korea

As memory-cell dimensions continue to shrink, the connection between capacitor lower electrodes and landing-pad structures becomes increasingly sensitive to local overlay error, landing-area loss, CMP/topography variation, and contact-interface geometry. This poster presents a public-disclosure-based manufacturing framework for landing-pad geometry engineering in scaled semiconductor memory integration. The framework is based on a landing-pad structure in which a lower landing pad, an upper landing pad with a cavity, and a conductive pattern in the cavity form additional contact-access geometry for a capacitor lower electrode.The objective is to treat landing-pad geometry as a process-margin design variable rather than only as a static interconnect feature. The proposed analysis maps key integration risks: capacitor-electrode shift from the landing pad, reduced effective contact area, contact-resistance increase, CMP-induced topography variation, and leakage/capacitance distribution spread. A qualitative failure-mode and effects analysis compares a conventional landing-pad contact scheme with a geometry-assisted landing-pad concept, identifying expected observable signatures and required metrology for each risk.The proposed validation path combines cross-sectional SEM/TEM, CD and overlay metrology, landing/contact-area extraction, capacitor contact-resistance monitoring, leakage and capacitance distribution, and optional process/device simulation. This work does not claim unpublished process recipes, product implementation, measured yield improvement, or node-specific dimensions. The intended contribution is a manufacturing-science poster framework showing how local landing-pad geometry can link process margin, contact accessibility, and device-level electrical robustness in scaled memory structures.

MS-ThP-2 Design of Ultra-Low Flow Microfluidic Peristaltic Pump for Neural Probe Based Drug Delivery with Refillable Reservoir, ***Haowei Ma***, *Allison Hess-Dunning, Melinda Lake-Speers,* Case Western Reserve University

Localized neurotherapeutic delivery requires compact microsystems that can store therapeutic agents, support repeated replenishment, and deliver small fluid volumes through a stable neural interface. Here, we present a tubing-based refillable microfluidic peristaltic pump for integration with a mechanically adaptive neural probe to deliver fluid at 0.15 microliters/hour. The device combines drug storage, tubing guidance, motor alignment, and rotary actuation within a compact footprint.

The pump was designed in SolidWorks as an integrated assembly containing a refillable reservoir, tubing groove, actuator chamber, and motor interface. A flexible microbore tube forms the fluid pathway and is seated within the groove to define the pumping region. The reservoir connects to the tubing inlet, while the outlet can be coupled to a downstream neural probe or other delivery module. A motor-driven rotary actuator periodically compresses the tubing to generate peristaltic displacement. The geometry maintains actuator-tubing alignment, limits tubing migration, and supports reproducible compression during low-speed rotation.

Housing and actuator components were fabricated from Anycubic Bio Resin by high-resolution resin-based 3D printing. Printed parts were washed in isopropyl alcohol, UV-cured, and inspected to confirm clearance in the tubing groove, rotor chamber, reservoir interface, and motor alignment region. During assembly, microbore tubing was manually seated into the printed pathway and connected between the reservoir and outlet. The geared micromotor was positioned in the alignment region and coupled to the rotary actuator for low-speed operation.

Preliminary proof-of-concept testing evaluated the mechanical and fluidic function of the assembled device. The pump was driven by a benchtop power supply at 0.5 to 3 V while the tubing compression region and outlet segment were observed under microscopy. Evaluation focused on actuator rotation, periodic tubing deformation, structural stability, fluid containment, and visible directional movement of liquid or air bubbles. These observations confirmed that the printed housing, flexible tubing, motor, and actuator can function together as a compact peristaltic pumping module.

This work demonstrates a modular tubing-based refillable pump architecture for localized neurotherapeutic delivery. Future work will quantify empirical flow rate to meet the target, low-speed stability, leakage resistance, and long-term operation, supporting integration with wearable neural probe interfaces for chronic localized therapy.

MS-ThP-3 Distal Electrofabrication of Chitosan Membranes on Printer Paper: A New Manufacturing Paradigm, ***Phuc Long Duong***, *Xiaolong Luo,* Catholic University of America

Traditional fabrication of biopolymer membranes relies heavily on solution casting or direct electrodeposition onto electrode surfaces. These methods restrict production scalability and limit control over the resulting material properties. This work introduces a novel macroscale manufacturing paradigm: distal electrofabrication of freestanding chitosan membranes directly onto a low-cost printer paper scaffold. By separating the fabrication site from the physical electrodes, this system enables membrane growth that is independent of electrode size, unlocking a highly scalable pathway for thin-film manufacturing.

The manufacturing setup utilizes two 3D-printed fluidic chambers containing a 0.5% w/v chitosan solution (pH 5.5) and a companion buffer solution. A regular piece of printer paper is sandwiched between the chamber apertures to serve as a porous interfacial matrix. By applying a direct current across the sandwiched fluidic chambers via remotely located platinum electrodes, a uniform chitosan thin film assembles directly on the paper surface. Crucially, the process offers precise controllability over the membrane's physical properties. Adjusting the current density (5 - 60 A/m^2) and deposition time (10 – 60 minutes) allows fine-tuning of the membrane thickness (a few hundred microns).

Material characterization confirms that the electrofabrication process microaligns the biopolymer's internal structure as compared to traditional casting. Electrochemical impedance spectroscopy (EIS) and tensile testing reveal that molecular alignment alters internal porosity, mechanical properties, and ionic pathways. This versatile, paper-supported fabrication technique provides a cost-effective, controllable blueprint for manufacturing high-performance biopolymer thin films for energy and electromechanical systems.

Nanoscale Science and Technology
Room Ballroom A - Session NS-ThP
Nanoscale Science and Technology Poster Session

NS-ThP-1 Improving Mechanical Integrity in Wearable Solid-Carbon Microneedle Sensors, ***Nicolas Manning***, Commonwealth University of Pennsylvania - Lock Haven

Nanostructured carbon used as solid contact enables stable, calibration-free all-solid-state ion-selective electrodes (SC-ISEs) in miniaturized formats. It is typically coated on top of a metallic electrode, such as a microneedle, followed by an ion-selective membrane (ISM) coating. When this microneedle is inserted into artificial skin, the coatings do not always stay intact. Here we investigate an alternate approach by preparing self-supporting mesoporous carbon-based microneedles, which can be infiltrated and covered with the ISM. We hypothesize that this helps to maintain the ISM coating during insertion of the microneedle into skin. Silicone molds were prepared from steel microneedle arrays and then infiltrated with a resol containing colloidal silica as sacrificial template for the mesopores. After polymerization and carbonization, the resulting microneedle arrays were etched to remove the silica, introducing mesopores. Structural features were verified by scanning-electron microscopy. Future work will incorporate reference membranes and assess ion selectivity under physiological conditions, advancing SC-ISE microneedles for real-time on-skin or in vivo ion monitoring.

NS-ThP-2 Single-Molecule Spectro-Microscopic Visualization of Surface-Supported Configurational Flexibility and Intramolecular Transformations, ***Soumyajit Rajak***, *Nan Jiang,* University of Illinois, Chicago

Understanding physicochemical transformations at surfaces with molecular-scale precision is essential for advancing nanoscale materials characterization and the rational design of functional interfaces for catalysis, molecular electronics, and optoelectronic devices. A major challenge in surface characterization is the direct identification of

intermediates, adsorption geometries, and reaction products with simultaneous chemical specificity and sub-molecular spatial resolution, capabilities that are difficult to achieve with conventional ensemble-averaged techniques. Although scanning tunneling microscopy (STM) provides atomic-scale structural information, it often lacks definitive chemical sensitivity, particularly for nonplanar and conformationally flexible molecular systems. A single-molecule tip-enhanced Raman spectroscopy (TERS) methodology integrated with ultra-high vacuum (UHV) STM has been utilized to achieve correlative nanoscale structural and chemical characterization of thermally induced surface transformations and surface-dependent molecular arrangements. Coupling light with an atomically sharp plasmonic probe creates highly localized surface plasmons (LSPs), which allow the overcoming of the diffraction limit and confined enhancement of the Raman signals. As a model metal-organic interface, we investigate tetraphenyl tetrabenzoporphyrin adsorbed on Cu(100) and Cu(111), representative systems relevant to heterogeneous catalysis and organic electronic materials. Porphyrin derivatives are especially attractive for nanoscale studies because of their tunable electronic structure, metal-coordination functionality, and conformational flexibility arising from σ-bonded meso-substituents.Our measurements demonstrate that TERS provides chemically specific vibrational fingerprints of individual adsorbed molecules while simultaneously resolving symmetry variations and local conformational changes induced by molecule–substrate interactions at the sub-nanometer scale. Spatially resolved vibrational mapping enables discrimination between coexisting adsorption geometries and thermochemically transformed species that exhibit distinct chemical identities. The results further reveal how substrate interactions stabilize nonplanar conformations and alter molecular symmetry, establishing direct structure-property relationships at the single-molecule level.

NS-ThP-3 Intrinsic Stability of Rhodium Nanoclusters on HOPG: An Atomic-Scale Investigation of Heat Treatment and CO Adsorption, ***Charbel Tawny***, *Maxwell Gillum, Gallage KPA Ariyaratne, Mausumi Mahapatra,* Loyola University Chicago

Understanding structure-reactivity relationships in heterogeneous catalysis requires well-defined model systems that enable atomic-scale characterization. In this work, Rhodium (Rh) nanoclusters were deposited on Highly Oriented Pyrolytic Graphite (HOPG), an inert support, to investigate their nucleation, growth and changes in morphology under ultra-high vacuum (UHV) conditions. By systematically varying Rh coverage (0.09 ML to 0.6 ML), Scanning Tunneling Microscopy (STM) was used to resolve cluster size, morphology, and spatial distribution. Our experiments reveal the formation of highly dispersed Rh nanoclusters with a notably narrow size distribution; for instance, a 0.09 ML deposition produced particles with an average width of 1.74 ± 0.5 nm and height of 0.85 ± 0.1 nm. Crucially, these nanostructures exhibit exceptional thermal stability, maintaining their size and distribution even after annealing to elevated temperatures up to 850 K. Subsequent CO exposure at both 300 K and 500 K allowed for the visualization of surface interactions. While CO induced streaking was observed in STM images due to adsorbate mobility, the Rh clusters remained structurally stable without significant redispersion or morphological changes. This study establishes the robustness of Rh nanoclusters in response to various stimuli that would be present in an industrial reaction, such as high temperatures and gas exposure, further deepening our knowledge of surface catalysis.

NS-ThP-4 Characterization and Analysis of Rhodium Oxide Nanoparticles on HOPG Surface, ***Gallage KPA Ariyaratne***, *Maxwell Gillum,* Loyola University Chicago*; Charbel Tawny,* loyola University Chicago*; Mausumi Mahapatra,* Loyola University Chicago

This study investigates the characterization and analysis of rhodium oxide (RhO_x) nanoparticles formed on highly oriented pyrolytic graphite (HOPG), with the aim of understanding how oxygen influences nanoparticle stabilization and behavior on a weakly interacting support. HOPG serves as an ideal model surface for probing intrinsic nanoparticle properties in the absence of strong substrate interactions. Rh nanoparticles are vapor-deposited onto freshly cleaved HOPG under ultra-high vacuum conditions and subsequently oxidized at controlled temperatures (300–850 K) to generate RhO_x nanostructures. Scanning Tunneling Microscopy (STM) is employed to examine nanoparticle morphology, size distribution, and structural evolution as a function of temperature and Rh coverage. Oxidation at room temperature results in the formation of RhO_x nanoparticles with an apparent reduction in particle density and surface coverage relative to metallic Rh. At elevated temperatures, larger RhO_x nanoparticles are observed, with average widths of 9.14 nm. High temperatures like 850 K, result in the formation of triangular channels on HOPG surface, originating from step edges. These features are not due to direct structural failure of HOPG but rather arise from oxygen mediated anisotropic etching of the graphite surface. Oxygen can dissociate on RhO_x which then migrate onto the HOPG surface where the atomic oxygen react with uncoordinated carbon atoms at defect sites and step edges which lead to the removal of carbon atoms as CO/CO_2 and leads to anisotropic etching on surface. Post oxidation exposure to carbon monoxide (CO) is performed to evaluate redox reversibility and stability under reducing conditions, with the evolution of gaseous species such as CO_2, O_2, and CO observed, while the crack and particle size remains unchanged. In parallel, Density Functional Theory (DFT) calculations using (PBE-GGA) model RhO_x adsorption on graphite, identifying favorable configurations, and electronic properties with nanoparticle stability, reactivity, and catalytic performance on carbon supports.

NS-ThP-5 Spatiotemporal Defect Engineering of Charge Transport in TiO2 by Time-Resolved Atomic Force Microscopy, *Nuray Basaran, Mohammad Safikhani-Mahmoudi,* École de technologie supérieure, University of Quebec, Canada*;* ***Bugrahan Guner****,* Yale University*; Omur Dagdeviren,* École de technologie supérieure, University of Quebec, Canada

The performance of photocatalysts, sensors, and oxide-based devices is governed by how charge carriers migrate, recombine, and interact with defects at surfaces and interfaces. Titanium dioxide (TiO_2), a model photocatalyst, provides a versatile platform for exploring these dynamics. Recent advances in*time-resolved atomic force microscopy (TR-AFM)* now allow direct nanoscale mapping of carrier motion under realistic conditions, uncovering defect-controlled pathways that were previously inaccessible.

We establish findings from our recent studies to build a coherent picture of light-induced defect dynamics in TiO_2. In "thin" TiO_2films, it was shown that ultraviolet irradiation generates photoinduced surface oxygen vacancies (PI-SOVs) that shorten carrier migration time constants but raise activation barriers, indicating a trade-off between faster trapping and reduced mobility. Extending this framework,*we*revealed that PI-SOVs impact both fast and slow timescales, with spatially heterogeneous distributions leading to locally distinct transport regimes.*Moreover, we explored* surface chemistry by introducing methanol as a prototypical hole scavenger: methanol adsorption further reduced time constants and modified activation energies, demonstrating how molecular adsorbates tune vacancy-carrier interactions.

By bridging molecular adsorption, defect generation, and irradiation penetration, this body of work highlights spatiotemporal defect engineering as a promising strategy for controlling charge transport in oxides. TR-AFM emerges as a uniquely powerful platform for resolving these processes at the nanoscale, offering pathways to rationally design oxide-based systems with tunable photocatalytic efficiency, sensor responsiveness, and energy-conversion robustness.

NS-ThP-6 Ce-Doped TiO_2 Nanoparticles from Commercial P25 and Flame Spray Pyrolysis Synthesis Routes for Enhanced Visible-Light Photocatalysis, *Selda Topcu Sendogdular,* Stony Brook University, Turkey*;* ***Ilker Keseroglu****, Pelagia-Iren Gouma,* The Ohio State University

Ce-doped TiO_2 nanoparticles were synthesized by modifying commercial Degussa P25 and flame-made TiO_2 produced by flame spray pyrolysis (FSP), followed by thermal treatment at 500 °C. The effects of Ce doping on the structural, morphological, optical, and photocatalytic properties of TiO_2 were investigated for undoped and Ce-doped samples containing 5 and 40 wt% Ce.

X-ray diffraction (XRD) analysis showed that both P25 and FSP TiO_2 consisted primarily of anatase and rutile phases, while Ce doping suppressed the anatase-to-rutile transformation and promoted CeO_2 phase formation at higher Ce loading. Ce doping reduced the anatase crystallite size and altered the phase composition, with brookite contributions observed in CE5-P25 and CE5-TiO_2 samples. SEM and TEM analyses revealed morphological differences between P25 and FSP TiO_2 particles, where P25 exhibited irregular elongated and polygonal particles, while FSP-derived TiO_2 showed predominantly spherical particles. Ce doping decreased particle size to approximately 14–34 nm, whereas high Ce loading (40 wt%) resulted in particle agglomeration and cube-like Ce-rich structures. SAED and HRTEM analyses confirmed the coexistence of anatase and rutile phases and verified lattice fringes corresponding to anatase (101) and rutile (110) planes.

UV–Vis spectroscopy demonstrated enhanced visible-light absorption and a red shift in the absorption edge with increasing Ce content. The bandgap decreased from approximately 3.06 eV for pure TiO_2 to 2.48 eV for Ce-

doped samples, indicating improved visible-light response. Photocatalytic performance was evaluated through methylene blue degradation under visible-light irradiation using a Xe lamp with AM 1.5G and a 400 nm cut-on filter. Among all samples, CE5-TiO_2 exhibited the highest photocatalytic activity, achieving approximately 90% methylene blue degradation under visible light.

The enhanced photocatalytic performance is attributed to reduced crystallite size, suppression of rutile phase growth, modified phase composition, and improved visible-light absorption induced by Ce doping. These results demonstrate that Ce modification effectively enhances the photocatalytic activity of both commercial P25 and flame-made TiO_2 for environmental remediation applications.

NS-ThP-7 Roll-to-Plate Nanoimprint Lithography for Fabrication of Biomimetic Structures, ***Daniela Topasna***, *Juan Gonzalez, Sebastian Ziegler,* Virginia Military Institute

Nanoimprint Lithography (NIL) fabrication technique consists of transferring a pattern from a template by pressing it onto a resin coated substrate, yielding structures with nanometer resolution. The resin can be cured thermally or by exposure to UV radiation. This is a simple, low-cost and high-throughput technique, which has been used as an alternative to photolithography in semiconductor industry, optics and photonics, and biomedical field. NIL roll-to-plate method was used in this project to replicate microstructures of Cicada wings which are of interest due to their antibacterial properties. We report the results on the fabrication of these biomimetic structures and on their characterization by scanning electron microscopy.

NS-ThP-8 Nanoscale Surface and Interface Engineering of Asymmetric Electrode Screen Length for Advanced Nanoscale Ferroelectric Devices, ***Philip (Sanghyun) Lee***, University of Kentucky*; Kent Price,* Morehead State University*; M. David Henry,* Sandia National Laboratories, USA

The continued scaling of ferroelectric tunnel junctions (FTJs) has placed unprecedented importance on understanding and controlling nanoscale surface and interface interactions within ultrathin HfO_2–based ferroelectrics. At thicknesses below 6 nm, the electronic structure, bonding environment, and screening behavior at metal/ferroelectric interfaces dominate the tunneling landscape, often more strongly than the bulk ferroelectric properties themselves. Conventional symmetric Metal-$Hf_{0.5}Zr_{0.5}O_2$-Metal (MFM) stacks such as TiN/HZO/TiN exhibit negligible tunneling electroresistance (TER) because their interfaces screen polarization charges in an identical manner, suppressing any barrier asymmetry. While inserting dielectric interlayers can restore asymmetry, these additional interfaces introduce variability, trap formation, and integration challenges.

This contribution presents a materials–driven strategy that leverages intrinsic nanoscale surface and interface asymmetry between dissimilar metal electrodes to enhance FTJ performance without modifying the ferroelectric layer. We focus on five CMOS compatible metals such as TiN, W, Ru, TaN, and Mo about possessing distinct electronic screening behavior, interfacial bonding characteristics, and surface chemistries with HZO. These differences affect how polarization-bound charges are compensated at the interface, reshaping the tunneling barrier.

To assess these nanoscale interfacial effects, multiple devices including Ta/HZO/TaN were developed and their nanoscale interfacial structures and chemistry were compared in agreement with theoretical research for MFM devices. This study incorporates realistic ferroelectric switching, nonlocal tunneling transport, and metal–specific screening behavior, enabling direct correlation between nanoscale interface physics and device–level performance. Surface and interface characteristics with multiple HZO thicknesses were quantified to confirm how interfacial screening, depolarization stability, and surface-induced barrier shaping collectively determine TER, read current, and write voltage.

Our results show that electrode pairs with different interfacial screening length create strong asymmetry in the tunneling barrier, enabling enhanced TER without the need for additional interlayers. Energy band analysis reveals how nanoscale surface interactions such as metal-oxygen bonding, interfacial dipole formation, and screening charge distribution directly affect the tunneling mechanism in opposite polarization states. Finally, we mapped optimal metal combinations that support low–voltage switching and stable ferroelectric behavior <6nm HZO for interface–engineered MFM devices.

NS-ThP-9 Time-Delayed Measurements of Heterogeneous Dynamic Data, ***Petro Maksymovych***, Clemson University*; Sabine Neumayer,* Oak Ridge National Laboratory, USA

In neuromorphic and memory devices, accessible multistability is enabled by the dynamics of the constitutive materials rather than by their equilibrium structures alone. Hysteresis loops, oscillatory responses, and other time-dependent signatures reflect the multiplicity of accessible material states. Yet deciphering the underlying dynamics remains persistently elusive — in no small part because the dynamic information itself is treated qualitatively rather than as a quantitative observable.

I will present a systematic approach based on time-delayed embedding and dynamic mode decomposition that treats dynamic data as a structured object, extracting its nonlinearity, topology, and a predictive numerical model of the underlying process. Applied to resistive switching in memory oxide materials [1,2], nonlinearity alone can discriminate between specific microscopic mechanisms. In ferroelectrics, the same framework separates genuine switching from spurious hysteresis and detects the signatures of a multiwell potential [3,4]. Effective denoising strategies extend the approach to noisy nanoscale and device measurements without loss of physical interpretability.

Time-delayed methodologies provide a transparent and interpretable connection between hysteresis loops and physical mechanisms, complementing machine learning methods and enabling parameter-free comparison between modeling and experiments of driven dynamics. R

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NS-ThP-10 Chirality Retention in Aqueous Propylene Oxide Hydration: Chirality of the Transition State, ***Nisha Shukla***, Carnegie Mellon University, USA*; Marcus Yu,* University of Columbia*; Andrew Gellman,* Carnegie Mellon University, USA

The hydration kinetics of enantiomerically pure propylene oxide (PO) to chiralpropylene glycol (PG) in aqueous solution have been studied using FTIRwhile simultaneously monitoring the net chirality of the reaction mixture. The hydration reactionappears to be first-order in the PO concentration with a rate constant of 0.05 hr. Moreimportantly, the reaction is enantioselective; the product PG retains the chirality of the 2C carbonin PO with ~2:1 selectivity. The fact that there is some inversion of the chirality suggests thatthe dominant transition state is one in which the 2C-O bond in PO is cleaved, resulting in a closeto planar transition state capable of inversion during hydration. If the transition state involved1C-O cleavage it would retain the rigid chiral center of the PO reactant, preventing significantinversion.

NS-ThP-11 Understanding the Structural Orientation of Iron Tetraphenylporphyrin (Fe-TPP) on HOPG through Scanning Tunneling Microscopy for Electrocatalytic CO_2 Reduction, ***Hritvik Bhosale***, *Mausumi Mahapatra,* Loyola University Chicago

Homogeneous molecular catalysts provide precise control over the steric and electronic properties of active sites, enabling tunable catalytic activity and selectivity. However, these systems often suffer from limited stability, poor recyclability and reduced long-term durability under homogeneous operating conditions. Consequently, strategies that combine the tunability of molecular catalysts with the robustness of heterogeneous platforms have attracted considerable attention. Despite advances in catalyst heterogenization, developing structurally well-defined systems that bridge homogeneous and heterogeneous catalysis remains a challenge.

Porphyrin-based systems have emerged as attractive molecular platforms owing to their structural versatility, electronic tunability and catalytic

relevance. Among them, iron porphyrins are particularly promising for electrocatalytic CO_2 reduction through successive electron-transfer processes that have demonstrated efficient, CO-selective and durable catalytic performance.

Understanding molecule-surface interactions at the nanoscale is essential for rational catalyst heterogenization. Scanning tunneling microscopy (STM), with submolecular and atomic-scale spatial resolution, provides a powerful platform for directly visualizing molecular arrangements, conformations, electronic structures and intermolecular interactions at surfaces. STM has proven especially effective for investigating the adsorption behavior and self-assembly of porphyrin systems on conductive substrates.

The present study investigates the adsorption behavior of iron tetraphenylporphyrin (FeTPP) on highly oriented pyrolytic graphite (HOPG) using STM as the primary investigative technique. By correlating molecular structure with surface organization, intermolecular interactions, and local electronic properties, this work aims to provide fundamental insights into molecule-surface interactions relevant to catalyst heterogenization and to establish structure–property relationships for the development of heterogenized iron porphyrin systems for efficient electrocatalytic CO_2 reduction.

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NS-ThP-12 Nano-Projectile SIMS: Guiding EUV Resists Fabrication Process with Nanoscale Compositional Insights, ***Christelle Guillermier***, Biennetechnology*; Michael J Eller,* University of Mississippi*; Stanislav V Verkhoturov, Richard Rickman,* Biennetechnology*; Serge Della Negra,* Universite Paris Saclay, France*; Emile A Schweikert,* Texas A&M and Biennetechnology

The semiconductor industry is rapidly adopting extreme ultraviolet (EUV) lithography to pattern features below 10 nm. However, there remains a critical need for methods capable of probing nanoscale compositional uniformity throughout the multi-step fabrication process. Secondary Ion Mass Spectrometry (SIMS) has long been a key analytical technique in semiconductor process control due to its high sensitivity and high-resolution depth profiling capabilities, but its lateral resolution is limited to ~50 nm, restricting its application to critical dimension analysis. In this work, we present results from the newly commercialized Nano projectile Secondary Ion Mass Spectrometry (NP-SIMS) instrument, the Orion MkII, which overcomes this limitation by examining surfaces with individual nano-projectiles. Each projectile samples an area of ~10–15 nm in diameter and ~10 nm in depth, enabling nanoscale inspection with lateral resolution that matches the requirements of advanced EUV photoresist characterization. We demonstrate the capabilities of NP SIMS for identifying material inhomogeneities that can lead to defects during resist fabrication and compromise pattern quality. More specifically, NP-SIMS enables examination of characteristic molecular species for homogeneity and co-localization with other resist components. The integration of a multi-anode detector further allows identification and characterization of sites containing multiple instances of the same analyte. Finally, NP-SIMS provides detailed chemical analysis of defect sites, which can significantly affect the resist performance. Altogether, NP-SIMS delivers essential insights to guide the optimization of EUV resist chemistry and processing conditions.

NS-ThP-13 Probing the Electron Screening Process in 2d Semiconductor WS_2, *Alex Boehm, Christopher Smyth,* Sandia National Laboratories*; Kory Burns,* University of Virginia, USA*; Andrew Kim,* Sandia National Laboratories, USA*; Jordan Hachtel,* Oak Ridge National Laboratory, USA*; Don Bethke, Tzu-Ming Lu, Catalin Spataru,* Sandia National Laboratories, USA*; Hayden Barry,* University of Virginia, USA*; Jose Fonseca, Jeremy Robinson,* Naval Research Laboratory, USA*; **Taisuke Ohta**,* Sandia National Laboratories, USA

The confinement of charge carriers within an anisotropic two-dimensional (2D) geometry leads to reduced, variable dielectric screening, which gives rise to strongly bound excitons, correlated electron phases, and band gap renormalization. We employ electronic structure probes (photoelectron and electron energy loss spectroscopies) to assess the impact of the supporting substrate and the sulfur vacancy defects on the screening characteristics of the 2D semiconductor WS_2. Exploiting the contrasting external dielectric screening environments achieved in gold-supported and free-standing (i.e. suspended) configurations, we show how the electronic states of one-layer WS_2 align at a built-in junction across the effective and ineffective screening environments. Photoelectron spectroscopy points to the close alignment of the charge neutrality levels of WS_2 between each screening environment. We further reveal through ion irradiation that the introduction of a modest defect density (n_V) of 1×10^{13} cm^{-2} reduces the electronic band gap from 2.4 eV to 2.2 eV in poorly-screened suspended WS_2 because of the exciton binding energy reduction. The band gap renormalization accompanies the diminishing photoelectron core-hole relaxation and the expansion of the screened radius beyond the inter-defect distance around 4 nm when n_V reaches ~8×10^{12} cm^{-2}. Collectively, these findings provide key insights into the interrelationships of the polarizability of WS_2 with its electronic behavior and photoemission process.

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NS-ThP-14 Local Electronic and Transport Properties of Epitaxial Graphene on Sic(0001) Studied by Scanning Tunneling Microscopy and Spectroscopy, ***Marek Kolmer***, *Umamahesh Thupakula, Shen Chen, Yong Han,* Ames National Laboratory*; Michael C. Tringides,* Iowa State University

Despite long-standing efforts to understand the interface between epitaxial graphene and the Si-terminated silicon carbide (0001) substrate, the exact atomic-scale structure, its complex bonding configurations, and the resulting electronic properties of the first epitaxial graphene carbon layer (C_{buffer}) remain open problems. We will present how to control the local structure of the epitaxial graphene-SiC interface with a low-temperature scanning tunneling microscope (STM) [1]. We will show that the covalent bonds between C_{buffer} and the SiC substrate may be reversibly broken and restored using the polarity of the electric field from the STM tip, generating protrusions at the interface of slightly higher amplitude. This buried interface manipulation enabled us to pattern epitaxial graphene with lateral precision, reaching the scale of a single 1.8 nm unit cell of the graphene-SiC interface $(6\times6)_{SiC}$ moiré lattice. However, the STM manipulation experiments also provide direct evidence of silicon vacancies at the topmost reconstructed SiC(0001) layers [2]. Bias-voltage- and epitaxial graphene thickness-dependent characterization of the collective C_{buffer}-SiC interface showed that 'Si' vacancy sites exhibit stable, non-switching behavior under STM electric fields. Moreover, vacancies introduce localized electronic states below the Fermi level. Our experimental results directly elucidate the atomic-scale interface and the influence of atomic and bonding configurations on the local density of states for graphene of different thicknesses on SiC(0001). Finally, we will present the consequences of the local epitaxial graphene structure on electronic transport properties.

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NS-ThP-15 The Nature of Photodoping in van der Waals Heterostructures, ***Son Le***, Laboratory for Physical Sciences; *Thuc Mai, Maria Munoz, Riccardo Torsi, Angela Hight Walker, Curt Richter,* NIST; *Aubrey Hanbicki,* Laboratory of Physical Sciences; *Adam Friedman,* Laboratory for Physical Sciences

A unique photoinduced modulation doping is achieved via integration of common 2D materials and inexpensive light sources. Under applied electric field and incident light, the doping level of 2D materials heterostructures consisting of multiple dielectric layers can be precisely controlled and tuned *in situ*. This photodoping also offers local control of charge with submicron spatial resolution with lifetimes on the order of months to years. For 2D materials systems there is no current agreement on the exact mechanism underlying this effect, with studies pointing to charge generation and trapping in various layers/interfaces. In this work, we present photoinduced doping of van der Waals heterostructures with various compositions in order to pin-point the exact spatial location of the photoactive defects that responsible for the doping phenomena. Regardless of the mechanistic details, this photodoping effect yields high-quality reconfigurable devices in a variety of 2D material systems including graphene, TMDs, and 2D superconductors.

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NS-ThP-16 Ternary Gold Nanoparticle-Corona-Neurotransmitter Plasmonic Complexes for Probing Resonant Electronic Coupling, ***Tefera Entele Tesema***, *Kahmeria Smith,* Prairie View A&M University

Plasmonic gold nanoparticles generate localized electromagnetic fields under resonant excitation, making them powerful platforms for probing nanoscale metal–molecule interactions. Although the molecular corona is often treated as a passive stabilizing layer, its composition can regulate interfacial charge distribution, optical damping, adsorption geometry, and plasmon-mediated coupling. Here, we develop a ternary plasmonic complex consisting of a gold nanoparticle core, a plant-derived molecular corona, and neurotransmitter molecules as a model system for resonant electronic coupling at bioactive noble-metal interfaces, using surface-enhanced Raman scattering (SERS) as the primary readout.Purple sweet potato (Ipomoea batatas, PSP)-derived extract functions as a reducing/stabilizing medium and forms a molecular corona containing anthocyanins, phenolic acids, and related polyphenols. This corona is treated as an electronically active, chromophoric interface whose absorption can influence resonance conditions. Dopamine is used as an initial catecholamine model to probe how bioactive adsorbates perturb the corona-mediated optical and vibrational response.Preliminary UV–visible spectroscopy shows that extraction protocol, pH, and solvent environment influence the optical identity of the PSP extract and nanoparticle formation. Unpeeled PSP extracted in 0.05 M acetate buffer at pH 4.75 produces a wine-colored, colloidally stable AuNP suspension that remains visually stable for five days. In contrast, TFA extraction at pH ~3 preserves anthocyanin absorption near 522 nm but is associated with black precipitate during AuNP formation, consistent with uncontrolled nucleation or aggregation. These observations indicate that mildly acidic acetate conditions provide a more suitable window for controlled AuNP–corona assembly. Anthocyanin interconversion among flavylium, hemiketal, quinonoidal, and related forms provides a handle for tuning corona absorption relative to the AuNP plasmon and SERS excitation.The phenolic and catechol-like functionalities in the PSP corona overlap chemically with catecholamine neurotransmitters and may compete for or reorganize interfacial binding sites on gold. SERS will monitor these interactions through vibrational fingerprints that report adsorption geometry, orientation, and binding competition. Coupling corona electronic transitions, nanoparticle plasmon resonance, and laser excitation is expected to amplify neurotransmitter-sensitive interfacial signatures. This work provides a tractable model for signal transduction at biotic–abiotic interfaces and may inform plasmonic chemical sensing and bioactive nanoparticle design.

NS-ThP-17 Exciton-Polaritons in Metal-Organic Chalcogenolates: From UV to Visible, ***Deep Jariwala***, University of Pennsylvania

Exciton-polaritons (EPs), hybrid light–matter quasiparticles formed by strong coupling between excitons and confined photons, offer a route to engineer semiconductor optical response without chemical modification. Here, I present strong and ultrastrong coupling in metal-organic chalcogenolates (MOCs), layered van der Waals hybrid semiconductors that act as natural multi-quantum-well structures with strong excitons, large oscillator strengths, and high refractive indices. These properties make MOCs promising self-hybridized polaritonic materials from the ultraviolet (UV) to visible range.

I will first discuss silver phenylselenolate (AgSePh, mithrene), which has a direct optical bandgap of ~2.65 eV, exciton binding energy of ~400 meV, and refractive index of ~2.5. Mueller matrix ellipsometry reveals giant in-plane birefringence (~1.01) and three anisotropic exciton resonances, enabling polarization-dependent linear dichroism up to ~77% when coupled to an optical self-cavity. Thickness-controlled mithrene flakes on reflective substrates support self-hybridized EPs in the ultrastrong coupling regime, with normalized coupling g/Ex = 0.13–0.14 and Rabi splitting >650 meV, the largest reported for a non-organic semiconductor in the visible range.

I will then present self-hybridized EP photodetectors in mithrene, where thickness-tunable multimode polariton states enable sub-bandgap photodetection extending >130 nm (~0.55 eV) below the optical bandgap. Trap-assisted two-photon absorption sustains strong coupling under sub-bandgap excitation, addressing a key limitation for polaritonic light harvesting. The polariton dispersion yields ultrafast group velocities (~65 μm ps−1), extending effective exciton diffusion from hundreds of nanometers to several micrometers and producing a 2.38-fold enhancement in photo-to-dark current ratio.

Finally, I will extend these concepts to the UV using silver phenylthiolate (AgSPh, thiorene), a wider-bandgap MOC with a sharp excitonic resonance at 3.46 eV (~60 meV linewidth) and refractive index of ~2.1. In open and closed cavities, thiorene shows clear anticrossing with Rabi splittings of 488 and 512 meV, respectively, among the largest reported in the UV and 6–10× larger than conventional ZnO and GaN platforms. Together, these results establish MOCs as a versatile platform for polariton-enhanced optoelectronics.

Advanced Packaging
Room Ballroom A - Session PK-ThP
Advanced Packaging Poster Session

PK-ThP-1 A Numerical Investigation of Acoustic Void Detection in Through Silicon Vias using the Rayleigh-Ritz Method, ***George Antonelli***, Antonelli Research & Technology; *Shiva Mudide,* Massachusetts Institute of Technology

Voids formed in through silicon vias (TSVs) during metallization pose significant reliability risks and are challenging to detect using conventional optical, x-ray, and electron beam defect inspection and review techniques. Non-destructive acoustic approaches such as scanning acoustic microscopy (SAM) and photoacoustics have been proposed to fill this gap. The expected signals from voided TSVs can be investigated with mechanical simulations using the finite element method to guide the development of hardware; however, these calculations can be slow and tedious to setup. We propose the application of a frequency-domain modeling framework based on the Rayleigh–Ritz variational method. Closed-form expressions for monomial volume moments can be derived for spherical, conical, cylindrical, and composite voids, enabling rapid parametric evaluation of void-induced perturbations to the vibrational spectrum. Symmetry constraints imposed by photoacoustics and SAM excitation conditions reduce the accessible mode space, further reducing the complexity of the calculation. Numerical studies demonstrate strong mode-specific sensitivity to void size and shape and reveal the dominant influence of geometric parameters—such as aspect ratio and radius—on modal dispersion.

Plasma Science and Technology
Room Ballroom A - Session PS-ThP
Plasma Science and Technology Poster Session

PS-ThP-1 CO_2 as an Alternative Oxidant to N_2O in Plasma–Enhanced CVD Oxide Deposition, ***Lipeng Qian***, Micron technology, Singapore

Silane–based oxide and oxynitride films are widely deposited using plasma–enhanced chemical vapor deposition (PECVD) with silane (SiH_4) as the silicon precursor and nitrous oxide (N_2O) as the oxidant. Due to the high global warming potential and limited abatement efficiency of N_2O, alternative oxidants are being evaluated. In this study, a PECVD process is developed in which carbon dioxide (CO_2) replaces N_2O as the oxidation gas.

A schematic comparison of the conventional N_2O–based process and the CO_2–based process is shown in Figure 1. The primary technical challenges associated with this transition arise from the intrinsically lower reactivity of CO_2 relative to N_2O, which results in reduced oxidation efficiency during plasma activation. The higher bond energy of CO_2 limits its dissociation and oxide–forming capability with SiH_4, necessitating extensive process tuning to achieve acceptable film formation.

Significant differences in film composition are observed between the two processes, leading to challenges in matching key optical properties, including refractive index (n) and extinction coefficient (k), as shown in Figure 2. In addition, the CO_2–based process exhibits a shifted and narrower process window, with substantially degraded defect performance relative to the N_2O baseline. Defect sensitivity is strongly process–region dependent and requires targeted optimization to achieve manufacturable performance.

Integration impacts are also observed, as the CO_2–based films demonstrate different wet and dry etch behaviors, requiring adjustments to downstream photo and etch processes to maintain compatibility. Despite these challenges, successful implementation of an N_2O–free PECVD process is achieved through systematic optimization and process innovation. Representative film performance is summarized in Table I, showing reduced surface roughness, slower wet etch rate, and reduced dry etch rate compared to the N_2O reference process.

This work demonstrates the technical feasibility of CO_2–based PECVD oxide deposition for semiconductor manufacturing, providing a viable pathway toward N_2O–free deposition processes while maintaining film property control and integration compatibility.

PS-ThP-2 Effect of Electrode Configuration on Plasma Discharge Characteristics and PVDF Film Properties Using Atmospheric Pressure Plasma Jets, ***Eun Young Jung***, The Institute of Electronic Technolog, Kyungpook National University, Republic of Korea*; Heung-Sik Tae,* School of Electronic and Electrical Engineering, Kyungpook National University, Republic of Korea*; Choon-Sang Park,* Department of Electrical Engineering, Milligan University

The development trends of piezoelectric nanogenerators (PENGs) will be flexible light weight and wearable self-poweredelectronics for an industrial application. For this reason, polyvinylidene fluoride (PVDF) for piezoelectric polymer materials seem to be attractive candidates for flexible PENGs owing to mechanical flexibility and good properties of the piezoelectric and ferroelectricity [1,2]. Recently, these PVDF-basedpolymers are used to produce films using the various plasma techniques such as low-pressure and atmospheric pressure plasma (APP). In particular,the APP process is the appropriate method to deposit the polymer film on the point of view a simple and low cost process. ThisAPP process are effective method for polymer deposition under ambient air due to easy, simple process, and room temperature[3]. There are few research on the piezoelectric polymers using the APP process [1,4].However, there are some problems such as low deposition rate, loss of monomer precursor, and small deposition area of the APP processes. Thus, to resolve these problems, the structural improvement of plasma reactor is essential for enhancing the efficiency of deposition rate and deposition area.Accordingly,this study investigates the plasma discharge characteristics and structural properties of PVDF thin film deposited by using APP reactor in terms of two different electrode configurations (metal-mesh and planar-type). The characteristics of PVDF thin films investigated using field-emission scanning electron microscope (FE-SEM), Fourier transforms-infrared spectroscopy (FT-IR), X-ray diffraction (XRD), and LCR meter. Through new APP plasma reactor electrode configurations, the thickness of PVDF thin film was increased by using a planar-type electrode compared to that of a metal-mesh type electrode at room temperature using a mixed polymer solution composing of PVDF nano powder and dimethylformamide solution. FE-SEM results show that PVDF nanoparticles are clearly observed and uniformly coated. In the FT-IR spectra, two types of chemical bonds (α and β phases) were observed in the deposited PVDF thin film. Based on these experimental results, we may expect that a new APP plasma reactor will be a great attractive method in order to synthesis the PVDF thin film under atmospheric pressure.The APP with new APP plasma reactor, FE-SEM, FT-IR, XRD, LCR meter, and related mechanism of PVDF thin film are studied and will be discussed in detail.

PS-ThP-3 Time Stability of Hafnium Nitride Thin Films Deposited by Plasma-Enhanced Atomic Layer Deposition, ***Sandra Schujman***, NY Creates*; Natalya Tokranova, Christophe Valleé,* University at Albany*; Vidya Kaushik,* NY Creates

Transition metal nitrides are sought for semiconductor device applications due to their low electrical resistivity and because they can be excellent diffusion barriers for copper and oxygen. Such films prepared by Atomic Layer Deposition (ALD) have the additional advantage of spatial conformability to structured surfaces and tight thickness control.

In particular, for the ALD deposition of hafnium nitride there have been a number of studies demonstrating tunable electrical properties by controlling the process chemistry (varying the precursor and co-reactant), using thermal ALD versus Plasma-Enhanced ALD, using different plasma compositions, and by varying the deposition parameters (substrate temperature, plasma pressure, plasma composition, etc.). Even though very low electrical resistivity values have been reported, it has also been observed that over time, the resistivity of the layers tends to increase.

In this work, we concentrated on the analysis of electrical resistivity stability as a function of time for HfN thin films deposited on Si or SiO_2 substrates. Various ionic compositions of the plasma, different external RF bias of the substrate, and ALD cycle parameters, were used in order to obtain low electrical resistivity. The layers were characterized by X-ray Photoelectron Spectroscopy, Grazing Incidence X-ray Diffractometry, X-ray Reflectrometry, and Atomic Force Microscopy, and four-point probe measurements were done to determine resistivity.

The samples were kept under regular atmospheric conditions and remeasured over time to understand composition and crystallinity variations and their effect on layer resistivity.

PS-ThP-4 Study on Cryogenic SiO_2 Etching Mechanisms in High Aspect Ratio Contacts Using CF_3I-Based Plasmas with C_4F_6 and WF_6 Passivation, ***Junyeob Lee***, *Mingyu Kim,* Daejeon University, Republic of Korea*; Hyunjun Kim,* Daejeon university, Republic of Korea*; Woongsun Lim, Changhwan Kim, Sanghee Gwak, Sungin Kim,* Korea Advanced Nano Fab Center, Republic of Korea*; Jeongwoon Bae, Kyongnam Kim,* Daejeon University, Republic of Korea

As 3D NAND flash memory integration increases, securing High Aspect Ratio Contact (HARC) etching technology capable of penetrating multi-layer dielectric stacks of hundreds of layers has become essential. Conventional fluorocarbon (C_xF_y) processes are prone to defects such as etch-stop and bowing as aspect ratios increase. Recently, cryogenic etching has gained significant attention as a solution due to its ability to form precise sidewall passivation layers. In this study, a cryogenic SiO_2 etching process was investigated using a Capacitively Coupled Plasma (CCP) system with a base gas chemistry of CF_3I and $H_2/Ar/O_2$, while incorporating C_4F_6 and WF_6 as passivation gases to elucidate the cryogenic etching mechanism. An Amorphous Carbon Layer (ACL) was used as a hard mask, and the substrate temperature was varied from 20℃ to –90℃ to investigate the effects of temperature on passivation and etching mechanisms. In the gas chemistry, the H_2/O_2 flow rate ratio was selected as a key variable to analyze the effect of hydrogen radical concentration on ACL mask protection and sidewall stability. Furthermore, the etching process was performed under various conditions, including the individual and simultaneous injection of C_4F_6 and WF_6, to systematically investigate the effects of CFx polymers and tungsten-containing compounds on cryogenic etching.

Changes in the etch profile were evaluated through cross-sectional SEM analysis. Additionally, XPS analysis was conducted to examine the content and chemical bonding states of Iodine (I), Carbon (C), and Tungsten (W) within the formed passivation layers. Through these analyses, this study aims to verify and propose the correlation between the multi-layer passivation mechanism and etch profile formation.

PS-ThP-5 Impact of Secondary Electrons on Scaling Wafer Bias to High Power, ***James Prager***, *Josh Perry, Paul Melnik, Timothy Ziemba,* Eagle Harbor Technologies, Inc. (dba EHT Semi)*; Max Kellermann-Stunt, Mark J. Kushner,* University of Michigan

The semiconductor market demands high-aspect-ratio (HAR) features that can be produced at high etching rates. This requires a high ion current to the wafer surface to increase the etch rate. Simultaneously, the aspect ratio of these features is increasing towards 100:1. To achieve high aspect ratios, the ion angular distribution must be well controlled to reduce the sidewall damage to the feature. To accomplish this, tool manufacturers are requesting tailored waveforms wafer bias power systems that can operate at higher voltage. As the wafer bias voltage increases, the secondary

electron effects also increase.In this work, we investigate the effect of secondary electrons on the power scaling of a tailored waveform wafer bias power system as the voltage increases. This experimental work was conducted with a capacitively coupled plasma, whose top-side electrode is driven by a 60 MHz radio frequency generator. The bottom-side electrode is driven by a high-voltage tailored waveform generator (Perseus) operating at 400 kHz. Plasma measurements made with a retarding field energy analyzer will be presented along with power system measurement. The experimental results will be compared with modeling results from the Hybrid Plasma Equipment Model. This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Fusion Energy Science under Award Number(s) DE-SC0024861.

PS-ThP-6 An RF Generator Without a Matching Network for Capacitively Coupled Plasma and Bias Applications, ***Timothy Ziemba***, *Josh Perry,* Eagle Harbor Technologies, Inc. (dba EHT Semi)*; Paul Melnik, Chris Bowman, Connor Liston, Stephanie Geeson, James Prager,* Eagle Harbor Technologies Inc. (dba EHT Semi)

Capacitively coupled plasma (CCP) sources are used throughout the semiconductor and thin film industries. CCPs are driven by a radio frequency (RF) generator with a fixed output impedance that must be impedance matched to the plasma. However, matching networks increase the cost, complexity, thermal management requirements, and response times of CCPs, which all scale with power of the RF generator. EHT Semi has developed a new RF generator that eliminates the need for a matching network while driving a capacitive load. This RF generator is being tested on a CCP for plasma generation and bias applications across a range of experimental parameters (power, neutral pressure, and gases). EHT will present the output and electrode waveforms of this new type of RF generator as well as plasma measurements.

PS-ThP-7 Modeling Atomic Wall-Catalyzed Recombination Kinetics and Weakly Bound Surface Species, ***Jonathan Tran***, *David Graves,* Princeton University

Radical surface recombination kinetics are important in plasma reactors, but mechanisms are still poorly understood. Improving the models for these processes is the main goal of this work. This requires a better understanding of weakly-bound species, but how to handle them in surface kinetics models remains an open question. Understanding the dynamics of non-chemisorbed species will also provide valuable insight into other important problems in plasma-surface reactions, for example, cryogenic etching.

In this work, we use molecular dynamics (MD) simulations to identify fundamental mechanisms of weakly-bound chlorine on chlorinated silicon surfaces. The reactive empirical bond-order (REBO) potential form is used. Insights from these simulations can be leveraged to develop reduced-order models (ROMs). The model parameters are then fit to MD results and combined with nudged elastic band (NEB) REBO calculations. Finally, the ROM results are compared to experimentally observed radical surface recombination kinetics. We identify plausible surface recombination mechanisms, propose models for how we may treat weakly-bound species in plasma surface systems, and suggest future experiments and computational studies that are necessary to clarify the role of weakly-bound species in these systems.

PS-ThP-8 Low Thermal Budget Dopant Activation via Spike Plasma Enhanced Annealing, ***Zhihao Ma***, University of Texas at Dallas*; Mahsa Shekarnoush, Yuanning Chen, Malcolm Bevan, Harvey Stiegler,* MicroSol Technologies Inc.*; Lawrence Overzet,* University of Texas at Dallas

The formation of highly activated ultra-shallow junctions remains a critical challenge for advanced semiconductor device scaling, where dopant activation must be achieved while suppressing thermal diffusion and preserving structural integrity. Conventional annealing approaches, including furnace annealing and rapid thermal annealing (RTA), typically require temperatures above 800 ℃, resulting in undesirable dopant redistribution, junction broadening, and degradation of thermally sensitive device structures and materials.

Plasma Enhanced Annealing (PEA) has demonstrated strong potential as low thermal budget annealing approach through localized and controllable energy delivery from plasma ions, which significantly reduce substrate temperatures (300-500 ℃) by adjusting ion kinetic energy, flux, dose, and species. In this work, a spike plasma enhanced annealing (spike-PEA, millisecond scale) process was investigated for phosphorus-, arsenic- and B-implanted silicon wafers and the post-process properties were systematically characterized by four-point probe measurement, Raman spectroscopy, and secondary ion mass spectrometry (SIMS). Compared with conventional thermal annealing (TA) and RTA under identical temperatures, spike-PEA demonstrated substantially enhanced dopant activation, producing significant reductions in sheet resistance across all implantation profiles, together with improved crystallinity. The effective activation fractions as high as 105% relative to 800 ℃ RTA reference were achieved at only 400 ℃ with minimal junction broadening.

The results demonstrate that spike-PEA enables efficient dopant activation through selective near-surface ion energy deposition while minimizing dopant diffusion. These findings establish spike-PEA as a promising low-temperature annealing strategy for next-generation semiconductor manufacturing and advanced ultra-shallow junction integration.

PS-ThP-9 Effect of Thin Dielectric Layer Boundary Conditions on Electronegative Plasmas in Capacitively Coupled Plasma Reactors, ***Jeong-hoon Son***, KWT Solution Inc., Republic of Korea

As semiconductor processes become increasingly precise, simulation-based plasma analysis is attracting growing interest due to the inherent limitations of direct experimental measurement. However, a persistent challenge remains the discrepancy between simulation predictions and experimental results, often arising from insufficient representation of actual experimental conditions in plasma simulations.

One commonly overlooked condition is the dielectric coating applied to electrode surfaces in real equipment. In industrial plasma reactors, electrodes are routinely coated with materials such as Al_2O_3 or Y_2O_3 to prevent plasma-induced corrosion and contamination. These coatings modify the effective sheath voltage through surface charge accumulation, yet most simulation studies continue to model electrodes as bare conductors.

In this study, we analyze the effect of dielectric electrode coatings in a capacitively coupled plasma (CCP) reactor using the thin dielectric layer boundary condition provided by a commercial fluid simulation software. Particular attention is given to electronegative plasmas, in which the presence of negative ions (O^-) fundamentally alters the discharge structure. Simulations are performed at 250 mTorr and 13.56 MHz with an applied voltage of 100 V, while the Ar/O_2 gas composition is systematically varied to examine how the influence of the coating changes as the negative ion fraction increases relative to the electropositive baseline.

As the O_2 fraction increases, the negative ion density rises and the overall plasma density distribution undergoes a significant transition. At low O_2 fractions, the radial electron density profiles with and without coating show little difference. However, as the O_2 fraction increases, the coating boundary condition produces a pronounced change in the radial electron density distribution. These results indicate that in highly electronegative plasmas, accurate representation of electrode surface coatings is not a minor modeling detail, but a physically significant factor that substantially affects simulation fidelity.

Given the growing use of electronegative gases in plasma processing, proper treatment of surface coating effects will be an essential element for obtaining reliable simulation results.

PS-ThP-10 Implementation of a Surface Coverage Module in K-PLASMA(0D) and Validation Against a C4F8 Inductively Coupled Plasma Global Model, ***Yongil Lee***, KWT Solution, Republic of Korea*; Deuk-Chul Kwon,* Korea Institute of Fusion Energy, Republic of Korea*; Dong-Hun Yu,* KWT Solution, Republic of Korea

In spatially-averaged plasma simulations, surface reactions are often represented as interactions with a single, time-invariant wall state characterized by fixed sticking or recombination probabilities. This simplification cannot capture the evolving surface state during etching or deposition processes, where adsorbed species progressively modify the wall composition and thereby change the probability of each subsequent wall reaction. To address this limitation, the wall must be resolved into multiple surface states whose fractional coverages are coupled with gas-phase kinetics. We report the implementation of a surface coverage module in K-PLASMA(0D), a 0D global plasma simulator currently under development and commercialization, and its validation against a reference C_4F_8 global model and inductively coupled plasma (ICP) measurements.

The new module couples gas-phase kinetics with a heterogeneous wall reaction set that distinguishes bare, fluorinated, and ion-activated sites of the fluorocarbon (fc) film. F atoms adsorb on the fc film and form a fractional surface coverage θ_F that blocks fc-radical deposition on bare sites and enables $CF_x + F(s) \rightarrow CF_{x+1}$ recombination (x = 0–3), including CF_4 formation. Ion-induced site activation and ion-enhanced etching releasing

CF_2 are also incorporated. The reaction probabilities and the C_4F_8 gas-phase reaction set, comprising electron impact, ion recombination, autodetachment, neutral recombination, and associative detachment, follow the reference formulation.

Simulations were performed for a C_4F_8 ICP reactor at 200 sccm C_4F_8 / 10 sccm Ar, pressure of 9.7 mTorr, T_gas = 305 K, and source power of 500–2,000 W. Using the reference global model as a benchmark, K-PLASMA(0D) successfully reproduces the F, CF_2, and CF density trends and the surface coverage evolution, with θ_F reaching ~0.19 at 2,000 W[1]. The agreement confirms that the surface coverage module, including F-blocking and surface recombination pathways, has been correctly implemented in K-PLASMA(0D).

In this work, only the fractional coverages of three surface states — bare site, F-adsorbed site (θ_F), and ion-activated site — were considered during polymer formation. As a next step, the surface reaction rates obtained here can be aggregated to derive the macroscopic polymer deposition rate, enabling the present module to be applied to PECVD process modeling. The framework will also be extended to other surface chemistries, in particular SiO_2 etching.

1 G. Kokkoris *et al*., J. Phys. D: Appl. Phys. 41, 195211 (2008)

PS-ThP-11 Positive Pulse Biasing for Directional Electron Extraction in Capacitively Coupled Plasma*, Kyoung-Jae Chung,* ***Junbeom Park****, Daehyun Kim,* Seoul National University, Republic of Korea

In high aspect ratio (HAR) etching, ions are directionally accelerated through the sheath, whereas electrons cross the sheath mainly by thermal motion. This difference causes positive charge accumulation near the bottom of narrow structures, which can distort the etching profile. Our previous work demonstrated through simulations that positive pulse biasing can extract directional electrons from capacitively coupled plasma (CCP) and transport them into HAR structures. In particular, the simulations showed that a shorter pulse rise time produces more directional electrons by enhancing the transient electron extraction process. However, experimental validation is needed to determine whether this pulse-induced electron extraction can be realized in an actual CCP system. In this work, positive pulse biasing is applied to a CCP system to observe directional electron extraction and to experimentally examine the correlation between pulse parameters and electron extraction behavior suggested by the simulations. The influence of plasma density on the extraction process is also analyzed, and the results provide guidance for the development of pulse bias waveforms that mitigate charge accumulation and improve profile control in advanced plasma processing.

This work was supported by Samsung Electronics Co., Ltd (IO251215-14597-01).

PS-ThP-12 Plasma Impedance Monitoring of SiNx Etching Processes with Different Grounding Conditions*,* ***hyun kyu Choi****, Heeyeop Chae,* Sungkyunkwan University (SKKU), Republic of Korea

Plasma impedance variations at the RF grounding interface were monitored to assess the system status in this work. The experiment was conducted in a 300 mm ICP chamber using Ar/CF_4 plasma at 30 mTorr. A 13.56 MHz source power and a 2 MHz bias power were applied to the inductive coil on a quartz window and to the electrostatic chuck, respectively. The grounding conditions were controlled by mechanically tightening the inner liner bolts using a torque driver. The bolt torque was adjusted from 1 to 15 torque levels, and the 15 torque condition was served as the reference for comparison. A VI probe captured the electrical variations of the plasma response to grounding status. The electrical resistance at 15 torque exhibited a standard deviation of 29.04% compared to the 1 torque condition, and the reactance showed a standard deviation of 21.06% under the same conditions. Theoretical analysis using the CMY models (Int. J. Heat Mass Transfer, 1969) and Greenwood models (Proc. R. Soc. Lond. A, 1966) was performed to predict the interface mechanics. These models show that increased torque expands the effective contact area and enhances the surface conductance.In addition, SiN etching experiments were performed under different torque conditions. The etch rate at 1 torque was 2.495% lower than the value at 15 torque. These results indicate that the bolt contact status alters the grounding stability of the chamber.

PS-ThP-13 Particle-in-Cell Simulation of the Synchronous Effect in Pulsed Dual-Frequency Capacitively Coupled Plasma*,* ***Jun Hee Mun****,* KWTSolution, Republic of Korea

This study investigates the synchronization effects between high-frequency (HF) and pulsed low-frequency (LF) voltages in a dual-frequency capacitively coupled plasma (DF-CCP) system, which is widely utilized in semiconductor processing and advanced plasma-based manufacturing. Dual-frequency operation enables independent control of plasma density and ion energy; however, the introduction of pulsed LF biasing introduces temporal complexity whose underlying mechanisms remain poorly understood. In particular, pulsed LF excitation has been proposed as an effective approach to tailor ion energy distributions for high-aspect-ratio etching, but the role of its phase relationship with HF excitation in determining plasma characteristics remains largely unexplored.

In this work, a two-dimensional particle-in-cell (PIC) simulation is performed to systematically analyze these synchronization effects. A 20 MHz sinusoidal HF voltage and a 400 kHz pulsed LF voltage are applied, with the LF duty cycle fixed at 50%. Two representative control strategies are considered: (1) varying the HF duty cycle from 50% to 100% to modulate the overall temporal overlap, and (2) maintaining a 50% HF duty cycle while introducing a controlled phase delay in the HF waveform within the LF pulse-on period. These approaches allow precise adjustment of the overlap ratio between HF excitation and the LF active phase, providing a consistent framework to isolate synchronization-driven phenomena.

The simulation results demonstrate that the degree of temporal overlap strongly affects the spatiotemporal evolution of plasma potential, sheath dynamics, and electron heating mechanisms. In particular, changes in overlap modify the phase-resolved electron power absorption and lead to distinct electron density distributions and potential structures. As a result, ion acceleration dynamics within the sheath are also altered, indicating that ion energy control is closely linked to waveform synchronization rather than solely to individual frequency components.

These findings highlight that synchronization between HF and pulsed LF voltages is a key operational parameter in DF-CCP operation. The results provide practical insight into waveform engineering strategies for precise control of plasma characteristics, provide pathways toward optimizing etching performance in next-generation semiconductor fabrication processes.

PS-ThP-14 3D PIC-MCC Simulation for Plasma Nonuniformity in off-centered DC Magnetron Sputtering*,* ***Yu Gyeong Suh****, Hae June Lee,* Pusan National University, Republic of Korea

DC magnetron sputtering (DCMS) remains a cornerstone of thin film deposition and is widely used for metal gap fill in semiconductor packaging processes. However, plasma nonuniformity arising from the closed E×B drift loop continues to limit target utilization and film uniformity. Nowadays, intentionally asymmetric magnet topologies offer an underexplored route to control plasma spatial structure and ion bombardment. This study utilizes a self-consistent 3D particle-in-cell with Monte Carlo collision (PIC-MCC) simulation to investigate a DCMS discharge driven by a non-circular off-centered magnet. Using an in-house-developed code, an Ar discharge at 5 mTorr with a planar Cu target has been investigated using a fully kinetic analysis under a realistic, azimuthally nonuniform magnetic field. We quantify how this non-circular topology reshapes the spatial distribution of electron and ion densities through the competition among E×B, ∇B, and diamagnetic drifts. Preliminary calculations confirm that the off-centered topology breaks the azimuthal symmetry of the trap region, inducing localized weakening of the curvature-driven gradients along the racetrack. These features drive azimuthally varying ion flux and measurable shifts in the IEAD high-energy tail. This work establishes a 3D kinetic framework for magnet design optimization, providing a physics-based basis for tuning film growth conditions in large-area, high-performance coatings.

PS-ThP-15 Two-Dimensional Particle-in-Cell Simulation of Electronegative Plasmas in Chlorine Capacitively Coupled RF Discharges*,* ***Dongmin Lee****, Hae June Lee,* Pusan National University, Republic of Korea

Capacitively coupled plasmas used in the etching process of advanced semiconductor fabrication include negative ions and reactive radicals. Unlike electropositive discharges, electronegative plasmas contain a large amount of negative ions, depleted electron densities, and enhanced bulk electric fields. It has been reported that these features modify sheath dynamics, electron power absorption, radical generation, and charged-particle motion. However, ion dynamics near the bulk–sheath boundary remain insufficiently understood under RF-driven etching conditions. In this work, frequency-dependent charged-particle dynamics in chlorine capacitively coupled plasmas are investigated using a two-dimensional particle-in-cell Monte Carlo collision (PIC MCC) simulation. Chlorine is selected as a representative electronegative etching gas, where dissociative attachment and negative-ion confinement can lead to an ion-dominated bulk plasma. By changing the RF driving frequency, different degrees of electronegativity are obtained, enabling comparison of charged-particle

motion. At lower driving frequencies, the discharge becomes highly electronegative. The bulk electron density is low because negative ions are confined in the plasma bulk, while positive ions are accelerated toward the electrodes through the RF sheath. This separation produces a localized space-charge density peak near the bulk–sheath boundary, thereby enhancing the local electric field. The resulting field perturbs the relative motion of positive and negative ions, generating a low-frequency ion-scale response that extends from the sheath edge into the plasma bulk. This ion motion is coupled to the electron power absorption, suggesting that the bulk–sheath boundary acts as an active region for energy exchange and charged-particle dynamics. As the driving frequency increases, the plasma becomes less electronegative, the localized space-charge peak weakens, and the ion-scale response near the sheath edge decreases. These results suggest that the localized electric field structure is governed by the balance among negative-ion confinement, ion inertia, and RF sheath motion. The results provide a kinetic interpretation of ion dynamics in electronegative chlorine CCPs and clarify how RF frequency can influence electronegativity and sheath-edge field formation. Understanding these mechanisms is important for high-aspect-ratio and profile-sensitive etching because the spatial distribution of ions, radicals, and energy deposition affects etch rate, selectivity, sidewall control, and process uniformity.

PS-ThP-16 Electrified C–N Coupling in Ethylene Glycol Using Nitrogen DC Plasma-Liquid Interactions, ***José Balena***, *Mikhail Vasilev,* University of Notre Dame*; R. Mohan Sankaran,* University of Illinois Urbana-Champaign*; Caue Ribeiro,* Embrapa Instrumentation, Brazil*; David Go,* University of Notre Dame

Direct-current (DC) plasma–liquid interactions have emerged as a promising strategy for electrified chemical transformations under mild conditions. Plasma systems are particularly attractive for nitrogen activation because cleavage of the N≡N bond is thermodynamically and kinetically challenging using conventional methods. Industrial nitrogen fixation still relies mainly on the energy-intensive Haber–Bosch process, and electrochemical and photocatalytic N-transformation often need highly active substrates, while suffering from low efficiencies and limited N_2 solubility in liquids. In this work, a nitrogen plasma generated directly over liquid ethylene glycol (EG) was employed to promote nitrogen incorporation into organic molecules. EG was selected as both solvent and carbon source due to its low cost, low volatility, biodegradability, and availability from biomass valorization, plastic recycling, and CO_2-derived routes. Reaction products were investigated by GC–MS using direct injection and silylation derivatization methods. The major nitrogen-containing product identified after derivatization was (2-hydroxyethyl) carbamate providing evidence for incorporation of nitrogen in the organic substrate. Total nitrogen analysis indicated a nitrogen fixation rate of approximately 370 μmol h^{-1} in EG. This rate was not significantly affected by either the reaction volume or reaction time, provided that the electrolyte concentration and gas flow rate were maintained constant at 0.17 M $NaClO_4$ and 50 sccm N_2, respectively. Control experiments using hydroxylamine (NH_2OH) and ammonium hydroxide (NH_4OH) under argon plasma yielded the same compound, suggesting NH_2• radicals as key intermediates. Comprehensive analysis of the samples revealed a broader distribution of nitrogen-containing compounds. GC-MS detected traces of amino acids after derivatization, while direct injection identified cyclic nitrogen compounds such as piperidinoacetonitrile. Ongoing studies are being performed to further elucidate reaction pathways and reactive intermediates. These findings demonstrate the potential of plasma-liquid systems for sustainable nitrogen fixation and electrified synthesis of value-added nitrogen-containing chemicals from abundant feedstocks.

PS-ThP-17 Effect of H_2O Additive Gas on Sio_2 and Si_3N_4 Films in C_4F_8 Self-Bias Plasma, *Heeyeop Chae,* ***Haegeon Jung***, Sungkyunkwan University (SKKU), Republic of Korea

Fluorocarbon (FC) layer formation affects surface reactions and profile evolution in low-temperature plasma processing. This study investigates the effect of H_2O addition on FC layer formation on SiO_2 and Si_3N_4 films in C_4F_8 self-bias plasma. An inductively coupled plasma chamber generates C_4F_8/Ar plasma without external RF bias. Substrate temperature ranges from 20 °C to −60 °C. FC layer thickness is evaluated by ellipsometry and VSEM, and surface bonding structure is analyzed by XPS. Low substrate temperature increases FC layer thickness on both SiO_2 and Si_3N_4 films due to enhanced polymer accumulation and reduced desorption. SiO_2 surfaces exhibit thicker FC layer formation than Si_3N_4 under identical plasma conditions. XPS analysis confirms increased C–C and C–CF bonding fractions at low temperature, indicating stabilization of carbon-rich FC structures. H_2O addition further increases FC layer thickness in C_4F_8 plasma, particularly on Si_3N_4 surfaces, while O_2 addition suppresses carbon accumulation through oxidation-related reactions. These results indicate that H_2O addition modifies FC surface chemistry and temperature-dependent polymer stabilization behavior in C_4F_8 self-bias plasma. The study suggests material-dependent FC layer formation behavior in low-temperature fluorocarbon plasma processing.

PS-ThP-18 Aqueous Electron Yields for Non-thermal Plasma in Contact with a Water Cathode: Effects of Plasma Gas Composition, ***Mikhail Vasilev***, *David Bartels, David Go,* University of Notre Dame

Nonthermal plasmas in contact with liquids present a unique plasma–surface interaction challenge: the liquid surface acts as the cathode and must supply electrons to sustain the discharge and maintain charge balance. Despite this fundamental role, the mechanism of secondary electron emission from the liquid cathode remains poorly understood. Proposed mechanisms include photoionization, field emission, and ion-induced emission. One candidate process involves plasma-generated reactive species producing free conduction-band electrons in the liquid, with a small fraction escaping into the plasma while the majority thermalize and solvate to form aqueous (solvated) electrons[1]. The probability of electron emission from the liquid surface is extremely low, with only ~10^{-6} of conduction-band electrons estimated to escape into the plasma, making direct measurement difficult and mechanistic assignment challenging.

Water has an ionization energy of ~10 eV, yet the average kinetic energy of ions impinging on the liquid surface through the plasma sheath is estimated at only ~1 eV for argon systems. This energy gap argues against simple ion-induced ionization of water and suggests that alternative interfacial processes, such as proton-transfer pathways or metastable-driven reactions, contribute to electron generation. Prior work using argon plasma–liquid systems and chloroacetate reduction as a liquid-phase electron dose probe has estimated apparent electron yields on the order of unity. In this work, we quantify how different gas ions affect electron generation at the plasma–liquid interface using in situ chloride ion measurements produced by the reaction of aqueous electrons with chloroacetate. By varying plasma gas composition (H_2, He, Ar, Kr, Xe), this work investigates how ion mass, metastable energy, and chemical reactivity govern electron generation pathways at plasma–liquid interfaces, with implications for secondary electron emission modeling in plasma–liquid systems.

PS-ThP-19 Plasma Monitoring for Chamber Conditioning Steady-State Detection Using He-Normalized SiF Saturation in Inductively Coupled Plasma, ***Suyoung Ko***, *Heeyeop Chae,* Sungkyunkwan University (SKKU), Republic of Korea

The He-normalized SiF Saturation Index (SSI) was developed as a real-time chamber wall condition indicator. SSI monitored chamber wall stabilization during post-preventive maintenance (PM) chamber conditioning in inductively coupled plasma etchers with Y_2O_3-coated walls. Optical emission spectroscopy (OES) monitored full-spectrum emission in situ during plasma cleaning cycles on a 300 mm ICP etcher with Y_2O_3-coated walls across three PM events. Partial least squares variable importance in projection (PLS-VIP) analysis identified SiF (440.1 nm) as the wall-state-sensitive emission line. SSI was defined as the cycle-averaged I(SiF)/I(He) ratio, using He (706.5 nm) as the normalization reference. Blanket oxide etch rate was measured to validate SSI. He normalization reduced the CV of SiF emission from 17.6% to 3.8%. This reduction isolated the wall-state-dependent SiF signal from plasma source fluctuations, enabling SSI to track chamber wall condition independently. SSI converged to a ±2% stability band at the 7th conditioning wafer across three PM events, indicating faster chamber stabilization than the conventional fixed 24-wafer chamber conditioning protocol. SSI correlated with blanket oxide etch rate at $r = 0.965$ ($p < 0.001$), confirming SSI as a process-relevant chamber wall condition indicator. SSI identified the chamber stabilization point in real time, replacing the conventional fixed-count chamber conditioning protocol. This work demonstrated that SSI is a practical in-situ wall condition indicator applicable to production ICP etchers.

PS-ThP-20 Time-Resolved Langmuir Probe Measurements of Pulsed RF Argon Plasmas, ***Collin Clay***, *Kylan Herring, David Ruzic,* University of Illinois

Pulsed RF plasmas are a powerful tool for etching and other plasma processes. The pulsing of the RF plasma provides a number of variables to control the plasma treatment process such as pulse repetition rate and duty cycle. While computational models have provided insight into the fundamental physics of pulsed RF plasmas, there is still a significant lack of experimental validation of these models. In this we work, we present progress on measuring the time-resolved evolution of the electron energy distribution function (EEDF) in a pulsed RF argon plasma. The energy

distribution of electrons in pulsed plasmas is unique because the electrons are constantly adjusting to the on- and off-states of the RF plasma. Models have predicted that the electrons at the beginning of a pulse have a low density with a high electron temperature, and over time, the density increases while the temperature decreases. This work uses time-resolved Langmuir probe measurements with a sub-nanosecond temporal resolution to experimentally determine the evolution of the EEDF in a pulsed plasma system. We present initial work measuring the IV traces of argon plasmas under pulsed RF ignition conditions at pressures from 30 – 100 mTorr. We explore the impact of pressure and pulse parameters on the EEDF. We will also discuss how the time-evolution of the EEDF can impact the application of pulsed RF plasmas for industrial processes.

PS-ThP-21 Optical Emission Diagnostics of Electron Temperature and Density in Argon ICP Assisted by Collisional-Radiative Modeling, ***JiHyun Park,*** Samsung Electronics Co., Republic of Korea

Optical emission spectroscopy (OES) is a useful non-invasive diagnostic technique for low-temperature plasmas, but measured emission intensities are governed by coupled collisional and radiative processes. Consequently, direct estimation of electron temperature (Te) and electron density (Ne) from emission intensities alone requires a collisional-radiative (CR) model. In this study, Te and Ne in argon inductively coupled plasma (Ar ICP) were estimated using OES combined with a CR model.

Ar I emission spectra were measured in a cylindrical quartz-tube ICP reactor operated at 13.56 MHz. RF power was varied from 30 to 50 W and gas pressure from 200 to 400 mTorr, giving nine operating conditions. For each condition, five repeated OES measurements were performed to evaluate repeatability. The spectra were corrected by wavelength-dependent and spectral-response calibration, and Ar I emission lines selected from the 696–978 nm range were used for analysis.

The CR model included the Ar ground state, four 4s metastable/resonance states, and ten 4p excited states. Electron-impact excitation and de-excitation, ionization, collisional quenching, diffusion loss to the wall, radiative transitions, and radiation trapping were considered. The diagnostic procedure was performed sequentially. First, Te was determined by minimizing the root-mean-square error between measured and CR-model-predicted line-intensity ratios. The 763.51 nm line was used as the reference, and five lines at 750.39, 772.38, 801.48, 826.45, and 912.30 nm were used to construct the ratio vector. Next, Ne was estimated by scaling the CR model intensity to match the experimental intensity at the determined Te. The Ar I 811.53 nm intensity at 300 mTorr and 40 W was used as the normalization reference.

The estimated Te ranged from 1.604 to 1.814 eV, while Ne ranged from 2.84 × 10^{12} to 8.07 × 10^{12} cm^{-3}. Te decreased with increasing pressure and showed a slight decrease with increasing RF power, whereas Ne increased with both pressure and RF power. The relative standard deviation was 0.14–0.96% for Te and 2.14–7.27% for Ne, indicating good repeatability. Comparison with a 0D global model showed that Te agreed within ±5%, while Ne showed larger quantitative deviations but reproduced the trends with operating conditions.

These results demonstrate that the sequential CR-OES approach provides physically consistent, non-invasive estimates of Te and Ne in Ar ICP, and is applicable to conditions where probe insertion is impractical or may perturb the plasma.

PS-ThP-22 ReaxFF Development by Latent Space Exploration for Plasma Etch Modeling, ***George Arsnow,*** *David Graves,* Princeton University

Extension of molecular dynamics (MD) etching simulations to industrially relevant plasma etching systems including silicon (Si), fluorine (F), chlorine (Cl), sulfur (S), and oxygen (O) necessitates the development of new interatomic potentials with suitable accuracy, transferability, and computational cost. These criteria can be balanced by the ReaxFF potential, which has sufficient flexibility and physicality to handle the highly non-equilibrium atomic environments replete in plasma etching simulations. Growing use of data-intensive machine learning interatomic potentials has spurred the creation of systematic and user-agnostic protocols for training set generation [1]; such active learning algorithms can also be harnessed to produce data sets for ReaxFF parameterization.

We demonstrate an active learning algorithm to sample an atomic configuration set's latent space, which comprises the first few principal components of the set's atomic descriptors. Latent space exploration enables efficient interpolation between user-defined boundary configurations, allowing the user to institute limits on the resulting potential's transferability [2]. We use this latent space exploration–based active learning algorithm to parameterize ReaxFF potentials for elemental subsets of the Si/F/Cl/S/O system. Parameterization is performed with version 2 of the JAX-ReaxFF global optimization software [3]. Validation entails comparison of ReaxFF-predicted energies and forces on a test data set to those calculated by density functional theory (DFT) and comparison of experimental etch rates and etch product selectivities to those manifested in MD etching simulations.

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PS-ThP-23 Enhanced Catalytic Performance in Plasma-Assisted Dry Methane Reforming via Ferroelectric Perovskites, ***Shanza Baig,*** University of Oklahoma

Non-Thermal Plasma technology holds significant potential for activating CH_4 and CO_2 molecules, enabling their conversion into H_2 and other valuable chemicals under mild conditions. However, conventional thermal catalysts which are primarily heat responsive often lack compatibility with non-thermal plasma environment, where reaction mechanisms and dominant species differ considerably. Moreover, as CO_2 has a higher bond dissociation energy than CH_4, there is a necessity to design a catalyst that can enhance CO_2 dissociation kinetics to improve overall DRM efficiency. This study integrates ferroelectric materials into plasma catalytic systems enhancing energy transfer to reactant molecules, increasing electron density in discharge regions, and elevating average electron energy – key factors critical to increasing the conversion rates of both CH_4 and CO_2 in plasma-assisted DRM. Perovskite oxides synthesized via the Pechini method were categorized into three classes: titanates ($BaTiO_3$, $CaTiO_3$, $SrTiO_3$), zirconates ($BaZrO_3$, $CaZrO_3$, $SrZrO_3$), and niobates ($KNbO_3$, $NaNbO_3$, $KNaNbO_3$), each exhibiting distinct curie temperatures and ferroelectric properties. Niobate-based ferroelectric catalysts, particularly $KNbO_3$ and $NaNbO_3$, demonstrated the highest CH_4 conversions of 71.7% and 71.9%, CO_2 conversions of 62.4% and 60.5%, H_2 yield of 33.6% and 33.3%, and CO yield of 33.5% and 32.9%, respectively. $KNbO_3$ resides in its orthorhombic ferroelectric phase at 800 V and 5 kHz enabling sustained polarization and enhanced surface charge effects. To further enhance performance and stability of traditional supports, ferroelectric $KNbO_3$ was incorporated into Al_2O_3 and SiO_2 using a co-precipitation method. This integration further improved CH_4 and CO_2 conversions to 75.5% and 54.6% with Al_2O_3, and 81.7% and 64.6% with SiO_2. To study the effect of loading active metal, nickel was introduced via incipient wetness impregnation. However, its addition to ferroelectric catalysts such as $KNbO_3$-Al_2O_3 and $KNbO_3$-SiO_2 led to reduced CH_4 and CO_2 conversions and a shift in product selectivity towards CO, highlighting the pivotal role of spontaneous polarization in directing plasma induced reaction pathways. In contrast, paraelectric perovskites exhibited poor catalytic performance due to their inability to maintain polarization under plasma conditions either due to inherently non-ferroelectric structures or low curie temperatures. Overall, among all tested catalysts, ferroelectric $KNbO_3$ based catalysts demonstrated superior control over electric field interactions at the catalyst surface, promoting localized micro-discharges, enhancing CO_2 dissociation, and reducing energy losses.

PS-ThP-24 Plasma-Enhanced CO_2 Dissociation for Chemical Synthesis: Modeling and Experimental Verification, ***Andrew Herschberg,*** *Nathan Bartlett, Jameson Crouse, Emily Greene, Jaime Robertson, David Ruzic,* University of Illinois at Urbana-Champaign

The conversion of carbon dioxide into carbon monoxide using non-equilibrium plasmas is of growing interest for carbon utilization, syngas generation, and plasma-assisted chemical synthesis. Radio frequency inductively coupled plasmas are attractive for this application due to stable operation, high plasma density, and efficient power coupling. In this work, a combined modeling and experimental study of CO2 dissociation in an intermediate-pressure RF ICP reactor is presented. A physics-based numerical model is being developed to simulate electromagnetic power deposition, plasma transport, and reaction pathways relevant to CO2 conversion. Parametric studies examine the influence of applied power,

pressure, residence time, and feed composition on predicted dissociation behavior and energy utilization.

Experimental validation is being conducted using an RF ICP reactor operated under comparable conditions. A combination of mass spectrometry and remote OES actinometry methods are used to measure species concentrations in the reactor effluent. Comparison of experimental measurements with model predictions will be used to refine the simulation framework and identify operating conditions for efficient plasma-assisted CO2 conversion. This work supports the development of scalable plasma reactors for chemical synthesis and carbon utilization applications.

PS-ThP-25 Effect of Steric Hindrance and Precursor Reactivity on Aluminum Oxide Area-Selective Atomic Layer Deposition, ***Sharmistha Bhattacharjee***, *Nicholas C. Strandwitz,* Lehigh University

Area-selective atomic layer deposition (AS-ALD) offers a promising route for bottom-up fabrication of advanced nanoscale devices by enabling deposition only on targeted surfaces while suppressing growth on undesired regions. However, maintaining selectivity during deposition remains a major challenge, particularly for highly reactive precursors that can penetrate blocking layers and nucleate on non-growth regions. In aluminum oxide AS-ALD, precursor properties such as molecular size, ligand structure, and reactivity play a critical role in determining interactions with self-assembled monolayer (SAM) blocking layers, surface defects, and precursor diffusion pathways. Small and highly reactive precursors such as trimethylaluminum (TMA) can readily infiltrate non-growth surfaces, leading to faster selectivity loss. Therefore, tailoring precursor chemistry is important for improving blocking efficiency and sustaining selective growth.

In this study, the influence of precursor molecular size and reactivity on Al_2O_3 AS-ALD was investigated using TMA, aluminum tri-sec-butoxide, and tri-i-butylaluminum with H_2O as the co-reactant. Dodecanethiol SAM deposited on copper substrates was employed as a blocking layer, and deposition behavior was examined over a temperature range of 100–160 °C. Film thickness and density were analyzed using spectroscopic ellipsometry and X-ray reflectivity, while blocking performance was evaluated through X-ray photoelectron spectroscopy measurements of Al atomic concentration. Compared with TMA, the larger precursors demonstrated substantially improved resistance to precursor infiltration and enhanced selectivity. Aluminum tri-sec-butoxide maintained 100% selectivity at low temperature, while tri-i-butylaluminum preserved selectivity above 90% after 100 ALD cycles of Al_2O_3. These findings highlight the importance of precursor design in AS-ALD and demonstrate that combining bulkier, lower-reactivity precursors with well-ordered SAM blocking layers provides an effective pathway for improving long-term selectivity performance.

PS-ThP-26 Evolution of Ion Energy Distribution Functions in High Aspect Ratio Features, ***David Kanfer***, North Carolina State University; *Krista Morris, Rex Anderson,* Micross; *Tanjina Akter,* North Carolina State University; *Chenyao Huang, Mark Kushner,* University of Michigan, Ann Arbor; *Steven Shannon,* North Carolina State University

The growing demand for High Aspect Ratio (HAR) features in micro and nanoscale devices motivates an understanding of the evolution of the ion energy distribution function (IEDF) as ions travel down a HAR feature. As the aspect ratio (AR) increases, features undergo bowing, tapering, and notching, deviating from the expected HAR geometry; these are largely attributed to AR dependent changes in the IEDF. By combining a retarding field energy analyzer (RFEA) with capillary plates (CPs) of varying ARs, the evolution of IEDFs as a function of depth into an HAR feature can be directly measured. This method has been previously demonstrated in inductively coupled plasmas.

Industry often uses capacitively coupled plasmas (CCPs) to perform the HAR etch. A CP design has been developed with feature diameters from 20 um to 90 um, and thicknesses from 200 um to 450 um, yielding features with ARs ranging from 2-22. The CPs are fabricated on backlapped silicon wafers. Copper is sputtered onto the back of the wafer as an etch-stop. A mask with an array of holes is exposed onto the wafer. The subsequent etch step varies, with larger diameter holes requiring a longer etch. The copper is then removed. Finally, dry thermal oxidation is used on some samples, forming a thin layer of SiO2 throughout the feature. An argon / oxygen / nitrogen dual-frequency CCP is used to test the fabricated CPs. The CCP is powered by a 60 MHz high frequency to sustain sufficient density, and a 13.56 MHz low frequency for sheath control.

By varying the AR of the CP used, power ratio of the dual-frequencies, pressure, and gas, the IEDF through the HAR can be measured with the RFEA. Additionally, by comparing the SiO2 HAR features to the non-oxidized features, the effect of insulating sidewalls is determined. These results provide insight into how IEDFs evolve within HAR features in dual-frequency CCPs.

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PS-ThP-27 Complex Transient Processes Observed During in-Plasma Nanocalorimetry, ***Carles Corbella***, National Institute of Standards and Technology (NIST)/ University of Maryland, College Park; *Caroline Adam, Holger Kersten,* Kiel University, Germany; *Feng Yi, Andrei Kolmakov,* National Institute of Standards and Technology (NIST)

Nanocalorimetry is a promising diagnostics tool to measure and analyze the energy fluxes from plasma discharges used for surface processing, such as film deposition, etching, and cleaning. Nanocalorimeter sensors consisting of silicon dies usually include a Pt thin film microstrip acting as a resistor, deposited on an ultrathin, free-standing SiN_x membrane. Recently, a two-timescale temperature profile upon plasma ignition has been observed: (1) initial fast sensor heating associated with the heat dissipation to the ultrathin SiN_x supporting membrane, followed by (2) slow heating of the silicon die in contact with the aluminum envelope. The reduced thermal mass of the membrane-supported Pt sensor enables a rapid temperature response down to the millisecond resolution. Nanocalorimeters' characteristic short response times, together with their sensitivity and selectivity, make such devices ideal for transient thermal processes' analysis during plasma processing. From plasma ignition to pulsed discharges, plasma-surface physics and chemistry are governed by transition processes where plasma parameters rapidly evolve. The energy fluxes during such non-stationary conditions can now be studied with nanocalorimetry sensors, whose thermal responses are validated using an array of independent plasma monitor techniques, such as electrical and optical probes. The time evolution of sensor temperature is correlated with RF discharge parameters (gas pressure, power, and residence time) and electrode materials (aluminum, copper, gold) to provide a unified description of the substrates' heating mechanisms. The roles played by the gas phase conditions and chemistry on the electrodes are discussed, as well as the separate contributions of gas, ions, electrons, and photons heat fluxes in the global heating of the nanocalorimeter.

PS-ThP-28 Three-Dimensional Kinetic Plasma Simulations for Predictive Modeling of ExB Plasma Processing Devices, ***Andrew Tasman Powis***, Princeton Plasma Physics Laboratory; *Jian Chen,* Sun Yat-sen University, China; *Igor Kaganovich,* Princeton Plasma Physics Laboratory

Three-dimensional kinetic plasma simulations are emerging as an essential tool for first-principles modeling of low-temperature plasmas used in materials processing. In many plasma sources, including partially magnetized discharges relevant to etching, deposition, surface functionalization, and ion-beam-assisted processing, device behavior is controlled by kinetic electron transport, self-consistent sheath formation, wave–particle interactions, and plasma–surface coupling. These effects are often reduced or parameterized in lower-dimensional models, but they can depend sensitively on the third spatial dimension, boundary conditions, and nonlinear instability dynamics. This talk highlights recent progress in high-performance 3D3V particle-in-cell simulations as a pathway toward predictive modeling of processing-relevant plasmas.

Two recent studies illustrate this point. In Hall-thruster-like crossed-field plasmas, 3D kinetic simulations show that radial boundary conditions can qualitatively alter density, temperature, electric-field structure, instability spectra, and cross-field electron transport [1]. In beam-generated partially magnetized plasmas, 3D PIC-MCC simulations reveal a transition from quasineutral lower-hybrid spiral arms to non-neutral diocotron-driven helical rotation, demonstrating that structures appearing spoke-like in projection may be intrinsically three-dimensional [2]. Together, these studies show that fully 3D kinetic simulations are not merely computational refinements, but necessary tools for connecting fundamental plasma instabilities to transport, wall interaction, and ultimately process control in advanced plasma technologies.

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PS-ThP-29 PICLas: An Open-Source Kinetic Simulation Framework for Plasma Science and Technology, ***Paul Nizenkov***, *Asim Mirza, Stephen Copplestone, Julian Beyer,* boltzplatz - numerical plasma dynamics GmbH, Germany; *Marcel Pfeiffer,* Institute of Space Systems, University of Stuttgart, Germany

PICLas (https://github.com/piclas-framework/piclas, GPLv3) is an open-source, massively parallel kinetic simulation framework combining Particle-

in-Cell (PIC), Monte Carlo Collisions (MCC), and Direct Simulation Monte Carlo (DSMC), Bhatnagar-Gross-Krook (BGK), and Fokker-Planck methods for rarefied gas and plasma dynamics. This poster demonstrates its versatility through three applications spanning plasma processing, beam physics, and radiation transport. First, reactive magnetron sputtering of titanium in an O_2/Ar atmosphere is simulated within an industrial coating chamber using DSMC. A reactive wall model (Tonneau et al. 2018, J. Phys. D 51, 195202) couples target surface coverage to incoming particle fluxes and sputter emission. Gas distribution, sputtered particle transport with configurable emission distributions, and deposition rates are analyzed under varying reactive gas inflow conditions, capturing the characteristic racetrack erosion pattern and the poisoning transition from metallic to compound target mode. A parametric racetrack model is introduced, enabling the simulation of rotating substrates by rotating the racetrack position accordingly, providing a computationally efficient approach for industrial coating geometries. Second, electron beam propagation in a PVD system is modelled with coupled PIC-MCC. Ionization of the background neutral gas, self-fields of charged species, and a superimposed magnetic field are included. The ionization-induced self-focusing of the beam is shown, and simulated beam widths are validated against burn-in diameter measurements within the beam generator. A species-specific time step bridges the different timescales of electrons and ions. Third, PICLas is bidirectionally coupled with a line-by-line radiation solver and a photon Monte Carlo transport method. The capabilities are demonstrated for an atmospheric entry plasma, a strongly non-equilibrium environment that shares key physical characteristics with high-power industrial plasma processes, enabling prediction of radiative transport properties and spectroscopic signatures in flow regimes inaccessible to continuum-based CFD. Together, these cases establish PICLas as a versatile kinetic simulation platform freely available to the plasma science and technology community.

PS-ThP-30 Time-Resolved Ion Energy Distribution Function Study of High Power Impulse Magnetron Sputtering with Positive Cathode Reversal using a Linear Magnetron for Cu and Ti, ***Collin Jeckell***, *Tag Choi, Matt Egly, Ricky Pickering, David Ruzic, Dren Qerimi,* University of Illinois at Urbana Champaign

High-Power Impulse Magnetron Sputtering (HiPIMS) is a physical vapor deposition (PVD) technique that, through short voltage pulses with high peak currents, is able to achieve higher density plasmas compared to traditional DC magnetron sputtering. This higher density leads to a significant increase in the ionization fraction, which leads to higher quality films by improving their adhesion, density, and roughness. A recent area of study has been how changing the polarity of the cathode affects the energies of the deposited ions. This work seeks to show how changing different parameters of the HiPIMS pulse with the positive cathodic reversal, and the position of the magnetron affects the time-resolved Ion Energy Distribution Function (IEDF). This data was collected using a Plasma Sampling Mass spectrometer (PSM) from Hiden Analytical Inc. For each experiment the IV trace was also collected allowing us to verify that the plasma is stable. By understanding how changing these parameters leads to changes in the IEDFS we can better design HiPIMS plasmas to obtain the desired film. For this both copper (Cu) and titanium (Ti) targets were studied changing 9 parameters to see how each of them affects the IEDF. Parameters such as main pulse length between 10 – 30 µs, peak current between 100 – 300 A, positive pulse length between 50 – 150 µs, with/without positive voltage of the cathode, angles of the PSM to target, etc. are varied. By testing all of these parameters we are able to see how they affect the behavior of the plasma. Secondarily by comparing the results between the two materials, we are able to observe if changing material properties has a large impact on the trends observed.

PS-ThP-31 Neural-Network Based Reconstruction for Limited-Line-of-Sight CT-OES Plasma Diagnostics, ***Jiseong Nam***, *Kyoung-Jae Chung, Sang Yoel Park,* Seoul National University, Republic of Korea

Computed-tomographic optical emission spectroscopy (CT-OES) is a non-invasive diagnostic technique for reconstructing the spatial distribution of local optical emissivity in plasmas from line-integrated emission signals. In practical plasma devices, however, the number and angular coverage of available lines of sight (LOS) are often limited by chamber geometry, viewport configuration, and optical-access constraints. Under such limited conditions, the reconstruction problem becomes highly ill-posed, and different non-axisymmetric emissivity distributions may produce similar projection signals. In this work, we propose a neural-network-based reconstruction model for CT-OES under limited-LOS conditions constrained by chamber structure and optical access. The model is designed to infer local emissivity distributions from sparse LOS signals while capturing non-axisymmetric and localized plasma emission structures. By learning physically plausible emissivity patterns from training data, the proposed model acts as an implicitly regularized inverse solver, enabling robust reconstruction from sparse LOS measurements with reduced dependence on manually tuned regularization parameters.

PS-ThP-32 Stannane Decomposition and Sticking Coefficients under Different Sample Conditions, ***Emily Greene***, *Jameson Crouse, Nathan Barlett, Eric Mushrush,* University of Illinois at Urbana-Champaign*; Niels Braaksma,* ASML*; David Ruzic,* University of Illinois at Urbana-Champaign

This is a placeholder abstract. I will update with the real abstract as soon as I receive sponsor approval. Thank you again for your patience and understanding!

PS-ThP-33 Plasma Torch Method for Silicon Carbide (SiC) Dopant Implantation, ***Victor Veltmeyer***, *Renato Beraldo, José Pissolato Filho, José Diniz, Marcos Puydinger dos Santos,* State University of Campinas, Brazil

Silicon Carbide (SiC) has been shown to be a capable semiconductor for power electronics applications, as it supports high forward currents whilst blocking high reverse voltages, while switching up to MHz frequencies. Those properties are enabled by an exceptionally durable crystalline lattice that allows it to withstand remarkably high temperatures, enabling it to sustain transient power regimes that would otherwise destroy standard silicon semiconductors.

This exceptional crystal lattice, however, also represents the main challenge in fabricating large SiC power electronics, as it is extremely difficult to dope (or alter in general) with standard fabrication techniques, whether it be thermal diffusion or ionic implantation. The former requires heating the substrate to temperatures as high as 2100 K for several minutes, while the latter requires 100-300 keV per µm of implant depth for aluminum, the standard p-dopant for SiC, while also requiring substrate heating up to temperatures between 500-1100 K during the entire process.

Our study aims to evaluate a novel method of dopant implantation, adapting an innovative plasma torch device to perform both thermal diffusion and ionic implantation concurrently by using accelerated ions within a thermal plasma discharge. The main source of ion energy are Lorentz electromagnetic forces, which also increase the plasma plume's temperature via magnetic self-confinement, a process which has been experimentally shown to reach temperatures to extremes of 4000 K in the original device.

This plasma torch, which originally operated at atmospheric pressure, was fitted with a fused-quartz high-vacuum (10-5 Torr) chamber to reduce the beam's temperature while also boosting ion energies by increasing their mean free path. A silicon carbide wafer coated on one side with aluminum will be placed perpendicularly to the plasma flight path, where nitrogen ions (n-type SiC dopant) will bombard the wafer, simultaneously heating it while pushing accelerated dopants into the crystal lattice, a novel hybrid method which combines the best aspects of the two existing alternatives, conceivably doping the uncoated side to an n-type semiconductor while the coated to a p-type, creating a standard diode junction, which will be tested to determine the quality of this new processing method.

PS-ThP-34 Machine-Learning-Assisted Investigation of CF_3–X (X=H, F, I) Plasma Kinetics In Semiconductor Manufacturing for Etch Effectiveness and Environmental Sustainability, ***Chi-Yun Lin***, *Jane Chang,* UCLA

Hydrofluorocarbons (HFCs) gases are commonly used in semiconductor manufacturing to etch silicon dioxide, an essential insulator in integrated circuits, either from chamber wall deposits or patterned features. CHF_3 plasma is utilized for its high etch rate (ER), comparable to CF_4, and favorable anisotropic etching characteristics, though its high global warming potential (GWP100) of 12400 and long atmospheric lifetime (LT) of 222 have prompted its phasedown by the EPA. CF_3I has a lower atmospheric lifetime (<0.005) and GWP100 (<1), which are 4-5 orders of magnitude smaller than those of HFCs, making it a promising alternative gas.

This work investigates CF_3X-based plasmas (where X = H, I) in etching SiO_2 with a focus on machine learning to extract meaningful kinetic parameters for modeling. CHF_3/O_2/Ar plasma was first used to evaluate the reduce and abate strategies. O_2 serves a dual role: process-gas additive to reduce the usage of CHF3 for improving SiO2 etching and abatement reactant for reducing high-GWP fluorocarbon emissions. The experimental and modeled SiO2 etch rate increased with measured emission of SiF_4 (kg-CO_2e) and the modeled ratio of fluorine flux to oxygen flux (Γ_F/Γ_O), reaching above 150 nm/min under selected conditions. The corresponding downstream composition was converted to $MMTCO_2e$ for CHF_3, CF_4, and C_2F_6. After

introducing O2 to downstream abatement, the modeled $MMTCO_2e$ decreased by approximately a few orders of magnitude relative to the untreated emission.

$CF_3I/O_2/Ar$ was evaluated as a lower-GWP alternative. A differentiable surface-kinetic model was developed to infer the unknown iodine adsorption and abstraction probabilities, using experimental SiO2 etch rates as the ground truth, while modeled ion fluxes and etch rates served as known inputs. Descriptor information from CF_3X (X = F, Cl, Br, and I), including C–X bond dissociation energy, Si–X bond strength, and electronegativity, was used to define physically reasonable bounds for the unknown iodine-related surface kinetics. Automatic differentiation through the ODE solver reduced the average absolute percent error from 23% for the initial assumption to 12.5% after applying new surface kinetic by AI/ML inference. As the SiO_2 etch rate increases from 50–80 nm/min to above 100–130 nm/min, the corresponding measured and modeled emission for CF_3I and CF_4 decreases by an order of magnitude in $MMTCO_2e$.

Overall, selected $CF_3I/O_2/Ar$ operating conditions showed the SiO_2 etch rate increased by approximately 70% while the estimated emission impact reduce by an order of magnitude, indicating that higher etch performance can be achieved with lower greenhouse-gas-equivalent emissions.

PS-ThP-35 Advanced Waveform-Modulated Pulsed Biasing for Seam Suppression in Dielectric Gap-Fill Processes*, Yejin Shin, *Tae Cho,* WONIK IPS Co., Ltd., Republic of Korea*; Junghoon Kim,* WONIK IPS Co., Ltd.*; Hyun-Jong Woo, TaeIn Kim, YongBaek Jeon, TaeJoon Kim, Gyu-Tai Kim, DongIl Choi, Eun Sun Jung,* WONIK IPS Co., Ltd., Republic of Korea

Advanced waveform-modulated pulsed biasing techniques were investigated for surface treatment and profile modification during dielectric gap-fill processes. The primary advantage of this approach is the precise control of ion energy, enabling optimization of the biasing effect while minimizing plasma-induced surface damage. Dielectric films are commonly deposited using CVD or ALD processes; however, as next-generation memory devices adopt increasingly high-aspect-ratio structures, the risk of seam formation in gap-filled features has increased significantly.

Various approaches have been explored to suppress seam formation, including post-deposition densification treatments and profile-shaping processes designed to prevent premature pinch-off near the trench opening. These plasma-assisted surface modification processes require carefully controlled ion bombardment to regenerate the surface and reshape deposited materials.

To independently control ion energy and ion flux, dual-frequency plasma excitation using low- and high-frequency sources has been widely adopted. However, achieving independent controllability remains highly challenging, particularly in capacitively coupled plasma (CCP) reactors commonly used for dielectric deposition systems. To minimize coupling between the two frequencies, the lower-frequency source is typically selected in the range of several kilohertz to a few megahertz. Although this approach improves the controllability of ion energy and ion flux, the low-frequency bias often produces excessively energetic ion bombardment, resulting in undesirable sputtering or excessive surface treatment.

In this study, a waveform-modulated pulsed biasing technique was developed to maintain sufficiently high ion energy while minimizing perturbation of ion flux. By tailoring pulse-shape parameters, precise control of ion bombardment characteristics was achieved. To implement this technique in a PEALD system developed at Wonik IPS, several chamber components were newly designed, including a ground-layer-embedded high-temperature heater pedestal and a broadband RF notch filter.

Initial experimental studies demonstrated effective reshaping behavior of the filled dielectric layer, indicating the strong potential of advanced pulse waveform modulation for future seam-suppression and gap-fill optimization processes.

PS-ThP-36 Wafer Edge Yield Improvement through SOH Mask Tilt Optimization by Edge Insert Ring Height Adjustment*, Junhyuk Choi,* Samsung Electronics, Republic of Korea

All values except radius are normalized to arbitrary units (a.u.) for confidentiality.

As DRAM design rules shrink, the impact of wafer edge yield on overall profitability has significantly increased. However, in the Spin-On Hard mask (SOH) etch process, edge yield degradation was observed as the accumulated Radio Frequency (RF) time increased. Specifically, the extreme edge (E1) Bit-Line Bridge Disturb (BBD)—a defect associated with the outermost chips—deteriorated over time (Fig. 1). Notably, standard mass production monitoring metrics, such as Non-Pattern Wafer Etch Rate (NPW ER), top edge Critical Dimension (CD), and Virtual Metrology (VM), did not exhibit meaningful correlations with this yield loss.

To investigate the root cause, non-destructive Slope CD (SCD) metrology was employed to measure the mask left-right tilt at nine different radii (Fig. 2). The analysis confirmed a clear correlation between RF time, SCD values, and E1 BBD (Fig. 3). The identified mechanism is that as RF time accumulates, the edge ring is eroded, which alters the edge plasma sheath characteristics. This modification shifts the ion incident angle distribution, inducing a subtle tilt in the SOH mask profile at the wafer edge. When this non-uniform profile is transferred to the subsequent bit line, it results in E1 BBD defects. The analysis indicated that this degradation was most pronounced before the Actinium (a mechanical ring-lift technology for sheath control) compensation function initiated at RF time 4.

To address the mask tilt and resulting defects caused by plasma sheath distortion, the edge insert ring height was optimized. Reducing the ring height shifts the edge plasma sheath curvature area outward, thereby minimizing the sputtering variance caused by ion incident angles (Fig. 4). Based on a measured etch rate of 1.22 and considerations for measurement and process tolerances, the ring height was reduced from 2.1 to 1.6. Additionally, the Actinium application point was advanced from RF time 4 to 0 to proactively compensate for ring erosion from the start of the process.

The implementation of the 1.6 ring, combined with the adjusted Actinium timing, significantly reduced the correlation between SCD and RF time, demonstrating enhanced mask profile stability against RF time accumulation (Fig. 5). Consequently, the E1 BBD defect rate improved by approximately 3.66 over the RF time 0–4 range (Table 1). This study presents a practical, cost-effective, and data-driven edge ring optimization methodology applicable to high-volume manufacturing lines.

Quantum Science and Technology
Room Ballroom A - Session QS-ThP
Quantum Science and Technology Poster Session

QS-ThP-1 from Quantum Device Output to Governed Compute Continuation: A Runtime Architecture for Heterogeneous Scientific Workflows*, Thomas Porter,* ACGEOS

The Issue:

Emerging quantum-enabled devices, including quantum computers, photonic devices, neuromorphic, superconducting, spin, and advanced microelectronic platforms, are increasingly presented as peer elements in heterogeneous computing scientific workflows. However, the boundary between experimental device output and runtime compute continuation remains creates isolation. Device configuration, execution conditions, telemetry, logs, uncertainty, AI/ML probability interpretation, and returned results are often handled through separate files, scripts, instruments, schedulers, or manual processes, limiting reproducibility and cross-platform comparison. Quantum computers are treated as stand-alone devices.

Presenting a solution:

This poster conceptually presents ACGEOS, a governed runtime orchestration architecture for integrating quantum-enabled devices into auditable heterogeneous workflows. The model treats each task, device, configuration, telemetry record, result, and continuation state as an identifiable object. A portable governed container, the .polyp , preserves the original request, device setup, execution context, telemetry, logs, error state, and returned data. A Binding Object Layer record links expected execution to actual returned state, allowing the workflow to continue without losing provenance.

Innovation:

A central feature is a triplet return model from the quantum-device integration:

1. un-edited quantum result preserved as a .polyp , the original evidence package,
2. a BOL-bound result returned to the compute runtime for deterministic workflow continuation, and
3. an AI/ML evaluation sidecar used for confidence scoring, anomaly detection, repeatability assessment, or interpretation of probabilistic device behavior. In this model, AI/ML does not replace the governed result of record; it becomes an attached evaluation layer.

The proposed architecture is intended for future testbeds where quantum, photonic, neuromorphic, GPU, CPU, and instrument-class devices must

participate in reproducible scientific workflows. The goal is to provide a systems-level bridge between device performance, experimental evidence, and compute continuation, supporting scalability, reliability, and translation of emerging quantum technologies into practical research and engineering environments.

QS-ThP-2 Josephson Effect at the Atomic Scale with High Energy Resolution and Microwave Irradiation, ***Soumyaranjan Jhankar***, *Christian Ast,* Max Planck Institute for Solid State Research, Germany

The Josephson effect is a fundamental phenomenon of a superconductor-insulator-superconductor (SIS) junction. The Josephson current encodes information about the Cooper pair condensate, and its spectral features can be exploited as a benchmark for the energy resolution of the system. Understanding the Josephson effect at the atomic level is directly relevant to superconducting devices such as SQUIDs and to emerging quantum technologies.

Using a low temperature scanning tunneling microscope (STM) with a superconducting tip and sample, it can be investigated at the atomic scale. In this work, we report high resolution STM measurements with a microwave source at the SIS junction. We have achieved an energy resolution of 9 μeV at 1.09 K, representing the lowest benchmark value reported at this temperature so far and on par with state-of-the-art mK systems.

Microwave irradiation allows the study of microscopic phenomena, including subgap bound states (e.g., Yu–Shiba–Rusinov states), tunneling processes such as Cooper pair and quasiparticle tunneling, and resonant processes such as electron paramagnetic resonance. This motivates us to study SIS junctions under microwave irradiation, where the energies of tunneling particles are varied non-adiabatically, giving rise to replica features in the differential conductance spectra and in the Josephson current–voltage characteristics. These features serve as a signature of quantum interference at the atomic scale.

QS-ThP-3 TOF-SIMS Depth Profiling of Tantalum Deposited with Ar and Kr Sputter Gas, ***Aleksandra Biedron***, *Vidya Kaushik,* NY Creates*; Maciej Olszewski, Lingda Kong, Simon Reinhardt, Daniel Tong, Xinyi Du,* Cornell University*; Gabriele Di Gianluca,* University of Florida*; Haoran Lu, Saswata Roy, Luojia Zhang, David Muller, Valla Fatemi,* Cornell University

Tantalum (Ta) is an attractive material for superconducting applications, and optimizing deposition conditions could improve compatibility with standard semiconductor processes. Ta is typically deposited on silicon at high temperature with argon (Ar) gas. This work examines how changing the sputter gas from Ar to krypton (Kr) promotes growth of high-quality Ta films at lower substrate temperatures. The Ta films were characterized with a variety of surface analysis techniques, including depth profiling with Time-of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS). Changes in the morphology and structure of Kr sputtered films were observed, as compared to ones deposited using conventional Ar gas. The results from SIMS and other thin film analysis were in agreement and complemented by cryogenic microwave and qubit performance data. We therefore promote Kr as a superior process gas for scalable deposition of Ta films for superconducting qubit applications. [1]Reference: [1] arXiv:2601.20091 [quant-ph]; https://doi.org/10.48550/arXiv.2601.20091

QS-ThP-4 A High-Yield "Baseline" Fabrication Recipe for Superconducting Resonators and Qubits at Cornell Nanoscale Facility, ***Xinyi Du***, *Maciej Olszewski, Simon Simon Reinhardt, Lingda Kong, Gabriele Gianluca, Ron Olson, Valla Fatemi,* Cornell University

The reliable scaling of superconducting quantum processors depends heavily on the reproducibility and yield of the underlying micro- and nanofabrication processes. As quantum computing research expands, open user facilities play a critical role in providing standardized, high-quality fabrication baselines that democratize hardware developmentand prototyping. In this work, we present a user-facility-compatible fabrication flow for coplanar waveguide (CPW) resonators and planar transmon qubits, developed using the equipment at the Cornell NanoScale Facility (CNF).

This baseline methodology focuses on process optimization to maximize device yield, establish a reliable foundation for quantum coherence, and improve overall fabrication efficiency. A primary challenge in planar qubit fabrication is mitigating Two-Level System (TLS) losses arising from interfacial defects and fabrication residues, a step that traditionally relies on labor-intensive processing. To address this, our process flow incorporates a streamlined wet chemical treatment protocol. This optimized approach significantly reduces hands-on effort while effectively minimizing polymer and oxide residues at critical material interfaces, providing an easier fabrication route that ensures no degradation of feature resolution or device quality.

We characterize the efficiency of this baseline flow through comprehensive room-temperature metrology, followed by cryogenic microwave measurements. The presentation details the step-by-step cleanroom recipe, emphasizing the correlation between our refined wet processing and the resulting quantum metrics. This baseline provides the broader materials for quantum information science community with a reliable approach to consistently achieve high-yield quantum hardware.

QS-ThP-5 Learning-Guided Variational Quantum Eigensolver with Circuit-Aware Parameterization and Post-Processing, ***Yan Li***, Penn State University

Variational quantum eigensolver (VQE) methods provide a promising hybrid quantum-classical framework for estimating low-energy states of complex Hamiltonian systems on near-term quantum devices. However, practical VQE performance is often limited by the strong dependence of the optimization landscape on circuit structure, parameter initialization, measurement noise, and the quality of classical post-processing. This work develops a learning-guided VQE workflow that integrates circuit-aware characterization, machine-learning-assisted parameter prediction, and classical post-processing to improve convergence and solution quality. First, the variational circuit is analyzed to identify structural features that influence the energy landscape and parameter sensitivity, enabling a more informed design of the ansatz and search space. Second, machine learning models are trained to predict promising initial parameters or parameter-update directions from Hamiltonian features and prior optimization data, reducing the reliance on random initialization and repeated classical optimization. Third, post-processing techniques are applied to refine measured quantum outputs, mitigate sampling effects, and improve the physical interpretability of the resulting eigenstate estimates. The proposed framework is demonstrated through representative Hamiltonian problems relevant to quantum simulation and energy-system optimization. Results show that incorporating circuit-informed learning and post-processing can accelerate convergence, reduce optimization variability, and enhance the reliability of VQE under realistic measurement constraints. This study highlights the potential of combining quantum circuit analysis, data-driven parameter learning, and classical refinement to make variational quantum algorithms more scalable and robust for near-term quantum science and technology applications.

QS-ThP-6 Scanning-Tunneling-Microscope-Defined Josephson Junctions as a Local Platform for Qubit-Relevant Phase Dynamics, ***Robertus Elbertse***, *Dengyu Yang,* NIST-Gaithersburg*; Fabian Natterer,* ETH Zürich, Switzerland*; Joseph Stroscio,* NIST-Gaithersburg

Superconducting qubits rely on the controlled dynamics of the Josephson phase across weak links, yet the microscopic relationship between junction structure, dissipation, electromagnetic environment, and phase coherence remains difficult to access directly. Scanning tunneling microscopy provides an unusual route to this problem: the tunnel junction itself can act as a local, continuously tunable Josephson junction between superconducting electrodes. Unlike lithographically defined devices, an STM-defined junction allows the critical current, normal-state resistance, capacitance, and local atomic environment to be varied in situ while preserving cryogenic operation and microwave access.

Here we develop STM-defined Josephson junctions as a platform for exploring qubit-relevant superconducting phase dynamics. Using superconducting tips and samples, we characterize Josephson coupling as a function of junction conductance, material parameters, and engineered microwave environment. We examine signatures associated with phase fluctuations, junction switching, and the crossover toward regimes where the junction potential becomes sufficiently nonlinear and isolated to support phase-qubit-like dynamics. Even when operated below the threshold for a fully realized qubit, this approach provides direct access to the ingredients that govern superconducting weak-link behavior: local structure, dissipation, impedance, and noise. The resulting platform bridges atomic-scale superconducting spectroscopy and circuit-level Josephson physics, offering a flexible route toward local studies of superconducting quantum devices.

QS-ThP-7 Structure-Transport Relationships of Epitaxial Superconducting Nitride Films, *Evangeline Beeching, Sabin Regmi, Amey Khanolkar, Ahmed Wasif Mustakim, Volodymyr Buturlim, Zach Cresswell, Kevin Vallejo,* Idaho National Laboratory*; Robert Makin,* Western Michigan University*; Krzysztof Gofryk,* Idaho National Laboratory*;* ***Brelon May****,* Montana State University

The high tunability of semiconductor platforms has enabled them to be leveraged for various technologies and applications. The aspects of superconductivity can also be engineered to have specific targets. Recent efforts surrounding superconducting films for quantum systems have largely focused on achieving higher critical temperatures. However, as consensus is reached surrounding the importance of defects in quantum systems there is increasing interest in elucidating and controlling other mechanisms and resulting parameters. Understanding how synthesis parameters influence structural disorder at various length scales and their impact on the physical properties is a complex problem. This work will look into aspects of disorder ranging from the atomic scale to longer range inhomogeneities in the crystalline lattice and the relationships with electrical transport.

We will discuss the deposition of epitaxial superconducting ZrN by molecular beam epitaxy, the separate roles of atomic and crystalline disorder, and relationships between synthesis parameters and resulting structural and physical properties. The use of various substrates and orientations allows for insight into the effects of lattice mismatch and the preferential growth directions. Under the conditions investigated, rocksalt ZrN appears to prefer formation along the (001) direction but (111) oriented inclusions are observed when the temperature is too low. There is a complex relationship between synthesis parameters and resulting short range (atomic scale) and long range (crystalline lattice) order, as measured by detailed X-ray diffraction. The resulting structure shows tunability of electrical transport and optical properties, which can both range from metallic to dielectric. A broad generalization shows that samples deposited at elevated temperatures were more metallic and have higher superconducting transitions. However, other properties change in unintuitive ways, which can be explained by the non-monotonic changes in the atomic scale disorder. This work integrating superconducting films with known semiconductor platforms provides an avenue for the pursuit of (001) oriented heterostructures for superconducting or optical quantum applications.

QS-ThP-8 High Purity CaO thin films for quantum information science, ***Jake DeChiara,*** Pennsylvania State University*; Bonnie Lin,* MIT*; Amirehsan Alizadeh, Edo Waks,* University of Maryland College Park*; James LeBeau,* MIT*; Saeed Almishal, Jon-Paul Maria,* Pennsylvania State University

Computational studies predict CaO as a promising host crystal suitable to sustain optically addressable QuBits with long coherence times due to low natural abundance of calcium isotopes with nuclei with net spin and low spin orbit coupling, allowing defect states to be well isolated from magnetic noise. In this work we experimentally engineer bismuth and rare earth lanthanide dopants in varying concentration levels in an ultra-high purity, low defect CaO thin film to experimentally verify defect structure and coherence times. Reactive RF Sputtering is selected as a desirable physical vapor deposition method allowing tunable deposition rates through changes in magnetron power and cathode working distance to the substrate. Relaxed (001) oriented CaO films are grown on r-plane sapphire single crystal substrates achieving film heteroepitaxy. Host crystal purity is paramount to achieving long spin coherence times, as any magnetic impurities may interact with defect states. To minimize chemical impurity, we develop an ultra-high purity calcium sputtering source by hydrothermal sintering. 1- and 2-inch calcium hydroxide (99.999% pure) to above 95 % theoretical density. Sintering temperatures below 150°C inhibit solid state diffusion of contaminants into the source target, maintaining exceptionally high target purity throughout all processing stages. Calcium oxide thin films and dopants are co-sputtered via an off-axis geometry to mitigate anion bombardment, allowing for increased deposition rates, smooth film morphology, high density, and low film mosaicity as quantified via XRD and XRR. High deposition temperatures (875°) allow for film deposition with high crystallinity. Dopant concentration down to the single part-per-million level is quantified by induction coupled plasma optical emission spectroscopy via film dissolution in aqueous solution. Dopant concentration is coupled with deposition rate from the calcium and dopant source magnetrons and is experimentally tuned by changing dopant magnetron working distance and power, in turn modifying calcium and dopant source flux to the substrate. Oxygen vacancy defects that scale with Er are identified in the CaO lattice via deep UV photoluminescence measurements performed with a 248 nm laser excitation at room temperature – these provide an interesting pathway to infer dopant concentrations. Finally STEM analysis, including electron ptychography, that shows film microstructure, lattice strains, and defects will be presented.

QS-ThP-9 Physical Vapor Deposition of Highly Crystalline Cerium Oxide (CeO_2) Thin Films for Quantum Information Technology, ***Andrey Shults,*** *Saeed Almishal,* The Pennsylvania State University*; Sooyoon Hwang,* MIT*; Amirehsan Alizadehherfati,* University of Maryland*; James LeBeau,* MIT*; Edo Waks,* University of Maryland*; Jon-Paul Maria,* The Pennsylvania State University

CeO_2 is a well-known host for defect-generated qubits that offers high relaxation and coherence times desirable in quantum computing applications. Scalable and reproducible qubit performance with large spin coherence lifetimes requires materials with high crystallinity, low point defect concentrations, and excellent surface quality. In this work, we investigate structural and electronic properties of erbium doped CeO_2 to better understand how the crystalline quality and the defect chemistry affect its performance in quantum information technology. Utilizing RF magnetron sputtering from CeO_2 ceramics, we can tune the crystalline quality by methodically adjusting the deposition parameters such as substrate temperature, total pressure, gas ratio, and stage bias. We find that high deposition temperatures and low oxygen flows yield films with smooth surfaces (<1nm RMS), outstanding crystallinity, and low mosaicity (<0.2° FWHM rocking curve) but also create oxygen vacancies. We demonstrate that a subsequent thermal anneal in oxygen atmosphere heals the films and improves electrical properties. By dilute-doping CeO_2 with optically-active erbium, we can introduce defect qubits without altering the overall crystalline quality. During the erbium co-sputtering, we can modulate dopant levels from tens to hundreds parts per million throughout the CeO_2 thickness, as confirmed by inductively coupled plasma atomic emission spectroscopy. Photoluminescence spectroscopy results show a strong erbium emission at ~1510 nm with a 3.7 ms lifetime in agreement with theoretical calculations. Transmission electron microscopy confirms homogenous erbium doping within the film, coherent film-substrate interface, dense and continuous growth, and a smooth surface. Ultimately, we use a rich combination of characterization probes to better understand the connection between thin film structure and electronic properties that give rise to high-performing defect qubits.

Advanced Surface Engineering
Room Ballroom A - Session SE-ThP
Advanced Surface Engineering Poster Session

SE-ThP-1 PLD or Magnetron Sputtering: Which to Choose for Functional Coatings?, ***Esteban Broitman,*** *Sven Kelling, Rickmer Kose,* SENTYS

This review evaluates pulsed–laser deposition (PLD) and magnetron sputtering (MS) through a practical, application–oriented lens to help researchers and engineers select the most appropriate route for functional thin films (oxides, nitrides, chalcogenides, carbon-based). Drawing on head–to–head studies that deposit identical materials with both techniques, the paper traces how differences in deposition physics translate into film composition, microstructure, defect populations, mechanical properties and device performance.

PLD is highlighted for its reliable stoichiometric transfer from complex targets, its ability to produce high bonding density and elevated sp^3 fractions in carbon films, and its suitability for epitaxial growth and high–hardness coatings; its principal drawback is the tendency to generate particulates from the energetic plume unless droplet–mitigation strategies are employed. Magnetron sputtering (DC/RF) is shown to excel at large–area uniformity, conformal coverage and low macroscopic droplet density; pulsed modes and HiPIMS further boost ionization and substrate bombardment, yielding dense films that can rival PLD in many functional metrics while offering established industrial throughput.

The review also surveys hybrid PLD+MS approaches that leverage PLD's compositional fidelity together with sputtering's smoother deposition to reduce defects and increase density. Advances in ultra–high vacuum (UHV) platforms enhance both methods: UHV PLD improves cleanliness and epitaxial control, and UHV MS reduces impurity uptake and tightens reproducibility. Manufacturers of scientific research equipment such as **PREVAC** exemplify systems that enable in–situ diagnostics and clean sample transfer. Finally, the paper places cost and scalability in context: bench–scale sputter tools are typically less costly to acquire and run than PLD

benches, whereas at production scale capital expenditures for high–end HiPIMS sputter systems and wafer–scale PLD platforms converge.

The review closes with a concise decision matrix and actionable guidelines to match deposition choice to stoichiometry, surface quality, throughput and budget constraints.

SE-ThP-2 Surface Engineering of Ni-Based Alloy Thin-Film Catalysts for Enhanced Hydrogen Evolution Reaction, *Zhe-Yu Liu, Jhih-Siang Yang, Fan-Bean Wu,* ***Wan-Yu Wu,*** National United University, Taiwan

Nickel-based thin-film catalysts have attracted increasing interest as cost-effective alternatives to noble-metal electrocatalysts for water electrolysis. In this study, Ni-Cu and Ni-Mo alloy thin films were prepared by magnetron co-sputtering as a surface engineering strategy to tune composition, morphology, and electrocatalytic performance for the hydrogen evolution reaction (HER). The sputtering process enables the fabrication of dense, adherent, and composition-controlled thin films, providing a useful platform for clarifying the relationship between alloy composition and catalytic activity.For the Ni-Cu system, Cu was incorporated into Ni to balance hydrogen adsorption behavior and improve charge-transfer properties. Pure Ni tends to bind hydrogen too strongly, whereas Cu has weaker hydrogen adsorption and high electrical conductivity. Therefore, the Ni-Cu alloy design is expected to provide a synergistic effect for HER. Electrochemical measurements in 1 M KOH showed that the Ni-Cu thin film with a near-equiatomic composition of approximately Ni:Cu = 55:45 exhibited the best HER performance, achieving overpotentials of 76 mV at 10 mA cm^{-2} and 180 mV at 100 mA cm^{-2}. This film also showed the lowest charge-transfer resistance of 0.71 Ω, indicating enhanced interfacial reaction kinetics.For the Ni-Mo system, Mo-Ni alloy thin films with different Ni contents were deposited by DC co-sputtering on silicon and carbon-paper substrates. Structural and surface analyses indicated that co-sputtering promoted composition-dependent thin-film structures with hydrophilic surfaces. In 0.5 M H_2SO_4, the Mo-Ni catalysts exhibited a volcano-type dependence of HER activity on Ni content. The catalyst with 72.8 at% Ni showed the optimal performance, with an overpotential of 149.0 mV at 10 mA cm^{-2} and a Tafel slope of 77.5 mV dec^{-1}. In 1 M KOH, HER activity generally improved with increasing Ni content, suggesting the important role of Ni in alkaline HER kinetics.Overall, these results demonstrate that magnetron co-sputtering is an effective approach for tailoring the composition and surface properties of Ni-based alloy thin-film catalysts. The Ni-Cu system highlights the importance of balancing hydrogen adsorption and charge transfer, while the Ni-Mo system shows that composition-dependent structural modification strongly influences HER kinetics.

SE-ThP-3 Mechanochemically-Driven Formation of Zero-Friction and Zero-Wear Lubricating Carbon Films, ***Diana Berman,*** University of North Texas

Mechanically-induced surface degradation creates a significant problem for currently-used mechanical assemblies and is the major cause for their loss of usefulness. Meanwhile, high-contact pressure and shear during relative movement of the sliding interfaces provide the unique capability for local heating and shear- and load-induced compression of the sliding surfaces. For a correct combination of materials in sliding contact, these conditions may induce tribochemical reactions that lead to the formation of a protective damage-suppressing tribofilm directly at the contact. In this presentation, we overview recent advances in establishing the fundamental understanding of materials interactions at sliding interfaces and use this knowledge as a guide to developing nanomaterials solutions that enhance reliability and efficiency of tribological systems. We demonstrate tribochemically-driven self-replenishment of materials inside the contact interfaces, thus enabling a zero-wear sliding regime.

Overall, the findings could open a new avenue for the development of new concepts and design strategies for next generation of tribologically efficient materials systems.

SE-ThP-4 Friction and Wear of Composite MXene/MoS_2 Coating Under Low-Viscosity Fuels, ***Ali Zayaan Macknojia,*** *Diana Berman, Andrey Voevodin, Samir Aouadi,* University of North Texas*; Stephen Berkebile,* Army Research Laboratory

Friction and wear-related failures remain major challenges in moving mechanical assemblies operating under various conditions. For example, the components of fuel systems made of AISI 52100 steel are susceptible to scuffing-induced wear when operated in a fuel environment. This study demonstrates the decreased friction and wear characteristics achieved by spray-coating 52100-grade steel surfaces with solution-processed multilayer Ti_3C_2Tx-MoS_2 blends. The study analyzed the performance of the coating under high contact stresses and sliding speeds in different fuels. Raman spectroscopy, scanning electron microscopy, and transmission electron microscopy results revealed the formation of a robust in situ tribolayer responsible for the outstanding performance observed at high contact pressures and sliding speeds. This study has broad implications for the development of solid lubricants that can operate under extreme conditions and low-viscosity fuel environments, inspiring further research and development in this field.

SE-ThP-5 Synthesis and Dehydrogenation of Thin Film Metal Hydride for Hydrogen Storage, ***Vladimir Gorokhovsky,*** *Grace Owens,* University of Colorado at Boulder*; Paul Smith,* Plasma Kinetics Corporation

Magnesium hydride (MgH_2) is solid-state hydrogen storage material, with a theoretical hydrogen storage capacity of 7.6 wt%, making it an attractive candidate due to its high hydrogen affinity, low cost and abundance. But high enthalpy of formation and high decomposition energy of MgH_2 requiring about 76 kJ/mol of heat for each mole of H_2 released lead to increase of hydrogenation temperature, slow hydrogenation and dehydrogenation kinetics. Ni is often used as a catalyst to improve the kinetics of MgH_2 formation in H_2-contained atmosphere due to reduced enthalpy of formation of Mg-Ni alloys (<65 kJ/mol) and also has a reduced activation energy of dissociation of molecular hydrogen in comparison to Mg, suggesting that Ni mainly catalyzes the dissociation/recombination reaction barrier for H_2 solid-state hydrogen storage material reducing the hydrogenation/dehydrogenation temperatures. MgNi thin film coatings were prepared via vacuum cathodic arc deposition on sapphire wafer, aluminum foil, and aluminized polyamide tape. The cathodic arc process conditions for deposition of MgNi coatings were chosen to keep the substrate temperature low for which the arc current was selected from 50 to 70 A, and substrates (both sapphire and metal foil) were installed in a free-standing position at floating potential. The coating architecture consisted of the bottom supporting NiTiCu sublayer having large open columnar microstructure promotes the formation of the columnar microstructure with open voids in the MgNi layer. The Pd top layer deposited by e-beam evaporation improves hydrogen absorbance capability. The films were hydrogenated in Ar/5%H_2 atmosphere at 300°C in atmospheric pressure. The hydrogenation changed the color of the coating surface from silver metal to dark color accompanied by reduced electrical conductivity and increased transparency of the film indicating shift from metallic to insulative ceramic The dehydrogenation of the magnesium hydride containing films was made via laser irradiation at room temperature using 808 nm wavelength CW laser. The hydrogen flow, consisting of both molecular and atomic hydrogen, generated by laser irradiation of one hydrogenated coating spot 1mm x 10mm during 1s ranging from 0.5 to 1 SCCM. It was demonstrated that almost 90% of hydrogen contained in hydrogenated NiTiCu/MgNi/Pd coating can be released by CW laser irradiation from the 1" x 1.25" sample. The partial light transparency and increased light absorbance of MgH_2 improved by columnar microstructure with open voids provide a basis for using amplified light beam to release hydrogen from the thin film, contributing to safe and efficient hydrogen storage.

SE-ThP-6 Photodegradable Thin Films for Dust Mitigation, ***Kira Sand,*** *David Allred,* Brigham Young University

High-contrast optical systems for space applications require effective dust mitigation strategies to maintain low-scatter surfaces and edges. A novel approach would be to use photodegradable thin films that can remove any dust particles after launch, thereby reducing the likelihood of further particulate accumulation.

In this work, we investigate the photodegradation behavior of polymers such as poly(olefin sulfone) (PMPS) and poly(1-hexene sulfone) (PHS) under space-like conditions, specifically in vacuum under UVC irradiation (254 nm and 172 nm). We demonstrate that these materials undergo efficient dissociative degradation, enabling the removal of dust from coated optical surfaces. Our results show a significant reduction in particle coverage following irradiation of dust-coated films.

Additionally, we report the use of more energetic thin-film materials, including ammonium nitrate, which exhibit similar photodegradation behavior. These materials may provide enhanced dust removal efficiency due to the higher energy stored in their chemical bonds.

Overall, this study highlights the potential of photodegradable thin films as an effective strategy for in situ dust mitigation in space-based optical systems.

SE-ThP-7 Surface Patterning with Unconventional Self-Assemblies by an *m*-Terphenyl Isocyanide Ligand, ***Liya Bi***, *Zhiyuan Yin, Krista Balto, Joshua Figueroa, Shaowei Li,* University of California San Diego

Self-assembled monolayers (SAMs) refer to spontaneously formed single-layer molecular sheets on surfaces, which have found applications in corrosion protection, catalysis, drug delivery, molecular sensing, etc. The assembling behaviors of a given molecule on the surface depend on both the molecule-surface interactions and the intermolecular interactions which include covalent bonding, van der Waals interaction, hydrogen bonding or a combination of these forces. Consequently, there are various tuning knobs towards controllable molecular self-assemblies by modifying either the surfaces or the molecules. Here, we report the unconventional self-assembled patterns of a rationally designed *m*-terphenyl isocyanide ligand, $CNAr^{Mes2}$, on Ag surfaces. This molecular ligand binds to metal atoms via its isocyanide group and experiences rich intermolecular interactions upon surface adsorption because of its *m*-terphenyl skeleton. We anticipated it to form a dimerized linear molecular chain on metal surfaces based on its profile, as confirmed on Cu(100) and Cu(111) surface. Surprisingly, $CNAr^{Mes2}$ self-assembles into a few unexpected structures on Ag(111) surface including ribbons, rings and hexagons at low surface coverage and forms closely packed monolayers at high molecule density. A detailed study on these unconventional patterns suggests that $CNAr^{Mes2}$ trimer other than the dimer is the building block and that the surface chemistry of Ag plays a vital role in this assembling mechanism change. These observations inspire us to engineer the metal-binding isocyanide group and/or the steric bulks of $CNAr^{Mes2}$ to achieve programmed SAMs with on-demand shapes, lattice constants and functionalities on metal surfaces.

SE-ThP-8 ASSD Student Award Finalist Poster: In-Situ Tribo-Sintering and Atomic Structure of 2D Silicate Interfacial Films derived from Sustainable Oleogels, ***Mohammad Eskandari***, *Diana Berman, Ali Zayaan Macknojia,* University of North Texas

Designing stimuli-responsive interfacial materials capable of adapting to extreme thermomechanical stresses remains a profound challenge in surface science. Conventional liquid lubricants typically exhibit catastrophic boundary film failure at elevated temperatures. Here, we report a paradoxical friction-reversing phenomenon in sustainable bio-oleogels thickened with organically modified montmorillonite nanoclay: an autonomous transition to a macroscopic superlubricity regime (COF <0.01) initiated solely by high contact pressures (500 N) and thermal activation (150°C).

To unravel the structural mechanisms underlying the observed superlubricity phenomena, we first performed a post-tribology Raman spectroscopy analysis that confirmed the formation of a clay-based tribofilm. The 3D topographical maps acquired with ultra-high-resolution confocal laser scanning microscopy (~140 nm) confirmed the contiguous nature of it. Electron diffraction and lattice fringe imaging using high-resolution transmission electron microscopy (HR-XTEM) revealed the in-situ self-assembly of ordered layers, sintered at the plastically deformed metallic asperities. Through the combined multi-scale microscopy approach, this research provides direct evidence of a shear-induced sol-to-solid phase transition at the sliding interfaces, revealing a new class of intelligent, bio-derived, adaptive liquid interfaces for extreme environments.

Surface Science
Room Ballroom A - Session SS-ThP
Surface Science Poster Session

SS-ThP-1 Development of Machine-Learned Models for Understanding Oxygen Adsorption on Silver Surfaces, ***Bright Daniel***, University of Tennessee, Knoxville*; Carson Mize,* Leiden University, Netherlands*; Lonnie Crosby, Sharani Roy,* University of Tennessee Knoxville

The interaction of atomic oxygen with silver surfaces plays a critical role in surface oxidation, oxygen-induced restructuring, and selective oxidation catalysis such as ethylene epoxidation. Capturing these phenomena across multiple adsorption environments, coverages, and subsurface regions using density functional theory (DFT) alone remains computationally prohibitive. In this work, machine-learned (ML) adsorption models were developed to accelerate and extend the study of oxygen adsorption on Ag(111) surface using periodic DFT datasets spanning surface and subsurface adsorption configurations across multiple oxygen coverages.

Coverage-aware SchNetPack models were trained to predict adsorption energetics with near-DFT accuracy at substantially lower computational cost. The optimized models achieved low RMSD values (0.047 eV/O) and strong generalization performance ($R^2 > 0.95$), while successfully capturing coverage-dependent stabilization, subsurface oxygen incorporation, and complex local and nonlocal oxygen interactions. Hyperparameter optimization, reproducibility testing, and learning-rate scheduler benchmarking were systematically performed to improve model robustness and transferability. Beyond the default ReduceLROnPlateau scheduler, additional learning-rate schedulers were implemented directly within SchNetPack workflows, with cosine annealing scheduling reducing RMSD by approximately 74–82% relative to alternative approaches.

In parallel, pretrained MACE foundation models were evaluated as transferable machine-learned interatomic potentials (MLIPs) through direct inference on DFT-generated O/Ag (111) configurations without additional retraining. Notably, the OC20-trained multi-head MACE variants demonstrated superior transferability and predictive performance relative to general-purpose MACE-MP models, highlighting the importance of surface-chemistry-focused pretraining for catalytic adsorption applications. These results demonstrate the promise of physically informed DFT–ML frameworks for scalable modeling of surface and subsurface oxygen chemistry relevant to catalytic surface science and rational catalyst design.

SS-ThP-2 Chemically Programmable Hole Migration on TiO2(111) Revealed by Time-Resolved Atomic Force Microscopy, *Nuray Basaran, Mohammad Safikhani-Mahmoudi,* École de technologie supérieure, University of Quebec, Canada*; Bugrahan Guner,* Yale University*; **Omur E. Dagdeviren**,* École de technologie supérieure, University of Quebec, Canada

Charge migration in metal-oxide semiconductors is often treated as a thermally activated process controlled by fixed energetic barriers. However, reactive oxide surfaces can reorganize carrier transport through facet-dependent defect chemistry, irradiation history, and adsorbate-mediated charge transfer. Here, we use time-resolved atomic force microscopy (TR-AFM) to directly probe hole-migration dynamics on single-crystal rutile TiO_2(111), a highly reactive facet relevant to photocatalysis and surface redox chemistry. Measurements were performed as a function of temperature under pristine conditions, after high-energy ultraviolet (UVC) irradiation, and following exposure to ethanol or methanol.

The temperature-dependent relaxation dynamics reveal that pristine TiO_2(111) does not follow a conventional positive activation barrier. Instead, the surface exhibits an apparent negative effective migration barrier of −313 ± 40 meV in the dark. UVC irradiation shifts this value to −55 ± 8 meV, indicating that photoinduced surface oxygen vacancies reorganize the carrier-defect landscape rather than simply accelerating a fixed migration pathway. Alcohol adsorption further reshapes the response. Ethanol preserves a negative-barrier regime that is nearly insensitive to UVC irradiation, with barriers of −123 ± 8 meV in the dark and −114 ± 11 meV under UVC. Methanol produces a stronger negative-barrier response, changing from −208 ± 21 meV in the dark to −263 ± 42 meV under UVC. These results show that methanol and ethanol, although often treated as comparable hole scavengers, are dynamically distinct modifiers of hole migration on TiO_2(111).

The negative apparent barriers indicate that the measured relaxation dynamics are not governed by simple thermally activated hopping, but by coupled migration, trapping, detrapping, and temperature-dependent redistribution among surface and near-surface defect states. More broadly, this work establishes TiO_2(111) as a dynamically distinct metal-oxide surface whose charge-transport behavior cannot be inferred from TiO_2(100). The results demonstrate that charge migration in TiO_2 can be programmed through facet selection, high-energy irradiation, and adsorbate chemistry, providing a surface-science framework for engineering carrier dynamics in photocatalytic and photoactive oxide materials.

SS-ThP-3 Controlling Catalytic Surface Chemistry and Interfacial Water Transport in CO-Based Oxidative Carbonylation, ***Yeonsong Lee***, KITECH, SKKU, Republic of Korea; *Min-zy Kim,* KITECH, Republic of Korea; *Ji Man Kim,* Sungkyunkwan University (SKKU), Republic of Korea; *Tae Yong Kim,* KOREATECH, Republic of Korea; *Yong Jin Kim, Jayeon Baek,* KITECH, Republic of Korea

The oxidative carbonylation of alcohols with CO and O_2 is an attractive phosgene-free route for producing dialkyl carbonates, but the reaction is strongly affected by the local liquid–solid reaction environment. In the synthesis of bis(2-methoxyethyl) carbonate (BMEC) from 2-methoxyethanol (MEG), water is formed as a by-product and limits equilibrium conversion. In addition, selenium-based catalytic species can undergo structural and chemical changes during continuous operation, including formation and leaching of soluble selenium–carbonyl species. These coupled issues indicate that control of both catalytic surface chemistry and interfacial mass transport is required for stable liquid-phase carbonylation.

In this study, we developed a recirculating packed-bed membrane reactor that combines a Se/Al_2O_3 catalyst bed with a hydrophilic LTA zeolite membrane supported on tubular α-Al_2O_3. The reactor was designed to regulate the liquid-phase catalytic environment by selectively removing water while retaining MEG, BMEC, and selenium-containing species within the recirculating phase. The LTA membrane provided water-selective transport through strong hydrophilicity and molecular sieving, whereas the recirculation configuration reduced net selenium loss from the catalytic zone. Thus, the membrane functioned not as a downstream separator but as an interfacial component that continuously modified the reaction environment during carbonylation.

The membrane showed preferential water permeation in H_2O/MEG and H_2O/BMEC mixtures, with effective retention of organic reactants and products. Molecular dynamics simulations using a machine-learned interatomic potential indicated that water molecules could enter the LTA pore structure, whereas MEG and BMEC were hindered near the pore entrance. Under CO/O_2 oxidative carbonylation conditions, in-situ water removal increased MEG conversion and BMEC selectivity compared with a conventional fixed-bed reactor. The effects of temperature, pressure difference, solvent dilution, and liquid flow rate showed that membrane performance was governed by water activity, concentration polarization, and interfacial mass transfer.

These results demonstrate that CO-based oxidative carbonylation can be improved by controlling both catalytic surface chemistry and interfacial molecular transport. By coupling selenium-mediated carbonylation with water-selective zeolite transport, this study provides a surface-science-based strategy for regulating the local reaction environment in liquid-phase heterogeneous catalysis.

SS-ThP-4 Revisiting MOF-Based Encapsulation for CO_2 Hydrogenation to Methanol: Metal–Oxide Interface Design in Cu-Based Catalysts, ***Yerin Lee***, Korea Institute of Industrial Technology, University of Science and Technology, Republic of Korea; *Yesub Keum,* Korea Institute of Industrial Technology, Republic of Korea; *Vu Nguyen,* Korea Institute of Industrial Technology, University of Science and Technology, Viet Nam; *Huiwon Jung,* Korea Institute of Industrial Technology, Konkuk University, Republic of Korea; *Yong Jin Kim, Jayeon Baek,* Korea Institute of Industrial Technology, University of Science and Technology, Republic of Korea

Metal–oxide interfaces are critical in CO_2 hydrogenation to methanol because they govern CO_2 activation, hydrogenation of surface intermediates, and the oxidation state of Cu active sites. In our previous work with Prof. Gabor A. Somorjai, Cu nanocrystals encapsulated in the Zr-based metal–organic framework UiO-66 showed enhanced methanol formation and high methanol selectivity. This behavior was attributed to strong interaction between Cu and the Zr-oxide secondary building units of UiO-66, indicating that MOF-derived oxide clusters can act as chemically active interfacial promoters rather than simple porous supports.

Here, we revisit this MOF-based encapsulation concept by designing a MOF-derived Cu–oxide hybrid catalyst for CO_2-containing C1 gas hydrogenation. An oxide-containing framework was constructed around Cu nanoparticles to increase metal–oxide interfacial contact while maintaining accessibility of reactants to Cu-based active sites. This architecture was designed to retain the advantages of encapsulation while introducing reducible oxide domains near Cu, which can contribute to CO_2 activation, intermediate stabilization, and methanol formation.

The structure and composition of the catalyst were examined by X-ray diffraction, inductively coupled plasma analysis, and scanning electron microscopy with elemental mapping. Continuous-flow hydrogenation of CO_2-containing C1 gas was conducted and compared with a conventional $Cu/ZnO/Al_2O_3$ catalyst. The MOF-derived Cu–oxide hybrid catalyst showed promising methanol formation activity, suggesting improved utilization of interfacial Cu sites. These results indicate that rational construction of Cu–oxide interfaces can be an effective strategy for enhancing methanol synthesis from CO_2-containing C1 gas streams.

This work connects the earlier Cu⊂UiO-66 encapsulation strategy with a new MOF-derived interfacial catalyst design. By revisiting MOF-based encapsulation from a surface and interface perspective, this study provides a route for developing Cu-based catalysts in which metal–oxide contact, redox functionality, and active-site accessibility are controlled for CO_2 hydrogenation to methanol.

SS-ThP-5 Plasmonic TiN/$BiVO_4$ Photoanodes for Enhanced Photoelectrochemical Water Oxidation, ***Minseok Lee***, *Hyewon Park,* Korea Advanced Institute of Science and Technology, Republic of Korea; *Dae Han Wi,* Chungnam National University, Republic of Korea; *Jeong Young Park,* Korea Advanced Institute of Science and Technology, Republic of Korea

Photoelectrochemical (PEC) water oxidation on $BiVO_4$ photoanodes is limited by inefficient charge transport, recombination, and sluggish surface reaction kinetics. Localized surface plasmon resonance (LSPR)-based strategies can address these limitations by enhancing light harvesting and enabling hot-carrier and photothermal energy conversion.[1] Here, titanium nitride (TiN) nanocubes were introduced onto $BiVO_4$ as refractory plasmonic components to promote hot electron transfer and local photothermal effects. TiN combines metallic conductivity, chemical/thermal robustness, and broadband visible-to-near-infrared absorption, making it a promising alternative to noble-metal plasmonic nanostructures.[2] TiN/$BiVO_4$ photoanodes with different TiN loadings were examined using structural, optical, and vacuum-based surface-sensitive analyses, and their PEC performance was evaluated under simulated solar illumination. Scanning electron microscopy and elemental mapping confirmed TiN integration on $BiVO_4$. UV–vis absorption showed enhanced broadband absorption, suggesting a TiN-derived broad plasmonic feature.X-ray photoelectron spectroscopy identified an ultrathin TiO_xN_y/TiO_x surface layer on TiN, indicating surface oxidation/passivation. PEC measurements showed loading-dependent photocurrent enhancement, with optimized TiN/$BiVO_4$ outperforming pristine $BiVO_4$. Incident photon-to-current efficiency, wavelength-selected chopped chronoamperometry, and electrochemical impedance analysis suggest that the enhanced response isassociated with local photothermal effects and hot electron transfer from broadband TiN plasmonic absorption, along with reduced surface charge-transfer resistance. These results provide insight into designing refractory plasmonic photoelectrodes that efficiently transfer plasmonic energy to semiconductor materials for PEC water splitting.

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SS-ThP-6 Surface Electronic Modulation in Au-Based Bimetallic Nanostructures for Photoelectrocatalysis, ***Dasol Kim***, *Hyosun Lee,* University of Seoul, Republic of Korea

Abstract

Bimetallic nanostructures have received considerable attention in catalysis because the integration of distinct physicochemical properties of different metallic constituents enables catalytic functionalities beyond those attainable with monometallic systems. In this regard, Au-based bimetallic nanostructures constitute a promising class of photoelectrocatalytic materials, where coupling between Au and catalytically active secondary metals enables simultaneous modulation of surface electronic structures, enhancement of catalytic activity, and efficient separation of plasmon-generated hot charge carriers. In this study, Au@Pd and Au@Ni core–shell nanoparticles with controlled Pd and Ni contents, respectively, were synthesized via seed-mediated shell growth on preformed Au seeds and integrated with TiO-₂ and BiVO-₄ photoelectrodes to evaluate their photoelectrochemical activity toward the oxygen evolution reaction (OER). Au@Pd nanoparticles formed well-defined core–shell structures with sub-monolayer-to-monolayer-level Pd shell coverage on Au seeds, and X-ray photoelectron spectroscopy (XPS) analysis revealed electronic interactions between Au and Pd through Pd-content-dependent spectral changes. Similarly, Au@Ni nanoparticles were synthesized with ultrathin Ni surface layers below the monolayer level, and successful Ni incorporation was

confirmed by Inductively coupled plasma mass spectrometry (ICP-MS) and XPS analysis. When integrated with semiconductor photoelectrodes, these Au-based bimetallic nanostructures enhanced photoelectrochemical performance under light irradiation. In particular, Au@Pd/TiO_2 exhibited improved visible-light-driven OER activity with increasing Pd shell coverage, while Au@Ni-modified TiO_2 and $BiVO_4$ photoelectrodes showed enhanced photocurrent responses under visible light irradiation. Overall, this study highlights the potential of Au-based bimetallic nanostructures as multifunctional photoelectrode modifiers that simultaneously promote plasmonic light harvesting, charge separation, and surface catalytic reactions within a single nanoscale architecture.

SS-ThP-7 Plasmonic 3D Au Mesh Gas-Diffusion Electrode for Photo-Assisted CO2 Electroreduction, ***hyunwoo Jeong***, *Yeneul Lim, Hyosun Lee,* University of Seoul, Republic of Korea

Abstract

The electrochemical CO_2 reduction reaction (ECO_2RR) driven by renewable energy is a promising strategy for mitigating CO_2 emissions and producing value-added chemicals. For plasmonic metals such as Au and Ag, photo-assisted ECO_2RR can provide an attractive route to facilitate surface reactions through localized surface plasmon resonance (LSPR)-induced hot-carrier transfer to adsorbates, local electromagnetic field enhancement, and localized heating effects. However, conventional Au nanoparticles (Au NPs) often suffer from limited plasmonic enhancement of primitive plasmon modes and insufficient utilization of photo-activated surface sites. Herein, we fabricate a multilayered three-dimensional mesh Au structure (3D-mesh Au) on gas-diffusion electrodes (GDEs) with different widths (20 - 200 nm) and pitches (80 nm - 1.2 μm). Under AM 1.5G illumination, the 3D-mesh Au exhibits significantly enhanced CO faradaic efficiency (FE) compared to both dark conditions and conventional Au NPs. This superior performance originates from a large electrochemically active surface area provided by abundant edges, junctions, and interconnected nanostructures, alongside enhanced plasmon effects. Furthermore, we demonstrate that tuning the geometric parameters of the 3D-mesh Au enables modulation of LSPR wavelengths, thereby giving rise to distinct CO selectivity. This work elucidates the mechanism governing the selectivity of surface reactions in plasmonic photoelectrochemical catalysis via precise surface structure control, while validating the feasibility of large-scale electrode utilization within a GDE system for practical photo-assisted ECO_2RR.

SS-ThP-8 Facet-Controlled Au-Cu2O Heterostructures for Selective Electrochemical CO2 Reduction, ***Yeneul Lim***, *Gangbin Ryoo, Hyosun Lee,* University of Seoul, Republic of Korea

The electrochemical CO2 reduction reaction (ECO2RR) provides a promising pathway for converting CO_2 into valuable chemical products. However, its reaction pathway is highly sensitive to the local surface and interfacial environment of the catalyst. In particular, metal-oxide interfaces can create distinct reaction environments by modulating electronic interactions and intermediate adsorption at the catalyst surface. In this study, we investigate facet-controlled Au-Cu_2O heterostructures as surface-engineered metal-oxide interfaces for selective CO_2 electroreduction. Au nanoparticles (NPs) were deposited on to cubic and octahedral Cu_2O particles with well-defined morphologies, exposing the {100} and {111} facet, respectively. These facet-controlled Cu_2O structures were used to investigate the influence of Cu_2O surface structure on the catalytic effects of Au incorporation. Compared with bare Cu_2O, Au-loaded catalysts exhibited enhanced electrochemical activity and improved CO selectivity, indicating that Au modifies the interfacial reaction environment and promotes the CO-formation pathway. Among the catalysts examined, Au-deposited octahedral Cu_2O showed the most significant enhancement in CO Faradaic Efficiency (FE) and CO partial current density, suggesting that the Au-Cu_2O interface formed on the {111}-faceted octahedral surface is more effective in directing CO_2 reduction toward CO production. Computational simulation results further revealed the same facet-dependent trend, supporting the critical role of interfacial surface structure in determining CO_2RR selectivity. These results highlight facet-dependent metal-oxide interface engineering as an effective strategy for regulating CO_2RR selectivity and emphasize the importance of surface structure in the design of heterogeneous electrocatalysts.

SS-ThP-9 DFT Study of Ru–Co Bimetallic Synergy in Ammonia Decomposition, ***Yujin Jeon***, Korea Advanced Institute of Science and Technology (KAIST) & Institute for Basic Science (IBS), Republic of Korea; *Soomin Kim,* Korea Advanced Institute of Science and Technology, Republic of Korea; *Mu-Hyun Baik,* Korea Advanced Institute of Science and Technology (KAIST) & Institute for Basic Science (IBS), Republic of Korea; *Jeong Young Park,* Korea Advanced Institute of Science and Technology, Republic of Korea

Ammonia decomposition is a key reaction for hydrogen production and NO_x emission control. Among transition metal catalysts, Ru exhibits high activity for ammonia decomposition, while Co is a cost-effective non-noble metal with promising catalytic performance. In addition, Co and Ru share the same hcp crystal structure, making Ru–Co bimetallic catalysts a promising platform for enhancing catalytic activity through alloying effects. Experimentally, Ru_3Co_1/MgO exhibited higher ammonia conversion than monometallic Ru/MgO, indicating pronounced bimetallic synergy. In this study, density functional theory calculations were performed to elucidate the origin of the enhanced activity of Ru–Co bimetallic nanoparticles supported on MgO. To model the Ru_3Co_1 hcp(0001) surface, 2 × 2 × 1 supercells with different atomic configurations were optimized, and the most stable structure was selected based on formation energy. The calculations reveal that Ru–Co alloying substantially lowers the N–N recombination barrier relative to bare Ru. This enhancement cannot be explained solely by N* adsorption strength. Instead, Bader charge and PDOS analyses show charge transfer from Co to Ru in the Ru_3Co_1 alloy, generating electron-deficient Co sites. These Co sites serve as active centers for N–N bond formation, lowering the activation barrier for recombination. These results provide molecular level insight into the bimetallic synergy of Ru_3Co_1 catalysts and offer design principles for improved ammonia decomposition catalysts.

SS-ThP-10 Ligand Field and Spin-Orbit Competition in a Pb-π System, *Fahri Alkan,* Bilkent University, Turkey; *Paul Bagus,* University of North Texas; ***Sefik Süzer***, Bilkent University, Turkey

There has been a strong recent interest in the large spin-orbit coupling (SOC), a relativistic effect, in Pb moieties adsorbed on graphene and related 2D materials. Since the SOC is inherently an atomic property, a conceptually simple and bold approach might have been pursued to relate the underlying physical/chemical origin of the large SO splitting to the lead atom's outermost valence 6p atomic level. To examine this possible origin at the most fundamental level, we investigated a minimal heavy-adatom–π model system consisting of a single Pb atom positioned at various distances above the center of a benzene (C_6H_6) molecule. In order to analyze the evolution of the electronic structure of this model system, fully relativistic four-component Dirac–Hartree–Fock (4c-DHF) calculations, which took account of the angular momentum coupling of the open shell, Pb 6p, electrons, as well as quasi-relativistic approaches are used. Our results show that the ligand field effects exerted by benzene on the excited states of Pb are comparable in magnitude to the intrinsic 6p SOC of the Pb atom when it is at short distances above the C_6H_6. Indeed, in this regime, the SOC and ligand-field interactions cannot be cleanly separated. In addition, single-determinant and quasi-relativistic SOC treatments are shown to overestimate the Pb–benzene interaction and the associated SOC transfer to the π system, whereas the inclusion of multiconfigurational effects significantly reduces SOC within the open-shell space. A key result of our findings is that the SOC in heavy-adatom–π systems is not a simple projection of atomic SOC, but rather a consequence of hybridization, which depends critically on the correlated description of the heavy-atom valence shell.

SS-ThP-11 Inelastic Electron Tunneling Through Adatoms and Molecular Nanomagnets, *Daria Kývala,* ***Jindrich Kolorenc***, Institute of Physics (FZU), Czech Academy of Science, Prague, Czechia

The inelastic electron tunneling spectra (IETS) measured in a scanning tunneling microscope (STM) have repeatedly proved very useful for investigation of spin excitations in transition-metal adatoms placed on various surfaces. More recently, more complex STM-IETS measurements were achieved, involving tunneling through multiple coupled magnetic centers (multiple partially filled atomic shells). These measurements include a sequential tunneling through a magnetic molecule (nickelocene) attached to the STM tip and through another magnetic nanosystem placed on the surface [1,2], or a tunneling through multiple partially filled shells located at a single adatom [3]. To model the inelastic spectra measured in these arrangements, we employ a variant of the cotunneling theory [2,4,5] with the magnetic nanosystems being represented by means of a cluster Hubbard model [6]. In the case of an iron adatom probed by a nickelocene-

terminated STM tip [1], we show that our model reproduces the experimentally observed bias asymmetry of the inelastic spectra without introducing the apparent spin polarization of the surface electrode as a fitting parameter as done in [1]. In the case of tunneling through the 6s shell that is exchange coupled to the partially filled 4f shell in a rare-earth adatom [3], we demonstrate that our theory faithfully captures not only the spectral features corresponding to relative reorientation of the 6s and 4f spins, but also the features corresponding to the crystal-field excitations of the 4f magnetic moment. Finally, we discuss the exchange between the spin of the tunneling electron and an adatom that carries a large orbital moment, and we show that this exchange is richer than the usually assumed Heisenberg form. This richer exchange induces more features in the inelastic tunneling spectra than would be expected with the Heisenberg exchange [5].

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SS-ThP-12 Interfacial Electronic and Optical Responses in Au-Based Bimetallic Systems, ***Sieun Yang**, Hyosun Lee,* University of Seoul, Republic of Korea

In plasmonic nanostructures, the interplay between plasmonic light absorption and interfacial electronic structure plays an important role in controlling optical and catalytic functionalities. Au nanoparticles (NPs) are attractive plasmonic cores because of their strong localized surface plasmon resonance (LSPR) in the visible-light region. However, their relatively inert surface chemistry can limit catalytic functionality. Coupling Au with another metal in a core–shell geometry offers an effective strategy to integrate plasmonic light-harvesting with interfacial electronic modulation and enhanced surface reactivity. Herein, we investigate the interfacial electronic and optical responses of Au-based bimetallic core–shell NPs (i.e., Au@Pd NPs and Au@Ni NPs) with sub-monolayer shell coverage. The surface coverage of the metal shell modulates the Au LSPR response, leading to attenuation and broadening of the plasmonic absorption band, while X-ray photoelectron spectroscopy (XPS) analysis suggests interfacial electronic interactions between the Au core and the surrounding metal shell. Furthermore, femtosecond transient absorption measurements of core–shell NPs reveal accelerated hot-carrier relaxation dynamics, highlighting the role of the metal shell in regulating plasmon-driven carrier behavior. These findings provide insight into how metal-shell formation modulates the coupled optical responses and interfacial electronic properties in Au-based bimetallic nanostructures and provide design insight for plasmonic photocatalytic systems.

SS-ThP-13 Visible-Light-Driven Metal/Cu2O/Fe2O3 Janus Micromotors with Engineered Interfacial Charge Transfer, ***Park Yijun**,* Universy of Seoul, Republic of Korea*; Son Jihan, Lee Hyosun,* University of Seoul, Republic of Korea

Microplastics have emerged as a critical global pollution issue, and micromotors are increasingly recognized as promising tools for their efficient collection and degradation in aquatic environments. Among them, metal-oxide-based Janus micromotors exhibit high photocatalytic activity; however, the risks of secondary contamination, such as corrosion of noble metal caps, remain a practical concern. To address this challenge, we develop α-Fe_2O_3-based heterostructure micromotors incorporating Cu_2O semiconductor shells and metallic caps (Cu, Au, Pt). Compared with conventional TiO_2-based micromotors, α-Fe_2O_3-based micromotors exhibit enhanced visible-light-driven propulsion and photocatalytic activity, while the introduction of Cu_2O further improves micromotor performance through heterostructure-assisted charge separation and interfacial charge transfer. Among the metallic caps examined, Cu-capped micromotors show the highest propulsion efficiency and photocatalytic activity under visible-light irradiation. In addition, methylene blue degradation is examined as a model reaction to evaluate the pollutant-removal capability of the micromotors under light irradiation. The enhanced performance of Cu-capped micromotors isattributed to the synergistic effect of Cu-based redox cycling, which efficiently activates H_2O_2 to sustain reactive oxygen species (ROS)-mediated oxidative degradation and self-diffusiophoretic propulsion, combined with favorable interfacial charge transfer at the Cu/Cu_2O junction. These findings highlight that interfacial band alignment and catalytic synergy are critical determinants of micromotor performance and provide design principles for eco-friendly photocatalytic micromotors for environmental remediation, including microplastic removal.

SS-ThP-14 Exploring a New Functionality for Surface Modifications, Organo-Azides, ***John R. Mason**, Andrew V. Teplyakov,* University of Delaware

Organo azides are a reactive nitrogen containing species that have been puzzling chemists for almost 200 years. These species readily eliminate molecular nitrogen, and can insert an organo-nitrene, and have been studied for various applications in click chemistry of clean surfaces, but very little work has been done on modified (terminated) semiconductor substrates, that are currently more industrially applicable as compared to ultra-high vacuum surfaces that these compounds have been studied on. This work aims to look at liquid organic azides, and their ability to functionalize a wide range of semi-conductor surfaces including silicon and metal oxides, to attempt to elucidate the reaction mechanism of the azide on the surface, and what surface products are formed after the reaction, through the use of Fourier-transform infrared spectroscopy (FT-IR), X-ray photoelectron spectroscopy (XPS) and time-of-flight secondary ion mass spectrometry (ToF-SIMS). This work could then be used in area-selective atomic layer deposition to attempt to further explore a new class of small molecule inhibitors from this underexplored molecular species.

SS-ThP-15 Facet-Engineered Cu Nanocatalysts for Efficient Nitrate Electroreduction to Ammonia, ***Zhen Meng**, Xiaofeng Feng,* University of Central Florida

Electrochemical nitrate reduction reaction (NO_3RR) shows great potential for the recycling of nitrate from wastewater sources for the denitrification of wastewater and sustainable ammonia production. Development of this technology requires electrocatalysts that can enable high activity and selectivity for nitrate conversion to ammonia. Here we report a Cu nanoflake electrocatalyst with tunable morphology and exposed crystal facets, synthesized directly on a Cu foam substrate. Compared with their Cu nanowire counterparts, the Cu nanoflakes showed a 5-fold increase in the NO_3RR activity with 81% Faradaic efficiency for ammonia production at a low overpotential of +0.15 V vs RHE. Furthermore, the surface-area-normalized NO_3RR activity of the Cu nanoflakes remains three-times higher than that of the Cu nanowires, which is attributed to the synergistic exposure of Cu(100) and Cu(111) facets. The Cu nanoflake electrode was further evaluated in a single-pass flow cell for continuous nitrate electrolysis, which achieved high activity and >90% Faradaic efficiency for nitrate-to-ammonia conversion at 0 V vs RHE cross a wide range of nitrate concentrations, while maintaining stable performance over ~100 h of continuous operation. Our work provides insights into the rational design of NO_3RR electrocatalysts for practical nitrate remediation and sustainable ammonia production.

SS-ThP-16 Monte Carlo Simulation of Dynamic CO Oxidation on Pt(111), ***Ignacio Vargas**, Eliseo Pérez,* Brookhaven National Laboratory and State University of New York at Stony Brook*; Qin Wu,* Brookhaven National Laboratory*; J. Aníbal Boscoboinik,* Brookhaven National Laboratory and State University of New York at Stony Brook

This project presents a Python-based kinetic Monte Carlo (kMC) simulation developed to model catalytic CO oxidation on a Pt(111) surface under dynamically varying reactant conditions. The catalyst surface is represented as a two-dimensional lattice that captures the nearest-neighbor interactions characteristic of the Pt(111) crystal structure. The model incorporates the elementary surface processes involved in CO oxidation, including CO adsorption/desorption, dissociative O_2 adsorption, and surface reactions leading to CO_2 formation, with the stochastic evolution of the system governed by temperature-dependent rate constants within a kinetic Monte Carlo framework. A key aspect of this work is the implementation of time-dependent CO partial-pressure pulses in the presence of a constant O_2 background, enabling the investigation of non-steady-state catalytic behavior. The simulation is designed to reproduce experimentally measured transient CO_2 signals obtained under pulsed conditions, and the simulated transient responses are directly compared with experimental data, including CO_2 production profiles and temperature-dependent kinetic regimes such as CO-poisoned and oxygen-rich surface states. Particular

attention is given to understanding how dynamic forcing influences the interplay between adsorption, reaction kinetics, and surface coverage evolution. Simulation outputs include time-resolved surface coverages, transient CO_2 production rates, and evolving surface configurations, providing insight into how stochastic surface processes contribute to experimentally observed catalytic behavior under dynamic conditions. This work establishes a computational framework that can be further refined to improve agreement with experiment and extended to investigate larger surface models, more realistic catalytic environments, and additional kinetic processes relevant to dynamic heterogeneous catalysis.

SS-ThP-17 Methanol Dehydrogenation and Combustion Pathways on Oxidized Cu (111), ***Vishwa Don Lokugan Hewage***, *Michael Trenary,* University of Illinois - Chicago

Methanol dehydrogenation is an industrially important reaction for the production of formaldehyde and hydrogen as valuable chemical feedstocks. Previous studies on oxidized copper surfaces have identified methoxy as the dominant intermediate in the formation of formaldehyde and hydrogen at elevated temperatures. More recent investigations of alcohol oxidation on Cu surfaces have also revealed competing combustion and hydration pathways that produce ethylene, CO_2, and H_2O through oxygen-assisted surface reactions. In addition, prior studies have suggested that CO_2 formation may proceed through a minor formate intermediate at elevated temperatures. In this study, methanol reactions on oxygen-precovered Cu(111) surfaces were investigated under ultrahigh vacuum (UHV) conditions using reflection absorption infrared spectroscopy (RAIRS) and temperature programmed reaction spectroscopy (TPRS) to elucidate reaction pathways and surface intermediates.TPRS experiments showed the formation of both CO_2 and H_2O at elevated temperatures on oxygenated Cu(111), while clean Cu(111) surfaces remained largely inert under identical conditions. Although previous studies reported only a single CO_2 desorption feature near 466 K, our TPRS results at higher oxygen coverages (100 L O_2) exhibited four distinct CO_2 desorption peaks at 359 K, 373 K, 403 K, and 466 K, with the lower-temperature features contributing the highest CO_2 yield. A single H_2O desorption feature was observed near 375 K and shifted to higher temperatures with increasing oxygen exposure. Methane formation was also detected near 320 K on both oxygenated and clean Cu(111) surfaces and is attributed to methanol fragmentation to surface methyl species followed by hydrogenation by adsorbed hydrogen atoms. RAIRS measurements identified a formate intermediate with a characteristic OCO stretching feature at 1343 cm^{-1} that formed near 200 K and remained stable on the surface up to 360 K together with the dominant methoxy intermediate. The formate yield reached a maximum at approximately 150 L oxygen exposure before decreasing at higher coverages. The persistence of surface formate over the temperature range associated with CO_2 desorption suggests that formate acts as a precursor to CO_2 formation on oxygenated Cu(111). These findings demonstrate that methanol on oxygenated Cu(111) proceeds through coupled dehydrogenation and combustion pathways involving dominant methoxy and minor formate intermediates, while no significant dehydration products were observed.

SS-ThP-18 Atomic-Scale Studies of Electron- and Hole-Induced Desorption at Single-Atom Alloy Active Sites, ***Nima Rajabi***, Tufts University; *Phillips Hutchison,* Princeton University; *Kai Shen,* UC Santa Barbara; *Charles Sykes,* Tufts University; *Emily Carter,* Princeton University; *Phillip Christopher,* UC Santa Barbara

Single-atom alloys (SAAs) have attracted significant attention as thermo-, electro-, and more recently plasmonic photocatalysts due to their unique electronic and chemical properties. Unlike thermal catalysis, plasmonic photocatalysis enables energy-efficient and selective molecular activation via localized surface plasmon resonances. However, the mechanisms governing adsorbate reaction and desorption remain unclear. Here, we explore how charge injection contributes to bond weakening, leading to more efficient CO removal – a major challenge in catalytic processes where CO acts as a poison. Using scanning tunneling microscopy (STM) and spectroscopy (STS), we investigate the geometric and electronic structure of four different SAA surfaces—NiAg(100), PtAg(100), PdAg(100), and RhAg(100)—and their role in electron-stimulated CO desorption. STS and density functional theory (DFT) allow correlation of local densities of states with electron/hole energies to help probe the mechanism of desorption. Specifically, we probe charge injection induced desorption, often postulated to involve transient negative ion (TNI) states formed by plasmon-induced charge transfer. Our results indicate that SAAs exhibit drastically different CO desorption rate dependence on electron energy than would be expected solely from their CO binding energies. To further support our experimental findings, we employed nanoparticle studies, DFT, and embedded correlated wavefunction (ECW) theory. These studies provide insight into electronic structure modifications induced by charge transfer during the induced desorption process. Specifically, ECW reveals similar charge transfer mechanisms – involving intermetallic excited states - for RhAg, PtAg, and PdAg, with NiAg alone indicating possible TNI formation. Our findings provide deeper insights into the electronic and catalytic properties of SAAs and offer guidance for designing more efficient and sustainable photocatalysts that minimize the use of precious metals.

SS-ThP-19 Pulsed Dosing of Platinum Topography Effects in CO Oxidation and ZIF Film Diffusion, ***Eliseo Perez Gomez***, Stony Brook University/Brookhaven National Laboratory; *Esteban L. Fornero,* Universidad Nacional del Litoral (UNL), Argentina; *J. Anibal Boscoboinik,* Stony Brook University/Brookhaven National Laboratory

A comprehensive understanding of surface reactions requires isolating the distinct contributions of chemical kinetics, surface topology, and mass transport. This study utilizes a pulsing valve system to precisely control dosing parameters, including valve opening/closing intervals and cycle repetitions, to drive transient surface reactions. By coupling this controlled dosing framework with simultaneous in situ infrared spectroscopy and mass spectrometry, we are able to monitor the resulting surface phenomena and gas-phase products with millisecond-scale time resolution. By systematically modifying these experimental parameters, we investigate two distinct regimes: defect-driven catalysis and framework-confined diffusion. First, we explore the impact of surface morphology on CO adsorption and oxidation kinetics by comparing flat, annealed Pt (111) against rough, sputtered Pt (111) and Pt films (deposited by sputtering). Enhanced CO_2 production on rougher surfaces indicates a key role of undercoordinated active sites. Second, we extend this pulsing methodology to evaluate molecular transport and gas diffusion resistance through porous zeolitic imidazolate framework (ZIF) overlayers synthesized on both inert (Au) and active (Pt) substrates. Together, these parallel investigations showcase the exceptional utility of transient pulse systems to precisely monitor reactions, map surface coverage, and decouple the intricate relationships between physical surface roughness, catalytic activity, and localized molecular diffusion.

SS-ThP-20 Next-Generation Momentum Microscopy, *Andreas Janzen,* Scienta Omicron GmbH, Germany; *Gerd Schönhense, Olena Tkach,* Johannes Gutenberg-Universität, Institut für Physik, Germany; *Andrew Yost, Xin Zhang,* ***Daniel Beaton***, Scienta Omicron Inc.

Momentum Microscopy (MM) offers an alternative to performing ARPES and photoelectron diffraction (PED) for energies from the VUV to hard X-rays. MM captures (k_x,k_y) momentum images with diameters ranging from 2 to 12 $Å^{-1}$, easily covering a full Brillouin zone in parallel for virtually all materials.

In this contribution, we present a new momentum microscope that combines a single high-resolution hemispherical energy analyser with a photoelectron microscopecolumn that can easily be switched between generating real and reciprocal space images from a selected region of interest. The key ingredient is the versatile objective lens that enables several operation modes.

With the novel objective lens design [1], the electric field at the sample surface can be shaped from strongly accelerating (similar to a conventional PEEM) to zero-field and retarding. Retarding fields effectively reduce the space-charge interaction by redirecting slow electrons back to the sample. The 'repeller mode' is useful for ARPES at high energies and time-resolved experiments involving intense pump pulses. Space-charge suppression has been proven at the free-electron laser FLASH [2] and at high-harmonic-generation sources [3].

We present first experimental results demonstrating the ultimate energy resolution of the instrument in gas-phase electron spectroscopy.

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SS-ThP-21 Investigating the Properties of Transition Metal-Doped Ceria Thin Films Grown by Pulsed Laser Deposition, ***Rosa Virginia Melinda***, *Nishan Paudyal, David King, Jinke Tang, Jing Zhou,* University of Wyoming

Ceria ($CeO_{2-\delta}$, $0<\delta<0.5$) has attracted increasing attention for a wide range of important catalytic applications due to its reversible Ce^{3+}/Ce^{4+} redox pairs and tailorable oxygen vacancy concentrations. The incorporation of

transition metal dopants in ceria has been reported to cause modifications in the lattice structures and electronic properties of the material, thereby enhancing its catalytic performance. Additionally, doped ceria has been reported to exhibit improved thermal stability, further extending its applicability in high-temperature catalytic environments. In this study, transition metal-doped ceria ($Ce_{1-x}M_xO_{2-\delta}$, 0<x<0.5, M=Ti, Ni, Co, Fe) thin films were synthesized on Si(111) substrates using the pulsed laser deposition (PLD) technique under an O_2 environment. X-ray diffraction (XRD) and energy-dispersive X-ray spectroscopy (EDS) data revealed that the resulting thin films are polycrystalline and stoichiometric with respect to the intended metal-dopant concentrations. Atomic force microscopy (AFM) images showed that the synthesized thin films have flat surface morphologies with roughness of about 130 ± 30 pm and are composed of nanostructures with a width average of 28 ± 3 nm. X-ray photoelectron spectroscopy (XPS) was used to examine the chemical state of the incorporated metal dopants. Ti exhibits the +4 state, while Ni and Co are in the +2 state. Based on the analysis of the Ce 3d region in XPS, the thin films grown without O_2 are highly reduced. The presence of O_2 during deposition is effective for tuning the degree of reduction of ceria thin films. Our studies demonstrate that PLD offers a straightforward approach for tailored growth of transition metal-doped ceria thin films with controlled composition, thickness, and structure, which can be used as model systems of ceria to elucidate the effect of dopants on its redox properties and catalytic activity.

SS-ThP-22 Molecular Adsorption of CO at 110 K on the ZrB2(0001) Surface, ***Cosmic Gober,*** University of Illinois at Chicago

Zirconium diboride (ZrB_2) is a candidate material for extreme-environment applications such as for aerospace and hypersonic vehicles due to its ultra-high melting point and high hardness.[1] Yet a significant gap exists in the literature regarding its surface chemistry: specifically, no prior work has investigated carbon monoxide (CO) adsorption on ZrB_2(0001) at cryogenic temperatures. For many other metals, the adsorption of CO is often used to characterize the chemistry of the metal's surface. The adsorption of CO on the ZrB_2(0001) surface at 110 K was investigated with reflection absorption infrared spectroscopy (RAIRS). While CO undergoes dissociative adsorption at room temperature,[2] it is molecularly adsorbed at 110 K. It reaches saturation coverage after exposures of 0.2–0.3 Langmuir (L) with a characteristic C-O stretching frequency of 2098–2100 cm^{-1} and a narrow peak width (FWHM) of ~8.5 cm^{-1}. A saturation coverage of oxygen achieved after an O_2 exposure of ~20 L reduces the CO peak area by over 60% and increases the C-O stretch FWHM to ~15 cm^{-1} ,indicating a transition to a more disordered adlayer. However, the C-O stretching frequency remains nearly constant, suggesting that the electronic nature of the binding sites is largely unaffected by co-adsorbed oxygen. These results provide new experimental data on the surface chemistry of ZrB_2 relevant to its application in the oxidizing environments of hypersonic flight.

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SS-ThP-23 Ultrafast Photodissociation Dynamics of CH_2I_2 on SiO_x, ***Keith Blackman,*** University of Central Florida

Diiodomethane (CH_2I_2) remains an important molecule for use as a model system in gas-phase and gas-solid spectroscopic studies. In particular, the dissociation of the C-I bond provides a useful probe of the diverse reaction pathways of CH_2I_2 upon UV photoexcitation. Despite this, the overall ultrafast dynamics of CH_2I_2 is still not fully understood.

In this work, the ultrafast reaction dynamics of CH_2I_2 adsorbed on a SiO_x thin film is investigated.Temperature programmed desorption is used to investigate the interaction of CH_2I_2 with the SiO_x surface, while the photoinduced reaction of CH_2I_2 is investigated using mass spectrometry in combination with ultrafast pump-probe laser spectroscopy. In these experiments, low intensity 266 nm pump laser pulses initiate the dissociation of the CH_2I_2 molecule, while precisely delayed, high intensity 266 nm probe pulses ionize the reaction intermediates and final products, which are subsequently analyzed by a time-of-flight mass spectrometer.

Results indicate a complex photodissociation pathway, in which intermediates such as H^+, CH_2^+, and I^+ are detected at the surface. Interestingly, I_2^+ is detected in the gas phase, likely originating from recombination of iodine atoms generated during photodissociation at the surface, followed by desorption into the vacuum. Additionally, $H_2^+$is detected at the surface, while reaction products such as CH_3^+ and $C_2H_4^+$ indicate the likely presence of hydrogenation and carbon-carbon bonding at the surface. While not detected at the surface, $CH_2I_2^+$ and CH_2I^+ are observed as gas-phase products, likely resulting from ionization and excitation into cationic dissociative states of the parent molecule, respectively. Time-resolved data for the ultrafast dissociation and subsequent reactions at the surface will be presented.

These findings provide a framework for future investigations of the ultrafast dynamics of CH_2I_2 across a range of surfaces, including semiconductors and metal particles and clusters, where stronger adsorbate–surface interactions are expected to significantly influence the reaction dynamics.

SS-ThP-24 Self-limiting Oxidation of Li_xAg(111) Surface Alloys, ***Yuchen Niu,*** ***Janice Reutt-Robey,*** University of Maryland, College Park

The environmental stability of Li-Ag alloys is of immense interest due to their wide-ranging technological applications. Their stability against oxidation is particularly noteworthy, as the alloy pairs an extremely O_2-reactive metal with one of much lower chemical reactivity. This difference suggests a pathway for Li surface segregation in Li-Ag surface alloys, which will lead to facile oxidation on heterogeneous alloy films via oxidation of lithium component.

Despite the great potential of Li-Ag alloys in solid-state battery applications, the atomic structures of Li-Ag alloy surfaces and the site-specific reactivity of different Li-Ag alloy phases to O_2 remain largely unexplored. In this study, Li_xAg(111) and Li/Li_xAg surfaces were prepared via lithium deposition on an Ag(111) substrate under UHV conditions. The chemo-structural evolution of alloy surfaces under oxidative conditions was studied *in situ* with scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS). At 5 Langmuir(L) of O_2 exposure, Li_xAg(111) surfaces underwent negligible oxidation, indicating low reactivity to oxygen. At high (200 L) O_2 exposure, structural evidence for oxidative transformation emerged, where atomically smooth Li surfaces on Li_xAg(111) developed a corrugated and particulate morphology. Such oxidation was self-limiting, which is attributed to a sub-stoichiometric Li_xO_y surface passivation layer. Further oxidation of Li_xO_y islands could be driven by a strong local electric field from the STM tip, in accordance with the Cabrera-Mott-type oxidation mechanism. A model for Li_xAg surface evolution during the oxidation is proposed.

SS-ThP-25 Insight Into Subsurface Adsorption Behavior Over the Material Pressure Gap, ***Carson Mize,*** Leiden University, Netherlands; *Sharani Roy,* University of Tennessee Knoxville

Transition metals are heavily utilized in catalytic reactions due to their ability to participate in a variety of reactions. While the fundamental focal point has been on deciphering the processes happening on the surface, the role subsurface adsorbed species play in the evolving chemical environment is less understood. It is suspected subsurface adsorption influences a variety of material effects, such as corrosion, metal oxidation, and even reconstruction, making characterizations in this region important in understanding the full properties of a material. However, to properly study subsurface adsorption, one must think of the concerted coadsorption of many atoms or molecules, as high coverage surface atoms promote diffusion into the subsurface, suggesting the demand to capture the adsorption behavior over a large coverage regime. To this end, we have developed an *ab initio*, lattice-gas model designed to include surface and subsurface adsorption in a solid[1]. We applied our model study the adsorption of atomic oxygen on Ag(111) over a wide range of coverages and O_2 pressures, representing experimental pressures (high vacuum) and industrial applications (high pressures)[2]. The coadsorbate interactions in the model are treated in a pairwise manner and all parameters of the model are calculated using density functional theory. This study demonstrates modelling this coadsorption behavior provides insight into the fundamental issue of the "pressure gap" that exists when studying adsorption and reactions at surfaces.

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SS-ThP-26 Investigating the Ultrafast Dynamics of CH_2I_2 on Metal Oxides, ***Sebastian Cimino,*** *Lucas Macri, Keith Blackman, Mihai Vaida,* University of Central Florida

As a model system, CH_2I_2 is a molecule that has highly documentable dissociation and recombination behaviors. While the gas-phase ultrafast

dynamics have been extensively characterized throughout previous femtochemistry research efforts, surface-aligned CH_2I_2 is still a relatively novel topic that is yet to be fully explored. One of the most significant dissociation products of CH_2I_2 is CH_2, since it has been theoretically determined that it is aligned towards the gas phase as opposed to the iodine in the compound which forms bonds with the surface. Therefore, dosing a metal oxide substrate such as titanium oxide or silicon oxide with both CH_2I2 and O_2, or ozone, leads to the creation of one of the simplest Criegee intermediates, CH_2OO or formaldehyde oxide. In current physical chemistry research, there is very little understood about the surface-aligned ultrafast dynamics of CH_2OO. While purely gas-phase formaldehyde oxide is the most prevalent form of this molecule in the environment, CH_2OO molecules in the air frequently adsorb to dust particles and unbound metal oxide matter. Understanding how CH_2OO interacts with a surface substrate can greatly assist current environmental efforts to reduce the amount of CH_2OO in the Earth's atmosphere, since its highly reactive nature leads to the creation of several harmful compounds found in the air.

SS-ThP-27 First-Principles Study of CF_4 and C_2F_6 Hydrolysis Pathways on $ZnAl_2O_4$ and Al_2O_3 Catalysts, ***Chi Hun Lee***, *Sang Hyeon Ju, Gyeong Won Seo,* Inha University, Republic of Korea*; Hyuk Jae Kwon, Jong-Min Lee, You-Hwan Son, Jeong Yun Kim,* Samsung Advanced Institute of Technology, Republic of Korea*; Hyung Chul Ham,* Inha University, Republic of Korea

Growing environmental regulations on the semiconductor industry have placed urgent demands on the development of effective abatement technologies for perfluorocompounds (PFCs) emitted from FAB exhaust streams. In particular, carbon tetrafluoride (CF_4) and hexafluoroethane (C_2F_6) are regarded as exceptionally challenging targets due to their outstanding thermochemical stability and extremely long atmospheric lifetimes. Against this backdrop, spinel-structured zinc aluminate ($ZnAl_2O_4$) and gamma alumina (γ-Al_2O_3) has emerged as a promising catalytic platform for PFC decomposition, owing to its superior thermal and chemical robustness. However, transition states — the highest-energy species along the reaction coordinate — are spectroscopically silent and thus fundamentally inaccessible through experimental observation alone, imposing inherent limitations on the elucidation of precise reaction mechanisms and catalyst deactivation pathways. To address this challenge, density functional theory (DFT) calculations are employed to systematically investigate the major reaction pathways of CF_4 and C_2F_6 on a $ZnAl_2O_4$ and γ-Al_2O_3 slab models with the most stable surface termination determined by surface energy calculations, considering both direct dissociation and hydrolysis routes. Our DFT calculation identified the most critical step that can simultaneously maximize the hydrolysis of both CF_4 and C_2F_6. In addition, the transition metal-doped $ZnAl_2O_4$ catalyst was examined to tune the surface reactivity toward CF_4 and C_2F_6 hydrolysis. The findings of this study are expected to provide molecular-level mechanistic insights into PFC hydrolysis on metal oxide surfaces and offer practical design principles for the rational development of next-generation catalytic abatement systems targeting FAB exhaust emissions.

SS-ThP-28 X-Ray Photoelectron Spectroscopy of Organo-Metallic Compounds Designed for Homogeneous Catalysis, ***Farzad Bastani,*** University of Virginia*; Daniel Ess,* Brigham Young University*; T. Brent Gunnoe, Petra Reinke,* University of Virginia

Organo-metallic compounds where one or several metal or metalloid centers are surrounded by organic ligands are highly efficient homogeneous catalysts. This toolbox for optimization is limited by the "synthesizability" of an imagined compound. Our focus here is on XPS which has the advantage of quantitative elemental analysis but brings the complications of final state effects which influence chemical shifts and spectral shapes.

Compound functionality relies on the distribution of charge between ligands and metal center(s) and functionalization with strongly electronegative groups, F, O, Cl and combinations thereof modulates said charge distribution. XPS offers, via the chemical shift of core level peaks, insight in the charge on the metal, and as an extension on other elements within the compound. We propose that XPS characterization can be used to map the relative changes in bonding and oxidation state within and between related compounds.

We have analyzed a set of 20 organo-metallic compounds which include Cu, Sb, Pt and Ag as single or double metal centers with a wide range of ligands and electronegative groups [1]. We developed a workflow to test for compound stability, and will discuss the choice of reference energy for these insulating substances. The chemical shift for core levels relies on the modulation of the oxidation state, respectively the charge state of the element. However, the shift is element and core level specific. We developed a calibration method based on data of inorganic materials, type and electronegativity of the bonding partner. We will discuss this benchmarking and its limits of transferability between inorganic and organic compounds. The relative shifts are compared to results from DFT calculations for the respective compounds. All elements within each compound are included, and fitting of the core levels is used to identify bonding configurations and corresponding ligand induced shifts. We will discuss several examples with various ligands and metal centers and develop from there a general approach to use XPS and construct a charge distribution map of the respective compound.

One of our examples are quinoline-based Sb ligands coordinated to Pt which are modified by attachment of Cl, F and $C_6Cl_4O_2$ to Sb or Pt. The charge distribution between Pt and Sb is modulated and explained with a next nearest neighbor interaction. However, changes in the Cl atom bonding and charge is traced back to a long range interaction enforced by the ligand geometry. Surprisingly switching Cl for F next to the Sb center is inconsequential to the Pt and all other oxidation states.

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SS-ThP-29 Evaluating MLIP Representation of Reaction Mechanisms on Ni-Based High-Entropy Alloy Surfaces, ***Chiezugolum Odilinye,*** *Liney Arnadottir,* Oregon State University*; Gregory Herman,* Argonne National Laboratory, USA

Understanding reaction mechanisms on complex alloy surfaces remains a key challenge in catalyst design. In this work, we investigate how Machine Learning Interatomic Potentials (MLIPs) capture adsorption energetics and reaction pathways for CO_2 hydrogenation reaction on a Ni-based High Entropy Alloy (HEA). Using the Universal Model for Atoms (UMA) MLIP, we evaluate adsorption properties of key intermediates (CO, O, and H). Nudged Elastic Band (NEB) calculations are used to probe the CO hydrogenation step (CO + H >CHO). MLIP predictions are benchmarked against Density Functional Theory (DFT) calculations and ML-NEB implementations (eOn and CatLearn) to assess their ability to represent reaction energetics on multi-element surfaces. Results show that UMA systematically overestimates adsorption energies, leading to deviations in predicted activation barriers. It also reveals composition-dependent trends in adsorption energetics and activation barriers across the HEA surfaces. These findings highlight both the potential and limitations of MLIPs in capturing surface reaction physics in high-dimensional compositional spaces and provide insight into their role in AI-driven materials discovery.

SS-ThP-30 Topology-Directed Silicide Formation: An Explanation for the Growth of C49-$TiSi_2$ on the Si(100) Surface, *Lukas Hückmann,* Leiden University, Netherlands*; Jonathon Cottom,* ARCNL*; **Jörg Meyer**,* Leiden University, Netherlands*; Emilia Olsson,* ARCNL

The optimization of metal-semiconductor (MS) junctions is a fundamental prerequisite for advancing electronic device performance. Titanium disilicide ($TiSi_2$) is a widely used material due to its low electrical resistivity, good chemical stability, and low Schottky barrier height at the MS interface [1]. In practice, the existence of multiple polymorphs makes it challenging to grow phase-pure films. Among these, the C54-$TiSi_2$ phase exhibits the desired beneficial properties; yet it is the metastable, high-resistivity C49-$TiSi_2$ modification that preferentially nucleates on Si substrates. The origin of C49-selective nucleation, however, remains debated [2]. We present a first-principles atomistic model of Ti adsorption on the c(4x2) Si(100) surface that highlights the key role of surface symmetry and reconstruction for the initial stages of the interfacial TiSi2 formation process [3]. Based on DFT calculations ranging from the dilute limit to a coverage of two monolayers, we identify the energetically most stable configuration as a Ti-Ti dimer pair consisting of a surface adatom and a first-subsurface interstitial. This specific pairing coincides with the local reversal of the Si(100) surface reconstruction, which creates a characteristic low-symmetry adsorption pattern that is unique to the C49-$TiSi_2$ phase and thereby serves as a nucleation template for C49.This model aligns with experimental observations like the Stranski-Krastanov growth mode, the preferential formation of C49-$TiSi_2$ despite being less favorable than the competing C54 phase, and why disrupting the surface structure via amorphization removes the nucleation template and restores thermodynamically driven growth of the latter. This atomistic perspective on phase-selective growth suggests that such surface pre-treatment could obviate the need for the C49 to C54 transformation, thereby minimizing the thermal budget in the fabrication of next-generation nanoelectronic devices.

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Thin Films
Room Ballroom A - Session TF-ThP
Thin Film Poster Session

TF-ThP-1 Phase Control in Flash-Evaporated Perovskite Thin Films, ***Jack Lawton***, *Milo V. Ferrara, Carlo A.R. Perini, Juan-Pablo Correa-Baena,* Georgia Institute of Technology

Thermal evaporation has become a well-established technique for the deposition of large area, uniform hybrid metal halide perovskite (MHP) thin films. Despite extensive literature on MHP evaporation, little progress has been made in high-rate MHP deposition, which is key to the eventual commercialization of MHP optoelectronics.Flash evaporation is a deposition technique that can produce MHP films at rates of 500 nm min-1. Such high deposition rates are due to high evaporation temperatures, but these temperatures can also have deleterious effects. In particular, the organic components of the hybrid material may partially decompose. This can lead to organic-deficient, nonstoichiometric films that are rich in secondary phases and possess undesirable properties. Furthermore, high evaporation temperatures can induce precursor powder spitting, whereby powder is ejected from the boat before vaporizing, leading to poor process reproducibility and films with spit defects.In this work, we demonstrate that particle spitting can be eliminated through evaporation boat design. A baffled boat architecture is introduced that hinders the ejection of particles by forcing precursor material to pass through a tortuous path before leaving the boat. We identify that the complex boat geometry produces transient vapor plume stoichiometries, whereby organic species that take longer to exit the boat experience greater heating and are therefore more likely to decompose. Such behavior leads to a gradient in the phase composition, with initial film growth being organic-rich, yet later film growth being dominated by organic-deficient phases.We introduce two novel approaches to achieve phase purity in flash-evaporated MHP films. First, we deposit an organic capping layer atop the MHP and induce intermixing through a modified annealing regimen. This technique replenishes organic material that is deficient in the upper layers of the films and films deposited by this method exhibit phase purity and favorable optoelectronic properties.Second, additive chemistry is shown to control phase composition in evaporated MHP films. Phosphonic acids can be incorporated into precursor powders to increase the organic material's sticking coefficient. Thus, we show that additive chemistry can control film stoichiometry, allowing for phase-pure and high-quality films to be achieved without the need for a second processing step. This work demonstrates how both processing and additive chemistry can be used to control the phase-purity of MHP films deposited at high rates, which could be key in their eventual commercialization.

TF-ThP-2 Low Energy Ion Scattering Surface Analysis of ALD Coated Ti-Based Porous Transport Layers, *Philipp Brüner,* ***Thomas Grehl***, IONTOF GmbH, Germany; *Athina Tzavara Roussi, Rens Kamphorst, Ruud van Ommen,* Delft University of Technology, Netherlands

Porous transport layers (PTLs) are essential components in water electrolyzers, facilitating efficient electrochemical reactions. Situated between the electrodes and current collectors, PTLs offer structural integrity, enable the diffusion of gases and the removal of water from reaction sites, ensure electrical connectivity between the electrode and current collector, and assist in thermal management by dissipating heat.

Titanium-based PTLs are widely used due to their good conductivity, corrosion resistance, and mechanical robustness. However, they are susceptible to long-term degradation under the aggressive chemical environments typical of electrolyzer cells. To address this, protective coatings are applied to enhance PTL performance by enhancing surface chemical stability and modifying surface characteristics.

Atomic layer deposition (ALD) is a highly effective technique for applying these protective coatings, particularly for porous substrates. Its conformal and precise nature allows for the fine-tuning of thin-film properties. In this study, we present findings from low-energy ion scattering (LEIS) analyses of ALD-coated Ti-based PTLs, utilizing a variety of coating materials.

LEIS, with its exceptional surface sensitivity, enables the quantification of surface coverage by the ALD film, offering critical insights into film growth and layer closure. Additionally, film thickness is evaluated to understand the ALD growth mechanism and growth per cycle. We also address the analytical challenges posed by the highly three-dimensional structure of the substrate, which impacts surface quantification and thickness measurements.

TF-ThP-3 Effects of Substrate and Deposition Temperature on the Morphology and Electronic Characteristics of Bismuth Thin Films Grown at 77 K and 296 K, ***Yulia Kirina***, *Prakash Sharma, Wyatt Thomas, Tristan Anderson, Arya G. Pour, Victoria Soghomonian, Jean J. Heremans,* Virginia Tech

Quench-condensed bismuth thin films deposited at substrate temperatures T_s = 4 K can exhibit superconductivity. However, the origin of this phenomenon is still debated [1]. Here, we report on the effect of T_s on the microstructure and transport properties of 100 nm thick Bi films evaporated onto single-crystalline Al_2O_3(0001), amorphous SiO_2, and van der Waals structured mica substrates. Two sets of samples are deposited, one at low T_s = 77 K and the other at T_s = 296 K [2]. Using atomic force microscopy, X-ray diffraction, transmission electron microscopy, and variable temperature multicarrier magnetotransport characterization techniques, we determine morphologies, crystallinities, carrier mobilities, carrier densities and sheet resistances of the as-deposited films. For the Bi films deposited on Al_2O_3(0001) and SiO_2 at T_s =77 K, the measured root-mean-square roughness values are comparable and are 3 to 4 times smaller than those obtained for the films grown at T_s = 296 K. In comparison, for the Bi films deposited on mica at the two different T_s, while the surface roughness is similar, the film morphologies are different. On all three substrates, rhombohedral (R-3m) 110-textured films at T_s = 77 K and 111-textured films at 296 K are obtained, with grain sizes 1.7 times larger for the films grown at T_s = 296 K. We find evidence of multicarrier transport in the films, originating from electrons and holes in the bulk in addition to surface state electrons in Bi(111) and Bi(110) oriented films [3]. Overall, on all three substrates films deposited at T_s = 77 K exhibit lower carrier mobility and higher sheet resistance when compared with films deposited at T_s = 296 K. Interestingly, annealing Bi films grown at 77 K results in a transition from a predominantly 110-texture to a predominantly 111-texture. In contrast, annealing Bi films deposited at 296 K leads to dewetting. Our results show the effects of deposition temperature and the substrate structure on morphology, microstructure, and charge transport characteristics of Bi thin films.

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TF-ThP-4 Reactive Atomistic Simulation Workflows for Thin-Film Growth and Surface Modification in ALD and ALE, ***Fedor Goumans***, Software for Chemistry & Materials, Netherlands

Thin-film processing increasingly depends on controlling chemistry at the scale of individual surface sites. In atomic layer deposition and atomic layer etching, precursor exposure, ligand removal, surface activation, and product desorption determine the final film structure and process selectivity. Atomistic simulations can provide mechanistic insight into these steps, but realistic process modeling requires methods that can describe reactive events while remaining efficient enough to sample complex surfaces and repeated process cycles.

This poster presents a simulation workflow for studying thin-film growth and surface modification using reactive force fields and machine-learned interatomic potentials. Representative systems include HF interaction with SiO_2 surfaces, relevant to oxide etching and surface modification, and TMA reactions with hydroxylated Al_2O_3, relevant to alumina atomic layer deposition. The workflow combines model surface generation, reactive molecular dynamics, trajectory analysis, and comparison with higher-level reference calculations. Key observables include surface functional group populations, bond rearrangements, volatile product formation, local coordination environments, and changes in film density or surface roughness.

By comparing etching and deposition examples, we illustrate how similar atomistic tools can be used to study both material removal and film growth. For HF/SiO_2, simulations can probe how hydroxylation, strain, and local network structure affect fluorination and etch susceptibility. For TMA/Al_2O_3, simulations can examine ligand exchange, methane formation, steric blocking, and the persistence of reactive surface sites over repeated exposure steps. These results support a mechanistic picture of how local surface structure controls macroscopic process behavior.

The poster emphasizes practical workflow choices, including the role of ReaxFF for exploratory reactive dynamics, the use of machine-learned potentials for improved accuracy and transferability, and validation strategies based on quantum chemical reference data. The approach is

intended to help bridge molecular-scale reaction mechanisms with thin-film processing outcomes such as growth per cycle, etch selectivity, nucleation behavior, and interface quality.

TF-ThP-5 A Calibrated Oxidization Model and Software Application for Predicting Silicon Dioxide Growth in a Muffle Furnace, ***Drew Ledger***, *Daniel MacAyeal, Alexander Kozen,* University of Vermont

Thermally growing Silicon Dioxide (SiO_2) remains one of the most fundamental processes in semiconductor research and education, but many labs relying on muffle furnaces often lack predictive growth models, leading to inaccurate predictions and wasted substrates. To address this, we adapted a simplified parabolic oxidization model based on the Deal-Grove model of the form $X_{nm} = 1 + \sqrt{(B_0 * exp((-E_a)/(k_BT)) * t)}$. 15 different SiO_2 films were oxidized across a wide range of temperatures and times, spanning from 800°C to 1200°C and 2 to 8 hours. The thickness and non-uniformity of these films were then measured using multi-point ellipsometry across each wafer. The dataset was then used to fit the B_0 and E_a variables under three different loss criteria: MAE, RMSE and MAPE. We will discuss model-experiment data similarity, deviation across loss functions, and the temperature and time ranges for which the model is reliable. The calibrated model was then packaged into a Python application, supporting direct thickness prediction, inverse recipe generation from target SiO_2 color or thickness, and re-calibration functionality for other labs.

TF-ThP-6 Processing-Structure Relationships in Superconducting Titanium Nitride Thin Films for Quantum Device Applications, ***Kiran Nyaupane***, *Ebenezer Vondee, Tianjun Xie, Raymond E. Samuel, Richard A. Taylor, Shyam Aravamudhan,* North Carolina A&T State University

The scalability of superconducting quantum computers is fundamentally limited by decoherence in Josephson junction–based qubits, where two-level system (TLS) defects at material interfaces are a major source of energy loss. Although aluminum remains the standard electrode material, its susceptibility to surface oxidation and coherence limitations have motivated the search for alternative superconductors. Titanium nitride (TiN) is a promising candidate because of its oxidation resistance, tunable kinetic inductance, and potential for reduced TLS-related losses. However, despite its use in superconducting resonators and capacitive elements, TiN-based Josephson junctions remain insufficiently optimized.

This research advances TiN as an electrode material for Josephson junctions by establishing reproducible fabrication protocols for TiN thin films with controlled stoichiometry, crystallinity, and superconducting properties. Using reactive magnetron sputtering with in-situ control of nitrogen partial pressure and sputtering power, this work systematically tunes film properties and correlates them with cryogenic device performance and quantum coherence metrics in TiN-based superconducting qubits.

By linking deposition conditions, materials quality, and qubit performance, this work addresses a critical materials-engineering gap in Josephson junction fabrication and establishes a pathway for integrating TiN into scalable quantum computing architectures. Future efforts will extend the platform to multi-qubit systems and all-nitride junction designs incorporating superconducting nitride barriers for improved materials compatibility and device performance.

TF-ThP-7 New Insights Into van der Waals Epitaxy of Layered Materials on Mica, ***Per Eklund***, Uppsala University, Sweden

There is a great deal of interest in rationally realizing van der Waals epitaxy (vdWE), a mechanism characterized by atomic-level registry across a weakly-bonded film-substrate interface. Weak interface bonding is conducive for stress-free crystal growth, and transfer to other substrates or stand-alone films. This is in contrast to conventional epitaxy with strong film-substrate interface bonding and lattice matching. The most intuitive examples of vdWE are seen in 2D materials like graphene and hexagonal boron nitride, where film-substrate atomic registry is mediated solely by vdW bonding.

The situation is more complex for substrates on which both conventional and vdW epitaxy are possible. A particularly important example is mica, a layered material commonly used for mechanically flexible thin films. Mica has been shown to support vdWE for layered materials such as chalcogenides. However, the current understanding of interface energetics and mechanisms of vdWE is inadequate to predict if a material will grow by vdWE or conventional epitaxy. As a result, vdWE is often *incorrectly presumed* simply because mica is layered, without establishing the conditions to indicate vdWE or even ignoring evidence to the contrary. We have shown that the growth of rocksalt ScN and NiO films on mica(001) occurs by conventional epitaxy. In fact, for any nonlayered materials such as transition metal oxides and nitrides grown on mica, conventional epitaxy should be the default assumption, and any claim of vdWE must, as a minimum, provide compelling evidence. Necessary conditions for vdWE are: a) in-plane and b) out-of-plane texturing, and c) nearly strain-free epilayers independent of lattice mismatch or film thickness.

In contrast, for layered materials on mica, the situation is far more complex, and an atomistic understanding of film/substrate interface structure that explains and predicts vdWE has remained elusive. We have unveiled atomistic interface mechanisms for vdWE of MoO_3 and VO_2 on mica showing negligible strain buildup in continuous epilayers, confirming vdWE. Ab initio computations showing interface energy minima for these orientations correlate with high cross-interface proximity between Mo atoms in MoO3 and K in mica conducive for maximal vdW attraction. These insights on interface structure and energetics provide a framework for predicting vdWE for different film/substrate combinations and designing of stress-free and/or standalone epitaxial films of layered materials on layered substrates such as mica.

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TF-ThP-8 Patterned Growth of Lead Halide Perovskite Thin Films via Stoichiometric Control, Surface Modification, and Templated Substrates, ***Jorge Rivera Romero***, *Nayeem Arefin, Sanchaya Pandit, Yanan (Laura) Wang,* University of Nebraska-Lincoln

All–inorganic lead halide perovskites (LHPs) combine tunable optical properties with strong excitonic behavior, making them attractive for integrated photonic and thin–film devices. Their chemical instability and complex phase behavior, however, make conventional lithographic patterning difficult. Here, we present a soft–lithographic approach that uses precursor stoichiometry, fluoroalkyl–silane-based surface modification, and micropatterned Si/SiO_2 templates to guide the selective nucleation and confined growth of $CsPbBr_3$ and $CsPb_2Br_5$ structures. Adjusting the $CsBr:PbBr_2$ ratio allows us to control the dominant phase, verified through photoluminescence and Raman measurements. Vapor–phase silanization of PDMS produces a lyophobic coating that can be transferred onto the template, creating a wettability difference that directs precursor infiltration and self–assembly during evaporation. This method yields patterned 1D perovskite arrays without the need for aggressive etching and provides a route toward thin–film structures with controlled morphology and crystallinity.

TF-ThP-9 Investigation of Lattice Interpenetration in Thin Film Growth of Microporous Coordination Polymers, *Hallie Matherne,* ***Greg Szulczewski***, The University of Alabama

Thin films were synthesized from a family of pillared, microporous coordination polymers with the general formula $M_2(BDC)_2L$, where M is Ni^{2+}, Co^{2+}, Cu^{2+} and Zn^{2+}, BDC is benzendicarboxylic acid and L is either is 1,4-diazabicyclo[2.2.2]octane (DABCO) or 4,4'-bypridine (bpy), by a hot-solvent technique and a room temperature layer-by-layer solution deposition. The thin films were grown on gold substrates and characterized by x-ray diffraction, x-ray photoelectron spectroscopy, ion-scattering spectroscopy, vibrational spectroscopy and scanning electron microscopy. The films were activated by heating under high vacuum and adsorption/desorption isotherms were measured for several volatile organic compounds. The mass uptake of the guest molecules into the coordination polymer host strongly depends on the extent of lattice interpenetration. In general, the extent of lattice interpenetration depends on the length of the diamine pillar. In the hot-vapor synthesis technique, lattice interpenetration is observed when using the longer bpy pillar, but not the shorter DABCO pillar. However, at room temperature, lattice interpenetration can be suppressed by using the layer-by-layer solution deposition technique with the bpy pillar. The key to suppress lattice interpenetration is use of a pyridine terminated thiol monolayer which templates the growth of a single phase.

TF-ThP-10 Modular High-Temperature Substrate Manipulation Platform for Wafer-Scale Semiconductor and Optoelectronic Thin Film Processing, ***Lukasz Walczak***, PREVAC, Poland

Recent advances in wafer-scale semiconductor and optoelectronic thin films have increased the demand for scalable and highly reproducible deposition environments capable of ensuring precise process control across large-area substrates [1–4]. In particular, substrate temperature stability, thermal uniformity, and motion precision are critical parameters influencing crystalline quality, interface formation, defect density, and thin-film

reproducibility during advanced deposition and epitaxial growth processes [2,5].In this work, we present a modular ultra-high vacuum (UHV)-compatible substrate manipulation platform designed for integrated thin-film synthesis and characterization workflows dedicated to semiconductor and optoelectronic material systems. The platform supports substrate diameters from 2-inch to 12-inch wafers and combines high-temperature operation with multi-axis manipulation capabilities, including continuous rotation, tilt, and precision XYZ positioning during deposition and transfer processes.Special emphasis was placed on thermal management and large-area process uniformity under conditions relevant for advanced PVD, ALD, MBE, and hybrid thin-film growth environments. Finite-element thermal simulations together with experimental temperature mapping were applied to optimize thermal distribution and minimize temperature gradients across large-area substrates. Stable high-temperature operation and improved spatial temperature uniformity were achieved, supporting enhanced reproducibility of thin-film deposition and wafer-scale material synthesis.The presented architecture enables integration of multiple process and characterization modules within a single interconnected UHV environment, including deposition, annealing, vacuum transfer, and surface analysis workflows. Such integrated processing environments are increasingly important for accelerated development of semiconductor heterostructures, functional thin films, and emerging optoelectronic materials [3,4].The influence of substrate thermal stability and motion control on process repeatability and scalable thin-film manufacturing will be discussed in the context of next-generation semiconductor and photonic material platforms.

TF-ThP-11 Synergistic Enhancement of Mechanical and Electrochemical Performance of Ni Doped Chromium Nitride Coatings Deposited on Nab Alloy Using Reactive Magnetron Sputtering, ***Aakanksha Jain***, *Ramesh Chandra, Rahul. S Mulik,* Indian Institute of Technology, India

The rapid degradation of nickel aluminium bronze (NAB) alloys in chloride-rich marine environments necessitates protective coatings with superior mechanical integrity, tribological durability and electrochemical stability. In the present work, nickel-doped chromium nitride coatings were deposited on NAB substrates by reactive DC magnetron sputtering using a co-focal arrangement of Cr and Ni targets in an Ar/N_2 plasma atmosphere. The incorporation of Ni was intended to improve the structural and multifunctional performance of CrN-based coatings for marine applications.

X-ray diffraction analysis confirmed the formation of crystalline Cr-N rich multiphase nitride structure consisting predominantly of FCC CrN/(Cr, Ni)N and HCP Cr_2N phases. A slight shift in diffraction peaks towards higher angles indicated lattice distortion and compressive residual stresses induced by substitutional incorporation of Ni into the CrN lattice. XPS investigations further confirmed the presence of Cr-N and Ni-N bonding states, confirming successful nitridation and the formation of a passive oxide layer for corrosion protection.

The deposited coating exhibited exceptional multifunctional performance. Contact angle measurements revealed a transition from hydrophilic to hydrophobic behaviour, where the water contact angle increased from 68.31 ± 1.21° for uncoated NAB to 135.32 ± 2.31° for coated NAB. Nanoindentation analysis indicated a hardness of ~37.14 GPa, attributed to hard nitride phase, grain refinement and lattice distortion. Tribological analysis revealed improved wear resistance, while the electrochemical study demonstrated nearly threefold enhancement in corrosion resistance under simulated marine conditions. The combined enhancement in hardness, hydrophobicity, wear resistance, and corrosion protection shows the potential of Ni-doped chromium nitride coatings for marine applications. The synergistic interaction between the dense nitride matrix and passive surface oxide restricted electrolyte penetration and material degradation, improving the reliability of NAB components exposed to harsh marine environments.

TF-ThP-13 Hydrogen-Manipulated Atomic Layer Epitaxy of Titanium Nitride for Superconducting Devices, ***Yi-Hsun Chen***, University of Queensland, Australia; *Miin-Jang Chen,* National Taiwan University, Taiwan; *Peter Jacobson, Arkady Fedorov,* University of Queensland, Australia

Advanced epitaxy techniques have become essential for superconducting quantum circuits due to their ability to fabricate high-quality and low-loss superconductors. Atomic layer deposition, which provides precise layer-by-layer growth, is widely adopted in advanced silicon manufacturing for complex 3D architectures, such as FinFETs and gate-all-around transistors. In this study, we investigate the structural and electrical transport properties of titanium nitride (TiN) thin films grown by hydrogen-manipulated atomic layer epitaxy (HM-ALE). Our twinned TiN film exhibits semi-coherent epitaxy with negligible oxide content, confirmed by synchrotron-based grazing-incidence wide-angle X-ray scattering (GIWAXS) and X-ray photoelectron spectroscopy, and X-ray absorption spectroscopy. Electrical transport measurements on Hall bar devices show a superconducting transition temperature of 2.2 K and a kinetic inductance of 15 pH/sq. Moreover, the superconducting coherence length of our TiN thin films is estimated to be 14.6 nm, comparable to the crystal coherent length measured by GIWAXS, suggesting that its fundamental superconducting properties may be correlated with the twinned structure. Our findings highlight HM-ALE as a promising epitaxial method for superconducting quantum research and applications.

TF-ThP-14 Thermal Degradation of ZIF-8 Thin Films in Vacuum, ***Eliseo Perez Gomez***, Stony Brook University/Brookhaven National Laboratory; *Pragya Parihar,* University of Minnesota, USA; *Mueed Ahmad,* Stony Brook University/Brookhaven National Laboratory; *J. Ilja Siepmann,* University of Minnesota, USA; *Michael Tsapatsis,* Johns Hopkins University; *J. Anibal Boscoboinik,* Stony Brook University/Brookhaven National Laboratory

Zeolitic imidazolate framework-8 (ZIF-8) is a promising candidate for advanced technological applications, including gas separation membranes, chemical sensors, and microelectronic devices. For many of these applications, thin film morphology is the most appropriate configuration, where defining critical operational limits like thermal stability is essential. However, while bulk ZIF-8 powder stability is well-documented, the thermal thresholds and structural degradation pathways of substrate-supported thin films under vacuum remain unexplored. Here, we track this degradation pathway using in situ IRRAS on a gold-supported film continuously heated under vacuum from 575 to 775 K. The framework remains structurally intact up to 700 K, followed by an abrupt, concurrent collapse of all characteristic vibrational modes at higher temperatures. This process was complemented by evaluating identically prepared parallel films via ex situ SEM, GIXD, and XPS. Interestingly, comparing these workflows demonstrates that the ambient air exposure encountered during ex situ analysis lowers the film's apparent stability threshold, inducing earlier structural collapse and severe film cracking. These results define a practical vacuum operating window of ≤ 700 K for the present ZIF-8 thin films and highlight the importance of maintaining controlled environments after activation.

TF-ThP-15 Ion Implantation and Ozone-Assisted Growth for Engineering Transport in CdO Thin Films, ***Amanda Ashby***, *Maxwell Tolchin,* Pennsylvania State University; *Bhaveshkumar Kamaliya,* McMaster University, Canada; *Angela Cleri,* Pennsylvania State University; *Youngji Kim,* Vanderbilt University; *Morvarid Ghorbani,* McMaster University, Canada; *Anton Ievlev,* Oak Ridge National Laboratory; *Nabil Bassim,* McMaster University, Canada; *Joshua Caldwell,* Vanderbilt University; *Jon-Paul Maria,* Pennsylvania State University

Cadmium oxide (CdO) thin films engineered by reactive radio-frequency–coupled high-power impulse magnetron sputtering (RF-HiPIMS) offer a versatile platform for infrared quantum photonics due to their highly tunable optoelectronic properties. In intrinsic CdO, electrical transport is dominated by native shallow donors in the form of oxygen vacancies ($V_o^{\bullet\bullet}$), which act as the primary source of free electrons and strongly influence mobility through ionized impurity scattering. As a result, unintentionally doped (UID) CdO routinely exhibits carrier concentrations of 1.6–3.5 × 10^{19} cm^{-3} with mobilities ranging from 235–290 $cm^2V^{-1}s^{-1}$, while extrinsically doped CdO incorporating aliovalent dopants demonstrates carrier concentration tunability from 0.15–5 × 10^{20} cm^{-3} with peak mobilities that can exceed 450 $cm^2V^{-1}s^{-1}$.This work investigates two methods for modulating CdO optoelectronic properties: ozone-assisted growth and localized ion implantation doping. Because formation energy and charge state of oxygen vacancies are highly sensitive to the oxidation environment, ozone-assisted deposition is explored as a method for suppressing oxygen-vacancy defects and improving carrier transport in both UID and RF-HiPIMS doped CdO films. Preliminary results show ozone-assisted UID CdO achieving mobilities near 330 $cm^2V^{-1}s^{-1}$ while maintaining low optical loss.Using a focused ion beam scanning electron microscope (FIB-SEM), 30 keV gallium-ion (Ga^+) implantation is employed to produce shallow donor-doped CdO at ion doses ranging from 10^{14} to 10^{16} ions/cm^2. Broad-beam indium- (In^+), fluorine- (F^+), and chromium- (Cr^-) ion implantation at 165, 35 and 60 keV, respectively, are also explored as an additional ion implantation approach. Varying incidence angles, ion doses, and annealing conditions prove to be suitable parameters to modifying CdO transport behavior in spatially and spectrally coherent plasmonic architectures. Ongoing work focuses on understanding the origin of the mobility enhancement through

oxygen vacancy healing, ionized impurity scattering, and microstructural evolution under highly oxidizing growth conditions.

TF-ThP-16 Molecular Dynamics Study of Amorphous Carbon Film Growth on Si (100): Effects of Incident Energy and Substrate Temperature, ***Jhonatan Gil Romero***, *Kenneth Lathrum, Seonhee Jang,* University of Louisiana

Amorphous carbon (a-C) films are widely studied as protective coatings for micro- and nanoelectromechanical systems (MEMS/NEMS), biomedical components, and engineering surfaces prone to wear or corrosion. Their hardness, friction, chemical stability, and optical/electronic response are highly tunable through the sp^2/sp^3 bonding structure. For silicon-based coatings, these properties depend on energetic carbon penetration, intermixing with the substrate, and relaxation into sp^2 or sp^3 bonded networks. This study uses molecular dynamics (MD) to investigate how incident carbon energy and substrate temperature govern a-C film growth on Si (100).

MD simulations were performed using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) with the Tersoff potential for C–C, C–Si, and Si–Si interactions. A diamond-cubic Si (100) substrate was modeled with fixed, thermostat, and free regions. A total of 3500 carbon atoms were deposited along the surface normal over 7 ns, followed by structural relaxation. Two primary parameter sets were evaluated: (1) incident carbon energy from 1 to 100 eV at 300 K, and (2) substrate temperature from 300 to 1200 K at a fixed incident energy of 40 eV. The resulting films were characterized by depth-resolved atomic distribution profiles, radial distribution functions, coordination-based $sp^1/sp^2/sp^3$ fractions, layer thicknesses, and density profiles.

The results show that incident energy controls the balance between surface film growth and Si–C intermixing. As energy increased from 1 to 100 eV, the interlayer thickness increased from 5.99 to 46.26 Å, while the stable carbon growth layer decreased from 33.60 to 11.11 Å. The strongest diamond-like character was observed at 40 eV, where the film reached the maximum sp^3 fraction of 26.90% and maximum density of 2.54 g cm^{-3}. Low incident energy limited carbon penetration and favored surface adsorption, while higher energy led to excessive penetration and partial sp^3-to-sp^2 rehybridization. On the other hand, substrate temperature primarily controlled post-impact relaxation. At 40 eV, increasing the temperature from 300 to 1200 K broadened the interlayer from 18.68 to 30.28 Å, reduced the stable growth region from 19.23 to 15.59 Å, decreased the sp^3 fraction from 26.90% to 17.32%, and increased the sp^2 fraction from 66.27% to 78.84%.

These findings demonstrate that achieving dense a-C growth on Si requires balancing subplantation-driven densification against relaxation. An incident energy of 40 eV provides the optimal deposition window for tetrahedral bonding, while elevated substrate temperature accelerates graphitization and interfacial broadening.

TF-ThP-17 Effect of Metal Precursor Size on Structural and Dielectric Properties of Terpineol-Doped Ald al2o3 for Low-κ Materials, ***Sovendo Talapatra***, *Nicholas Strandwitz,* Lehigh University

Research on low-κ dielectric materials is gaining significant importance in overcoming capacitance delays that arise from shrinking dimensions of integrated circuits. Herein, we will report the structural and dielectric properties of terpineol-doped Al_2O_3 films, where terpineol acts as a sacrificial agent or porogen, leaving porosity in the films after post-deposition annealing treatment. Terpineol-doped films were deposited by atomic layer deposition (ALD), and the modification of the film porosity was done by introducing a terpineol pulse in between the metal precursor and co-reactant, H_2O. The choice of metal precursor influences the porosity generation in the film because of the steric hindrance and reactivity of the precursor. Three metal precursors, trimethylaluminum (TMA), tris(dimethylamido) aluminum (III) (TDMAAl), and aluminum tri-sec-butoxide, will be used to study the density and dielectric constant of the films. X-ray reflectivity will be used to measure the density of the films. Initial results showed the density of terpineol-doped films with TMA decreased by ~17% from ALD Al_2O_3, whereas for TDMAAl, the density decreased by about ~27%. The dielectric constant of the films will be measured using capacitance-voltage measurement. For as-grown terpineol-doped films, the initial measurement also showed dielectric constants as low as 4 compared to a value of ~7 for ALD-grown Al_2O_3. Our work shows that incorporating small molecule inclusions during ALD is a useful strategy for growing porous, low-κ thin films while still retaining precise thickness control and conformality afforded by ALD.

TF-ThP-18 Vapor-Phase Synthesis of Fused Copper Porphyrin Thin Films for Highly efficient Electrochemical Nitrate Reduction to Ammonia, ***Mohammad Arham Khan,*** University of Nebraska-Lincoln, USA*; Tan Zhang,* University of Pennsylvania*; Drialys Cardenas-Morcoso,* Luxembourg Institute of Science and Technology (LIST), Luxembourg*; Hamidreza Mohajeri Khorasani, Syed Ibrahim Gnani Peer Mohamed,* University of Nebraska-Lincoln, USA*; Andrew M. Rappe,* University of Pennsylvania*; Nicolas D. Boscher,* Luxembourg Institute of Science and Technology (LIST)*; Siamak Nejati,* University of Nebraska-Lincoln, USA

Electrochemical nitrate reduction to ammonia (eNO_3RR) has emerged as a promising route and sustainable alternative to conventional ammonia production. However, its practical implementation remains limited by poor selectivity, the competing hydrogen evolution reaction, and insufficient long-term stability, particularly at industrially relevant current densities (>300 mA cm^{-2}). Here, we report conjugated microporous polymer films based on molecular copper-porphyrin tapes as heterogeneous electrocatalysts for nitrate-to-ammonia conversion. The electrodes are prepared by the solvent-free oxidative polymerization of phenyl-substituted Cu-DPP and mesityl-substituted Cu-DMP directly on carbon paper, producing binder-free catalytic coatings with extended conjugated networks. The pCuDPP-coated electrode reaches a current density of 590 mA cm^{-2} at -0.78 V vs RHE and an ammonia production rate of 26.86 mg h^{-1} cm^{-2} (287.7 mmol h^{-1} mg_{cat}^{-1}) at -0.58 V vs RHE, this represents one of the highest reported ammonia production rates for eNO_3RR using a polymeric electrocatalyst. It also maintains stable activity for 15 h at 250 mA cm^{-2} and for six days at 50 mA cm^{-2}. SEM-EDX mapping confirms that copper remains uniformly distributed across the electrode before and after electrolysis, while high-resolution XPS indicates that Cu(II) sites are largely preserved after operation, demonstrating robust structural stability. In comparison, pCuDMP shows lower activity, reaching 230 mA cm^{-2} at -0.78 V vs RHE and an ammonia production rate of 12.5 mg h^{-1} cm^{-2} (134.74 mmol h^{-1} mg_{cat}^{-1}) at -0.68 V vs RHE. This reduced performance highlights the importance of precursor molecular structure in controlling the electrocatalytic activity of catalysts prepared by oxidative polymerization. DFT calculations show that the phenyl substituents in pCuDPP remain in-plane with the porphyrin backbone, promoting extended π-conjugation, electronic delocalization, and improved charge transport. In contrast, the bulkier mesityl substituents present in pCuDMP twist out of plane because of steric hindrance, disrupting conjugation and limiting electronic conductivity. This nonplanar geometry may also restrict nitrate adsorption near the catalytic Cu sites, contributing to lower nitrate to ammonia activity. These results highlight substituent-controlled molecular geometry as an important design principle for developing high-rate conjugated porphyrin electrocatalysts for sustainable ammonia synthesis.

Keywords: Electrochemical nitrate reduction (eNO_3RR), Porphyrin-based catalysts, electrocatalyst, energy, Electrocatalysis, density functional theory (DFT).

TF-ThP-20 Effective Barrier for Chronic Implantable Device Encapsulation with Tri-Layer HfO2/Al2O3/HfO2 with Atomic Layer Deposition, *Rahul Manna, Hyeongjin Jo, Martin Niemiec, Fatih Bayansal,* ***Necmi Biyikli***, *Kyungjin Kim,* University of Connecticut

The long-term reliability of chronic implantable devices is fundamentally limited by the encapsulation layers to withstand the ion-rich harsh environment of the human body. Single-layer thin films often fail due to intrinsic pinhole defects or hydrothermal degradation. This study investigates a tri-layer nanolaminate strategy employing $HfO_2/Al_2O_3/HfO_2$ deposited with atomic layer deposition (ALD). By depositing the Al_2O_3 layer between two chemically resilient HfO_2 layers, a synergistic barrier that inhibits ion diffusion and prevents moisture ingress is created. To assess the barrier properties of the proposed tri-layer structure, monolayer of Al_2O_3 and HfO_2 samples were prepared.

Tri-layer $HfO_2/Al_2O_3/HfO_2$ thin films with a total thickness of 60 nm were deposited on 4 µm thick polyimide (PI) substrates at 100°C. Polyimide 2610 was first spin-coated onto a silicon wafer and thermally cured. HfO_2 layers were deposited using tetrakis(dimethylamido)hafnium (TDMAH) and water, while Al_2O_3 layers were deposited using trimethylaluminum (TMA) and H_2O. Each oxide layer was deposited to a thickness of ~20 nm. Growth-per-cycle (GPC) values of ~1.6 and ~1.0 Å were obtained for HfO_2 and Al_2O_3, resulting in an average GPC of ~1.4 Å/cycle for the tri-layer stack. Following deposition, the coated PI films were released from the wafer for characterization and testing.

Mechanical performance of the deposited films was evaluated through in situ tensile testing to quantify elastic modulus, crack onset strain, crack

density, fracture toughness, and interfacial shear strength. In addition, water vapor transmission rate (WVTR) measurements were performed according to ASTM F3299 to compare the moisture barrier performance of HfO_2, Al_2O_3, and $HfO_2/Al_2O_3/HfO_2$ coatings. Further, sorption testing with DI water was performed by submerging coated films at 37°C and periodically measuring changes in mass. For sorption studies, films were deposited on commercially available 25.4 µm Kapton HN substrates suspended within the ALD chamber to achieve conformal 3D encapsulation with full surface coverage.

We will present results that provide important insights into the viability and advantages of tri-layer $HfO_2/Al_2O_3/HfO_2$ thin films for encapsulation of chronic implantable devices. The proposed precision tri-layer coating demonstrated enhanced moisture barrier performance with improved mechanical robustness, including resistance to cracking and delamination. These combined properties indicate strong potential for long-term reliability in flexible and implantable biomedical device applications.

TF-ThP-21 Vapor-Phase Deposition of Ultrathin Porous Membranes for Organic Solvent Nanofiltration, ***Shadi Motamed***, *Mohammad Arham Khan,* University of Nebraska-Lincoln*; Hesam Jafarian,* University of Alabama*; Syed Ibrahim Gemini Peer Mohammad,* University of Nebraska-Lincoln*; Mostafa Dadashi Firouzjaei,* University of Alabama*; Mona Bavarian, Siamak Nejati,* University of Nebraska-Lincoln

Creating hybrid, organic/inorganic, and polymeric thin films using vapor-phase approaches has emerged as a powerful strategy for fabricating ultrathin functional coatings with precise control over thickness, porosity, and interfacial chemistry. Applying these approaches to membrane fabrication offers new opportunities to engineer solvent-resistant separation layers with high permeance, tailored selectivity, and robust stability in harsh organic solvent environments. Here, we introduce a novel three-layer membrane architecture consisting of a robust porous support, an intermediate porous polymeric layer formed by oxidative polymerization of tetra(4-aminophenyl)porphyrin (TAPP), and an ultrathin selective top layer fabricated via vapor-phase deposition of TAPP, interfacially crosslinked with trimesoyl chloride through stable amide linkages. This unique architecture combines intrinsic porosity, molecular sieving, and excellent chemical resistance. The resulting membranes demonstrate superior performance, achieving dye rejections exceeding 96% for challenging industrial dyes ranging from approximately 300 to 900 $g \cdot mol^{-1}$. The prepared membranes had a permeability value of 7.5 $L \cdot m^{-2} \cdot h^{-1} \cdot bar^{-1}$ and offered stable operation across various polar and nonpolar solvents. By combining oxidative and interfacial polymerization strategies in a multilayer design of membranes, we demonstrate a powerful approach to develop membranes with tailored selectivity, high permeance, and robust solvent compatibility for challenging separations.

TF-ThP-22 Nanofluidic Electrokinetic Analysis of the Isoelectric Point of Thin Films Deposited in Solid State Nanopores using Atomic and Molecular Layer Deposition, ***Jay Werner***, *Akira Pfeffer, Jens Gundlach, David S. Bergsman,* University of Washington

Solid state nanopores are commonly fabricated by etching through low isoelectric point (IEP) materials such as silicon dioxide or silicon nitride. As a result, these pores often have a negative charge around pH 8 (physiological pH). However, it is often desirable in biosensing applications to have the surfaces of microfluidic devices be positively charged to improve protein adhesion and promote crosslinking. Though a neutral or positive charge coating can be applied a surface through an amine-terminated self-assembled monolayer (SAM) such as 3-(aminopropyl) triethoxysilane, this approach may result in uncontrolled polymerization or an unstable film structure.

An alternative strategy for changing surface charge is to use atomic layer deposition (ALD) or molecular layer deposition (MLD),which are cyclic processes for depositing a thin film via exposure to reactive precursors in the vapor phase. These processes are attractive options for modifying the size and/or chemistry of solid state nanopores because they are highly precise and conformal. However, most water-stable inorganic thin films and organic polymer coatings that can be created through ALD and MLD similarly exhibit IEPs below 5. As a result, producing neutral or positively charged nanopore surfaces at physiological pH remains a significant challenge in nanopore surface engineering.

In this work, we investigate several new ALD/MLD coatings as candidate high-IEP surface modifications for solid state nanopores, comparing hafnium oxide to polyureas composed of 2,4-toluene diisocyanate (TDIC) combined with substituted diamines such as bis(2-aminopropyl)(methyl)amine (BAPMA) and 2,6-diaminopyridine (DAP). To measure surface charge, nanofluidic electrokinetic characterization (NEC) techniques were used, which involves the analysis of the ion current rectification behavior, surface conductance, and streaming current. With the exception of streaming current, which can be performed on flat surfaces, these characterization techniques involve properties which are unique to the nanofluidic nature of the system, offering a unique characterization tool for gathering surface properties. Overall, this work highlights the potential of ALD/MLD for surface modification of solid state nanopores to produce stable, high IEP surfaces as well as the utility of analyzing the breadth of physical phenomena present in a nanofluidic electrokinetic experiment.

TF-ThP-23 4h-Sic Schottky Barrier Diode Surface Passivation Based on o2/n2 Icp Plasma for Oxynitridation, ***Renato Beraldo***, UNICAMP, Brazil

In order to improve the surface quality of 4H-SiC for Schottky barrier diodes (SBDs), plasma oxynitridation (PON) was carried out on substrates using an ultrathin nickel film of 2 nm as the Schottky contacts, deposited via electron-beam evaporation. This passivation technique, until this publication, has no evidence in the literature for Schottky barrier devices based on 4H-SiC. Two pairs of devices were fabricated. In the first pair, the devices were fabricated following the ohmic contact formed using 100 nm of nickel, and the samples underwent the PON process for 20 minutes executed using an ICP-LAM, creating a 5 nm thick NyOx layer. Following this, the samples were annealed at 950 °C for 5 minutes, while for the second pair, the samples were not exposed to PON. Subsequently, a dip in HF 10% for 20 seconds was carried out to remove the passivation layer. A 2 nm layer of Ni was deposited on the top side to form the Schottky contact, and the devices were subjected to an annealing temperature of 650 °C. To create the metallic contact, 300 nm of Al was deposited by thermal evaporation and patterned into pads of 2 mm diameter without any shielding structure, finishing with a thermal treatment at 450 °C for 5 minutes. The influence of PON passivation on electrical performance and interface quality was evaluated. Electrical characteristics were measured using a parameter analyzer, revealing the rectification ratio and density of surface states. Also, the junction morphology was analyzed by high-resolution transmission electron microscopy (HRTEM).

The electrical results showed a difference between the passivated samples and unpassivated samples, where the passivated samples showed a rectification ratio about 6 times higher than the unpassivated ones. The leakage current at –5 V was 2 pA for passivated samples and 10 µA for unpassivated samples. Also, these results showed a shift in Schottky barrier height (SBH) values, besides improving the ideality factor to a maximum value of 1. The passivated samples also showed a difference between the surface states, where in this case, the surface states kept the same values as the unpassivated samples; however, the values shifted slightly far from the Ec band, possibly caused by band bending due to SBH surface density change.

For upcoming analysis, devices will receive a shielding structure for testing under temperature variation, and breakdown voltage tests will be performed to check reliability. Furthermore, characterizations such as XPS and Raman will be conducted for further investigation of the surface improvements achieved.

TF-ThP-24 Superior Radiation Tolerance and Annealing Recovery of a-IGZO TFTs Under Gamma Irradiation, ***Juwon Lee***, *Jin-Hong Park,* Sungkyunkwan University, Korea

Amorphous indium–gallium–zinc oxide (a-IGZO) is widely explored for advanced thin-film applications due to its high carrier mobility and uniform amorphous phase. While its basic electrical properties are well-understood, the defect generation mechanisms and interface stability of oxide semiconductor thin films under high-energy ionizing radiation require deeper investigation. This study explores the radiation tolerance and defect dynamics of a-IGZO thin-film transistors (TFTs) compared to low-temperature polycrystalline silicon (LTPS) TFTs under gamma-ray exposure.

Devices were irradiated with a 60Co gamma-ray source at total doses of 0, 0.5, and 1 kGy. Evaluating the electrical parameters provided direct insights into the generation of interface states and trapped charges within the thin films. For the a-IGZO TFTs, the subthreshold swing (SS) remained essentially constant at ~0.09 V/dec despite the irradiation, indicating that the generation of new interface trap states at the dielectric/channel boundary was heavily suppressed. The threshold voltage (Vth) exhibited only a slight negative shift ($\Delta Vth \approx -0.87$ V), suggesting a strong resilience of the amorphous oxide network against radiation-induced oxygen vacancy generation and positive charge trapping.

Conversely, the LTPS TFTs experienced drastic degradation. The Vth shifted negatively by −4.24 V, and the SS deteriorated significantly from 0.22 to 0.81 V/dec. This implies severe structural damage, likely due to the massive generation of deep trap states at the poly-Si grain boundaries and the gate dielectric interface.

Post-irradiation annealing further differentiated the materials: the amorphous network of a-IGZO allowed for partial structural relaxation and recovery of initial characteristics, whereas the crystalline damage in LTPS was largely irreversible under the same thermal budget. These findings underscore the superior defect immunity and interface stability of a-IGZO thin films in extreme environments.

TF-ThP-25 Substrate Oxidation in Atomic Layer Deposition (ALD): Role of Temperature and Precursor Selection, ***Nathan Younce***, UCF (CREOL)

We investigate how ALD oxidizer chemistry and chamber temperature impact the optical and morphological stability of metal/dielectric superlattices targeting epsilon-near-zero (ENZ) photonics. ENZ multilayers rely heavily on high-quality, continuous metal/dielectric interfaces, where increased roughness, oxidation, or aggregation increases effective extinction and dissipative losses, degrading the field enhancement and resonant behavior required for ENZ operation. Our superlattices alternate ~10 nm thermally evaporated metallic layers (Ag, Al, or 90/10 Ag/Al alloy) with ~1 nm ALD Al_2O_3 deposited from trimethyl-aluminum (TMA) using H_2O, O_3, or *t*-BuOH oxidizing co-reactants. Following ALD growth, multilayer ellipsometric responses become poorly described by otherwise reliable isolated (pre-ALD) metal film models, suggesting direct interaction between ALD processing conditions and the underlying metallic layers. To isolate these effects, we omit TMA and pulse oxidizer only under conditions typical of dielectric growth (~100 °C for H_2O/O_3 and ~280 °C for *t*-BuOH). Optical constants (n,k) and thicknesses were characterized through spectroscopic ellipsometry and transmission measurements, while morphology was characterized via SEM. We observe that oxidizer selection strongly impacts metallic optical behavior, with “harder” oxidizers producing the greatest optical degradation (O_3 > H_2O > *t*-BuOH). However, the comparatively “soft” *t*-BuOH chemistry requires elevated process temperatures to maintain a viable ALD growth window, introducing competing thermal aggregation in Ag films. Elevated temperatures drive Ag aggregation that increases with both temperature and exposure duration, while oxidizer chemistry primarily governs oxidation-driven optical degradation. Pure Al exhibits strong morphological stability but remains optically unfavorable for ENZ applications due to its comparatively high extinction coefficient and associated dissipation. Ag/Al alloy films demonstrate substantially improved aggregation resistance while largely preserving Ag-dominated optical behavior. Although elevated-temperature *t*-BuOH processes do not universally outperform alternative chemistries, the reduced optical degradation associated with “soft” oxidizer exposure, combined with the aggregation resistance of Ag/Al alloy films, shows strong promise for maintaining optical and morphological stability. Rather than constructing full ENZ devices directly, this work identifies degradation mechanisms and practical ALD processing windows necessary for reliable fabrication of ENZ-oriented metal/dielectric superlattice metamaterials.

The Future of Temperature Sensing
Room Ballroom A - Session TS-ThP
The Future of Temperature Sensing, Poster Session

TS-ThP-1 Progress Towards Simplified Measurement Schemes for Optomechanical Quantum-Correlation Thermometers, ***Daniel Barker***, National Institute of Standards and Technology; *Ana Rakonjac,* Measurement Standards Laboratory, New Zealand; *Biswarup Guha, Kartik Srinivasan, Nikolai Klimov,* National Institute of Standards and Technology; *Thomas Purdy,* University of Pittsburgh

Optomechanical thermometry is a promising route to portable primary thermometry from room temperature down to a few kelvin. Quantum noise arising from the zero-point motion of a mechanical oscillator can provide *in situ* calibration of the oscillator’s thermal motion. In an optomechanical system, the resonator undergoes thermal Brownian motion, driven motion from the light in the cavity, and optomechanical backaction. Noise correlators can be employed to separate thermal and quantum signals, thereby forming a quantum-correlation thermometer and enabling primary temperature measurements. The optomechanical cavity is chip-scale, which allows for integration with other chip-scale sensors. Fiber-optic readout makes optomechanical thermometers suitable for a variety of applications, including those in which conductive sensor leads cannot be used. However, the measurement precision of quantum-correlation thermometers is not presently competitive with existing secondary thermometers, and reducing systematic uncertainties is an ongoing challenge.

We use a waveguide-coupled GaAs nanobeam resonator with an optical resonance in the telecom wavelength range and a mechanical resonance around 2.6 GHz as our optomechanical thermometer. The optomechanical resonator is installed in a low-vibration cryostat along with a resistive cryogenic thermometer that independently monitors the temperature. Our detection scheme utilizes a double-mix-down technique, where optical carrier sidebands generated by an electro-optic modulator mix with the mechanical signal in the resonator and are then combined with a local oscillator in a heterodyne measurement. This method requires only a single channel for data acquisition, with subsequent phase-sensitive signal processing performed entirely in software. We report on progress towards primary thermometry using this simplified measurement scheme and provide an outlook for future work.

TS-ThP-2 Progress Towards Doppler Thermometry in Microfabricated Vapor Cells, ***Ryan Johnson***, *Yu-Ting Chen, Sean Bresler, Erin Adkins, Matthew Hummon, Benjamin Reschovsky, Vladimir Aksyuk, Stephen Eckel, Tobias Herman, John Kitching, Daniel Barker,* NIST

We report on our effort to develop Doppler thermometers using microfabricated atomic vapor cells. The Doppler broadening of spectral lines relates gas temperature to physical constants and immutable gas properties, enabling primary thermometry. We present measurements of the Doppler broadening in a microfabricated rubidium vapor cell from 25 °C to above 100 °C. The accuracy of the fitted Doppler temperature is limited by parasitic etalons in the vapor cell. To reduce the temperature uncertainty, we are implementing improved physical models of the etalon transmission. We also discuss prospects for improving the accuracy and increasing the operating temperature range of atomic Doppler thermometers using microfabricated cesium and ytterbium vapor cells.

TS-ThP-3 Thermal Noise Measurements in a Cavity Electro-Optic System, ***Griffin O'Neal-Freeman***, University of Pittsburgh

Resonant electro-optic transducers are a promising platform for high-sensitivity microwave detection and quantum frequency conversion. By utilizing a fully-resonant, all-dielectric architecture, we achieve high photon-number conversion efficiencies, enabling the up-conversion of thermal microwave photons into the optical domain. In this work, we explore the application of these transducers as high-precision temperature sensors. We are interested in investigating Raman sideband asymmetry thermometry, a technique employed in spectroscopy, fiber optic sensing, and cavity optomechanics to make calibrated temperature measurements. We present preliminary experimental results demonstrating the optical detection of the thermal occupation of a 16GHz microwave mode with a signal-to-noise ratio of a few. Ongoing efforts focus on mitigating material losses and optimizing resonator geometry to enhance coupling and further suppress technical noise. Ultimately, this electro-optic platform offers a path toward precision temperature sensing, quantum-limited radiometry and quantum communication.

TS-ThP-4 The Recent Advancement of Crystalline Core and Crystalline Cladding Sapphire Fibers for Extreme High Temperature Environment Sensing, ***Shizhuo Yin***, Penn State University

In this paper, we report the recent progress of crystalline core and crystalline cladding sapphire fibers and its potential applications for extreme high temperature >1500 oC sensing. In particular, we will discuss the single-transverse-mode clad sapphire fiber.

TS-ThP-5 Chip-Scale Photonic AC –DC Thermal Transfer Device, ***Pavan Challa***, *Kevin Douglass, Michal Chojnacky, Thinh Bui, Tam Duong,* NIST-Gaithersburg; *Michael Sherman, Dorin Shapira, Leeya Engel,* Technion Israel Institute of Technology, Israel; *Stefan Cular,* Howard Community College; *Nikolai Klimov,* NIST-Gaithersburg

We present a chip-scale photonic ac–dc thermal transfer device that provide an alternative to conventional multijunction thermal converters (MJTCs) for establishing the traceability link between dc electrical units and practical ac voltage and current measurements. While MJTCs offer the highest accuracy available today, they exhibit intrinsic ac–frequency–dependent transfer errors arising from parasitic capacitive coupling between the resistive heater and the thermocouple array. To overcome these limitations, we introduce an integrated photonics-based architecture

that replaces the thermoelectric sensor with an electrically passive, silicon photonic microresonator thermometer – the Standard Photonic Thermometer (SPoT). In the SPoT sensor, Joule heating under ac or dc excitation produces a highly sensitive shift in the optical resonance frequency. Because the optical readout is electrically isolated from the heater, the device measures Joule-heating-induced temperature rise without capacitive pickup, thus eliminating fundamental error mechanics present in MJTC-based thermal-transfer metrology.

We report the first prototype of photonic ac–dc thermal transfer standard device, termed the thermal-transfer SPoT (T-SPoT). The device integrates a waveguide-coupled SPoT sensor with an on-chip microheater and is interrogated using resonance-scanning optical readout. Ac–dc difference measurements are performed as a function of ac frequency at fixed voltage and benchmarked against a calibrated MJTC standard using a drift-rejecting triplet measurement sequence. The initial T-SPoT results demonstrate performance consistent with expectations for a first-generation photonic thermal transfer device and reveal clear pathways for further improvement through enhanced optical-frequency readout and thermally optimized device architectures. These results establish a foundation for next–generation photonic ac–dc transfer standards with improved robustness, scalability, and long–term stability.

Undergraduate Poster Session
Room Ballroom A - Session UN-ThP
Undergraduate Poster Session

UN-ThP-1 Deposition and Annealing of RF-Sputtered, Thin Film Gallium Oxide, ***Aria Lindberg***, *Jackson Anderson,* University of Vermont

Gallium oxide (Ga_2O_3) is a polymorphic semiconductor material whose β phase demonstrates potential for applications in power electronics due to high Johnson and Baliga figures of merit. When compared to other materials commonly used in piezoelectric MEMS, metastable ε-Ga_2O_3 demonstrates a promising electromechanical coupling coefficient (k^2) — highlighted in Table 1. Despite this, ε-Ga_2O_3 remains less studied than β-Ga_2O_3, which has been grown using melt, MOCVD, and PVD techniques.

This study presents initial results of the effects of different RF sputtering and annealing conditions on the crystal characteristics of thin-film Ga_2O_3 on <111> silicon substrates towards the goal of determining ideal temperature, gas type and flow ratio, and RF power values contributing to ε-phase stabilization. The study follows the process shown in Fig. 1.

Films were sputtered from a Ga_2O_3 target in 32 sccm of Ar at 3 mTorr with 50W RF power for 2 hours (Fig. 2) and subsequently annealed in an air-ambient tube furnace at 500 to 900°C in 100°C steps for 30 minutes at temperature. These temperatures were chosen based on literature showing the transition of ε- to β-Ga_2O_3 around 800°C. Samples were characterized before and after annealing with spectroscopic ellipsometry shown in Fig. 3 and XRR shown in Fig. 4.

Ellipsometry results indicate a slight decrease in film thickness at sub-600°C anneals with rapid expansion at higher temperatures (Fig. 3); XRR fringe spacing (Fig. 4), in contrast, indicates thickness expansion across all anneal temperatures, while critical angle right shift indicates densification and increasing slope indicates increasing roughness. This is supported by AFM (Fig. 5), which demonstrates a change in surface roughness from 66.59pm RMS (unannealed) to 1.858nm RMS (900°C) while also revealing the polycrystalline nature of the annealed films. XRD measurement did not yield clean spectra, likely due to the disoriented polycrystalline nature of the films.

Following literature on successful deposition of ε-Ga_2O_3, future work will explore deposition at elevated temperatures, while also varying O_2/Ar gas mixture, substrate bias, and deposition rate to enhance ε-phase stability and crystallinity.

UN-ThP-2 Temperature-Dependent Behavior of TaN Thin Film Resistors, ***Joshua Dykas***, *Alex Zaccardi, Alexander C. Kozen,* University of Vermont

Tantalum Nitride (TaN) is a thin-film resistive material that is widely used in the semiconductor industry for its temperature stability and CMOS compatibility. However, stoichiometry and deposition process conditions can heavily influence resistive properties. Additionally, cross-wafer nonuniformities in materials composition or thickness can vary the electrical behavior of devices from the center to the edge of a wafer. We developed an automated temperature-dependent electrical characterization system to perform thin-film resistivity measurements of TaN films as a function of temperature from 50°C to 130°C. A custom-built Python program automates data collection, analysis, and real-time data plotting. 200 mm oxidized silicon wafers, subsequently coated in sputtered TaN were provided by GlobalFoundries (GF). These wafers were cleaved into 3 cm squares selected from the center, middle, and edge of each wafer for TCR measurements. The average TCR for 48 nm TaN is -371.4 ± 10.8 ppm/°C, meanwhile the TCR for 15 nm High-Nitrogen TaN is -1066 ± 52 ppm/°C. Our data indicates that higher concentrations of nitrogen and thinner films cause the resistive properties of TaN to be less stable with temperature. Notably, the center of both wafers exhibits lower TCR values than the middle or edges of the wafer, indicating radial nonuniformities related to TaN deposition conditions.

UN-ThP-3 Analyzing Hardness of Poly (Methyl Methacrylate) (PMMA) Infiltrated with Trimethyl Aluminum (TMA) Through Vapor Phase Infiltration (VPI), ***Annie Powell***, *Mark Losego, Ronan Neill,* Georgia Institute of Technology

This research seeks to understand how the hardness of poly (methyl methacrylate) (PMMA), a thermoplastic polymer, can be altered when it is infiltrated with an inorganic via vapor phase infiltration (VPI). In VPI, the polymer sorbs inorganic vapors into the bulk of the polymeric material, transforming it into an organic-inorganic hybrid material. The resultant hybrid materials are known to have properties that differ from their parent polymer. In this work, we examine the VPI of PMMA blocks with trimethylaluminum (TMA) vapors and water to form PMMA-AlOx hybrid materials. We study the effects of infiltration temperature, time, and number of cycles on the hardness of the material using a microhardness tester. Additionally, chemical changes to the composition and chemical structure of the material are studied with SEM-EDX analysis and FTIR spectroscopy.

The results of this experiment in Figure 1 show that when PMMA is infiltrated at 120 °C, hardness initially decreases and then steadily increases. We observe a decrease in Vickers' hardness from about 23.1 ± 0.6 to 10.9 ± 0.5 between the pure polymer and 3 hours of infiltration. The hardness then rises to 16.1 ± 0.2 after 10 hours of infiltration, which is still lower than the pure polymer. These results are surprising to us, given we nominally infiltrate the softer polymer material with a harder ceramic-like material. This phenomenon may be explained by chemical bond disruption in the hybrid that is softening the polymer upon infiltration. Additionally, there is visible chemical change in the sample, as they increase in amber color with longer hold times as shown in Figure 2. These chemical changes will be discussed more fully at my poster presentation.

UN-ThP-4 Exploring Feasibility of Raman Spectroscopy for Identification of Nb Oxides on NASA Devices, ***Dorian Davis***, *Femi Akinrinola, Mikel Holcomb,* West Virginia University

Niobium thin films are widely used for superconducting applications due to their low-temperature superconductivity and corrosion resistance. This makes them well suited for NASA detectors for astrophysics, and quantum computing. However, NASA believes that the formation of oxide phases on the thin films tends to cause variability in device performance. To better understand the origin of this variability, we aimed to characterize the oxide phases forming on the device surface. To this end, we sought to determine whether Raman spectroscopy is a reliable identification method, in comparison of other methods — such as XAS — are not as accessible as Raman can be. We suspected our signal was going to be small, so we chose to compare it to samples which had been annealed to promote oxide growth. We were able to identify Nb_2O_5 oxides on an annealed sample and had difficulty finding any oxides on the devices, using Raman. Our findings suggest that Raman is best used when a thin film has a greater concentration of surface oxides, and is not the optimal identification method for devices that tend to have low oxide content.

UN-ThP-5 Spectroscopic Ellipsometry of High-K Dielectrics, ***Alexander Zaccardi***, *Joshua Dykas, Alexander Kozen,* University of Vermont

Spectroscopic ellipsometry is a characterization technique used for analyzing the optical characteristics of high-k dielectric films in advanced semiconductor devices. Using the J.A. Woollam M-2000D spectroscopic ellipsometer, we characterized monolithic and nanolaminate dielectric layers composed of hafnium oxide, aluminum oxide, and silicon dioxide to investigate the relationship between film composition, structure, and dielectric performance. Through the utilization of Cauchy and B-spline fitting models, we extracted the refractive index and the extinction coefficient across ultraviolet to near-infrared wavelengths. We compared monolithic and nanolaminate dielectric film stacks to determine which configuration yielded the highest dielectric constant. Wafer mapping was

used to reveal nonidealities and nonuniformities in the varying layer stacks across a 200 mm substrate. Results demonstrate that hafnium oxide and aluminum oxide nanolaminate structures exhibit the highest dielectric constants, and increased concentrations of aluminum oxide may further improve the dielectric constant. Our results provide crucial insight into thin-film dielectrics suitable for next-generation semiconductor devices.

UN-ThP-6 An Electrodeposited Iridium Oxide pH Sensor for Ingestible Capsule Localization, ***Micheal York***, College of Southern Maryland; *Justin Stine,* University of Maryland, College Park

Gastrointestinal (GI) disorders, such as inflammatory bowel disease (IBD), are commonly diagnosed using invasive endoscopy and biopsy. Ingestible capsules have emerged as a minimally invasive alternative for GI monitoring, sampling, and targeted drug delivery. As these pill-sized devices traverse different GI regions, localization becomes essential for interpreting measurements within the appropriate physiological context. Therefore, scalable and low-cost pH sensing solutions are desired to complement existing capsule size and electronics. This work presents the integration of an iridium oxide (IrO2) pH sensor into an ingestible capsule prototype for measuring dynamic pH gradients in GI environments to classify sensor readouts (Fig. S1).

The pH sensor consists of screen-printed electrode (SPE) with platinum (Pt) working and counter electrodes and a silver (Ag) reference electrode. An electrodeposition solution was prepared following existing protocols. Briefly, iridium chloride was dissolved in DI water (5.5 mM) and stirred for 30 minutes, followed by addition of 0.5 mL hydrogen peroxide and stirring for 10 minutes before adding 0.25 g oxalic acid. The solution was adjusted to pH 10.5 with potassium carbonate, heated under a water bath for 5h, then stored at 4 °C until use. Electrodeposition was performed using an Interface 1010E benchtop potentiostat (Fig. S2). The SPE was submerged in solution, within an ice-water bath, and the Pt working electrode was modified using either (1) chronopotentiometry (CP) at 0.2 mA/cm2 for 100 s or (2) cyclic voltammetry (CV) from 0 V to +0.7 V at 50 mV/sec for 90 cycles (Fig. S2b).

IrO2 film formation was characterized using open circuit potential (OCP) measurements in pH 4.00, 6.86, and 9.81 buffer solutions for 60 s (Fig. S3a). Calibration curves were generated for each electrodeposition method (Fig. S3a,b). Linear fitting yielded sensitivities of 71.25 mV/pH (R2 = 0.9861) for the CV-pH sensor and 65.07 mV/pH (R2 = 0.959) for the CP-pH sensor (Fig. S3b). Solution pH was verified using a commercial pH meter (Nanbei Instrument) prior to testing. Sensor drift was evaluated in pH 4.00 buffer solution for 30 minutes, yielding 2.36 and 28.80 mV/hr, respectively. This showed that the CV-pH sensors showed superior film formation and performance compared to the CP-pH sensor. This work further demonstrates the integration of the IrO2 sensor with a high-impedance voltage follower (LTC6078) and analog front-end (AD5940) into an existing ingestible capsule prototype (Fig. S3c), while implementing embedded on-chip calibration to improve signal fidelity, and evaluating performance in simulated gastric and intestinal fluids.

UN-ThP-7 A Hybrid Energy-Harvesting Ingestible Capsule: Piezoelectric Harvester, ***Kristin Wiens***, *Izabella Tucker, Ian Jackson, Jenna Pratt, Anika Prasanna, Daniel Hutman, Abinezer Abate, Sydney Overton, Justin Stine, Reza Ghodssi,* University of Maryland, College Park

Advances in microelectromechanical (MEMS) research has enabled the development of non-invasive ingestible capsule devices for medical interventions in the gastrointestinal (GI) tract. Further ingestible device miniaturization is limited by the necessity for batteries to power them. Onboard energy harvesters present an alternative power method, reducing the footprint of the ingestible device. Gastric battery and chemical energy harvesters have shown promising results integrating into ingestible devices, but operation is limited to the stomach and prone to energy leakage. To overcome these limitations, we propose a hybrid energy harvesting system that enables chemical harvesting in the stomach and piezoelectric harvesting in the intestines, thereby extending the overall region of operation (Fig. S1).

Here, we report a piezoelectric energy harvester to convert mechanical, peristaltic motion within the intestines to electrical energy. The harvester utilizes polyvinylidene fluoride (PVDF) thin films, known for their excellent biocompatibility, flexibility, and piezoelectric properties. Multiple thin film configurations under controlled mechanical excitation were evaluated to maximize voltage output and prevent back charging between the PVDFs. Two thin films with isolated H-bridges had the highest voltage output of 85 mV (Fig. S2). Integration with an integrated circuit (IC) improved energy collection efficiency from the PVDFs by preventing premature voltage dissipation. Our findings support the feasibility of piezoelectric energy harvesting for microscale biomedical applications.

To facilitate testing, we are developing a simulated small intestinal model consisting of a silicone sleeve and actuators that apply a realistic pressure wave via an external pump to move the capsule prototype through the model (Fig. S3). Testing the piezoelectric harvester in the simulated model will enable characterization of voltage outputs from peristaltic forces in the microscale (18–62 mmHg). We anticipate the supplemental energy collection supplied from the piezoelectric harvester will counteract capacitor leakage and allow for a decrease in overall capsule size once scaled appropriately. Integrating the piezoelectric harvester with a chemical harvester will enable an ingestible self-powered system capable of sustained operation in the GI tract.

UN-ThP-8 A Hybrid Energy-Harvesting Ingestible Capsule: Electrochemical Harvester, ***Ian Jackson***, *Abinezer Abate, Daniel Hutman, Kristin Wiens, Izabella Tucker, Anika Prasanna, Jenna Pratt, Sydney Overton, Justin Stine, Reza Ghodssi,* University of Maryland, College Park

Advances in microelectromechanical (MEMS) research has enabled the development of non-invasive ingestible capsule devices for medical interventions in the gastrointestinal (GI) tract. Further ingestible device miniaturization is limited by the necessity for batteries to power them. Onboard energy harvesters present an alternative power method, reducing the footprint of the ingestible device. Gastric battery and chemical energy harvesters have shown promising results integrating into ingestible devices, but operation is limited to the stomach and prone to energy leakage. To overcome these limitations, we propose a hybrid energy harvesting system that enables chemical harvesting in the stomach and piezoelectric harvesting in the intestines, thereby extending the overall region of operation (Fig. S1). This work investigates the design trade-offs of electrochemical harvester electrodes for current generation within ingestible capsule form factors.

Previously reported chemical energy harvesters have been demonstrated, utilizing stomach acid to induce oxidation-reduction reactions, producing electric current that can be used to power an ingestible device. While these systems can generate electrical current, maintaining sufficient power output over the capsule's residence time in the stomach remains a challenge. To address this limitation, this work integrates both piezoelectric and chemical energy harvesters; each system can be independently optimized for maximum power output within its respective operating region and duration. Thus, the chemical harvester seeks to maximize power for the amount of time the capsule will spend in the stomach.

Optimizing the power generation of the chemical harvester entailed material selection and evaluation of electrode dimensions and size. Anode and cathode materials were examined using galvanostatic discharge across a 1kΩ load with a benchtop potentiostat. Based on the average power density, the electrochemical cell comprises a magnesium (Mg) anode and molybdenum (Mo) cathode and was assembled on a thin polyimide film with 4 mm spacing (Fig. S2). Characterization of the Mg-Mo harvester at varied surface area (i.e., 8, 16, 24 and 32 mm2) in simulated gastric fluid revealed that power density increased with increasing electrode size (Table S3); however plateau at the 4 mm x 4 mm size anode/cathode, which produces 0.219 mW/mm. Integrating the chemical harvester with a piezoelectric harvester will enable an ingestible self-powered system capable of sustained operation in the GI tract.

UN-ThP-9 Exploring Novel CVD Synthesis Routes for Enhanced Optoelectronic Properties of VS_2, ***Amari Gayle***, *M. K. Indika Senevirathna,* Clark Atlanta University

Vanadium disulfide (VS_2), a member of the transition metal dichalcogenides (TMDs) family, has gained considerable attention from researchers owing to its remarkable properties. These include metal-insulator transition behavior, room-temperature ferromagnetism, a unique layered structure, and metallic conductivity. Additionally, VS_2 can form highly crystalline materials. With advances in achieving a more precise structure of this semiconducting material, VS_2 nanomaterials have the potential to be the most efficient TMDs for various photonic and optoelectronic applications. Chemical vapor deposition (CVD) has proven to be an effective method for synthesizing two-dimensional materials. Its simple process, compatibility with industry standards, and capacity to produce high-quality crystals make it an excellent choice for both researchers and industrial producers. This study will investigate the optoelectronic behavior of VS_2 thin films synthesized on different substrates using CVD, building on and extending conventional growth techniques. It will determine the optimal growth conditions, with particular attention to substrate type, growth temperature,

and carrier gas flow rate. The properties of the resulting samples, including surface morphology, crystalline quality, Raman phonon modes, and bandgap characteristics, will be systematically studied as a function of substrate type, growth temperature, and carrier gas flow rate using Raman spectroscopy, photoluminescence (PL), and confocal laser scanning microscopy.

UN-ThP-10 Electrochemical Protonation of ALD Oxide Thin Films, ***Kaydence Delgado***, *Daniel MacAyeal, Alexander Kozen,* University of Vermont

Electrochemical Protonation of ALD Oxide Thin Films

Kaydence Delgado, Daniel J. MacAyeal, Alexander C. Kozen

University of Vermont, Department of Physics

Hydrogen incorporation in ultra-thin atomic layer deposited (ALD) oxide films is important for understanding macroscale properties such as water diffusion barrier performance, dielectric behavior, chemical reactivity, and electrical breakdown strength, and, critically, suitability as a barrier material in fusion reactors. However, accurately measuring hydrogen content in films thinner than 10 nm remains difficult using conventional surface science techniques. An alternative approach is to use electrochemical ion insertion/extraction to quantify exchangeable protons in ALD-grown oxide films using an aqueous system. We investigate the protonation behavior of ALD oxide films (Al2O3, ZnO, and Nb2O5) growth with TMA, NbEtOH, and DEZ as metalorganic precursors and H2O, t-BuOH, and O3 as oxidation precursors, and discuss how differences in oxidation precursor selection impact protonation behavior in these oxide films. We examine electrochemical reactions with cyclic voltammetry and discuss how ALD film thickness and oxidation precursor selection affects electrochemical response, proton insertion behavior, and ion-transport kinetics using cyclic voltammetry. Lastly, we will use Dunn–Trasatti analysis to extract protonation redox kinetics, giving us insight into the relationship between ALD film thickness, transport behavior, and ion insertion/deinsertion kinetics.

UN-ThP-11 ALD Silica for Surface Passivation of Porous Stainless Steel, ***Alexander Randall***, *Richard Vanfleet, Robert Davis,* Brigham Young University

Atomic layer deposition (ALD) could allow surface passivation of porous metals which could enable their use in molecular separation or purification processes, including liquid chromatography. We explored ALD passivation of porous stainless steel metal monoliths (“metalliths”) formed by powder sintering with the goal of passivating all exposed stainless steel surfaces including interior surfaces. In the ALD process, tris(dimethylamino)silane (3DMAS) and ozone precursors were used to coat the metallith pores with a thin film of silica. For comparison, trimethylaluminum and H_2O ALD was also performed on the metalliths. The resulting passivated metalliths were characterized with energy dispersive x-ray spectroscopy and scanning electron microscopy to determine the penetration uniformity, conformality, and thickness of the silica film.

UN-ThP-12 Fourier Denoising of the C Auger XPS Signal for Subsequent D-Parameter Calculation, ***Jonathan C. Nelson***, *Alvaro J. Lizarbe, B. Maxwell Clark, Matthew R. Linford,* Brigham Young University

X-ray Photoelectron Spectroscopy (XPS) of carbon-containing compounds requires peak and derivative analysis to find the percent hybridization (sp^2 versus sp^3 ratio) via the so-called D-parameter, which is the separation between the minimum and maximum of the first derivative of the carbon Auger spectrum. However, taking the derivative of raw spectral data can yield incorrect minima and maxima, distorting the D-parameter, because of high-frequency background noise. Accordingly, the C Auger peak is usually smoothed prior to D-parameter calculation. We have developed a tool based on denoising via Fourier analysis that allows D-parameter calculation. Results from this tool are consistent with other known procedures for determining the D-parameter.

UN-ThP-13 The Effect of Aluminum Precursor on the Electrical, Optical, and Structural Properties of Atomic Layer Deposited Aluminum-Doped Zinc Oxide Thin Films, ***Addison McLean***, *Nicholas Strandwitz,* Lehigh University

Aluminum-doped zinc oxide (AZO) is a promising material characterized by high transparency and conductivity, emerging as a inexpensive transparent conductive oxide alternative to indium tin oxide. Atomic layer deposition (ALD) is a technique well suited for depositing AZO films with precise control over dopant composition and film thickness. While the effect of aluminum composition and growth temperature on electrical properties is well studied, understanding the role of aluminum precursors in the ALD process is essential for further optimizing optoelectronic properties. In this study, the effect of aluminum precursor size and reactivity on the electrical, optical, and structural characteristics of ALD AZO thin films was investigated. AZO films were grown via the ALD supercycle method, in which matrix (ZnO) film layers are periodically interrupted by single dopant (Al) layers. The fraction of aluminum atoms contributing to carrier donation (doping efficiency) is dependent on the distribution of dopant atoms in the doping layer. Four aluminum precursors were investigated, including trimethyl aluminum, aluminum tri-sec-butoxide, tributyl aluminum, and tris(dimethylamino)aluminum. It was found that larger, less reactive precursors resulted in a lower Al concentration while maintaining a similar carrier concentration to smaller precursors by limiting the clustering of Al in the ZnO film, suggesting higher doping efficiencies. Additionally, mobility and conductivity both increased with precursor size, while refractive index, absorption coefficient, and transmittance remained largely unchanged.

UN-ThP-14 Plasma Diagnostics for the Modification of Plant-Based Biopolymers, ***Morgan Schnell***, *Joshua Blechle,* Wilkes University

Seed biopolymers, such as chickpeas, are commonly utilized in kitchens and are grown worldwide. Known for their great yield, health benefits, and versatility – agriculture and everyday suburbia depend on chickpeas. However, due to their thick outer cuticle structure, germination varies from seed to seed and results in a slow growth rate. As such, there is a desire to develop procedures that produce more consistent and faster germination processes. One potential method is the utilization of plasma-enhanced modification techniques. It has been suggested by surface analysis that the use of cold air plasma treatments will etch at the outer layer of the seed coat, inducing hydrophilicity. If this translates onto the chickpea biopolymer, germination should consequently be enhanced.

In order to achieve more reproducible etching processes, the mechanism driving the etching of the seed coat must be explored. Here, optical emission spectroscopy (OES) is used to monitor gas-phase species during chickpea treatment. A low-temperature, inductively-coupled plasma system formed from a mixture of breathing air and argon (90% and 10%, respectively, by pressure) is used for all treatment conditions, with the Ar serving as an actinometric addition. Various treatment times (30 - 120 s), pressures (50 - 250 mTorr), and applied powers (50 – 100 W) were assessed. Densities (measured via OES) were determined for plasma systems, with and without the chickpeas present, to help identify key reactive species and etch products. Notably, the presence of chickpeas increased the density of CO* gas while simultaneously reducing the density of NO*. These relationships help verify the predicted etching and break down of the hydrophobic cuticles. This is further explored by increasing the number of chickpeas present in the reactor, as well as further comparison with other conditions previously described. Etching into the hydrophilic cuticle as planned will allow for easier water access into the seed and higher consistency in the germination process.

Vacuum Technology
Room Ballroom A - Session VT-ThP
Vacuum Technology Poster Session

VT-ThP-1 Maintenance, Upgrade, and Vacuum System Optimization of the LCLS Superconducting Injector During 2026 Long Downtime, ***TC Chen***, SLAC National Accelerator Laboratory

The LCLS-II superconducting (SC) photoinjector at SLAC National Accelerator Laboratory is designed to produce high-brightness electron beams at repetition rates up to 1 MHz. The injector system integrates a Cs_2Te photocathode, RF gun, buncher, cryomodule, and extensive vacuum infrastructure to maintain ultra-high vacuum (UHV) conditions critical for cathode lifetime and beam quality. Following extended operation, component aging, vacuum degradation risks, and reliability concerns necessitate a comprehensive maintenance and upgrade campaign during the scheduled 2026 long downtime (LDT).

The maintenance strategy involves coordinated interventions across three major subsystems: the photocathode loadlock system, RF gun, and low-energy beamline (LEB). Key activities include removal of auxiliary hardware, such as cables, waveguides, tuners, cooling water hoses, and the 1.3 GHz cryomodule (CM) endcap support to provide access of parts being replaced , followed by replacement of failed and aging components including vacuum pumps, pneumatic gate valves, residual gas analyzers (RGAs), and

RF waveguide windows.

VT-ThP-2 Design and Construction of a Calibration Chamber and Pressure Control System for Automated Calibration of Capacitance Diaphragm Gauges and Other Vacuum Standards, ***Jacob Ricker***, *Jay Hendricks, Kevin Douglass, Ifenna Anakor, Thomas Howard,* NIST

The calibration of vacuum gauges from 13 mPa to 130 kPa has been done for the last 40 years using liquid column manometers. NIST new Fixed Length Optical Cavity (FLOC) pressure standards will be replacing these standards, however because they are based on gas refractivity, they require high purity gas. The current manifold is contaminated with mercury and oil from the manometers, so NIST has been designing and constructing a new manifold capable of automatically adjusting pressures and calibrating customer gauges against the standard. The automated system must be able to precisely control flow to set pressures in the chamber to within mPa accuracy at low pressure, however it must have capability for fast flow when filling pressures near atmospheric pressure. This presentation will describe the design, assembly, and testing of a low-cost calibration system capable of calibrating vacuum gauges over the range of 13 mPa to 130 kPa.

VT-ThP-3 Vacuum Considerations for the Next Generation of DC High Voltage Polarized Electron Gun at Jefferson Lab, ***Marcy Stutzman***, Thomas Jefferson National Accelerator Facility, United States Minor Outlying Islands (the)

The polarized electron source at Thomas Jefferson National Accelerator Facility (JLab) has delivered highly polarized electron beams for the nuclear physics program for over 20 years using a series of custom DC high voltage electron guns. We achieve pressure approaching 10^{-12} Torr in the electron gun by applying NEG coatings to heat treated stainless steel chambers, installing a large array of NEG modules and an ion pump, and baking the system for several days prior to use. The operational lifetime of the system is strongly affected by the vacuum level, as residual gasses ionized by the electron beam can damage the photocathode. Recent research on the electron guns has focused on improving high voltage performance by iterating the cathode electrode and insulator designs necessary for operation at a DC bias of -200 kV, with only minimal changes to the vacuum systems. However, the next generation polarized electron gun is now being designed to deliver at least 10x higher current to generate a polarized positron beam. The design for the high voltage, vacuum, and electrostatic beam optics must all be optimized, and some of the design choices that improve one aspect adversely affect other aspects. Vacuum system options will be discussed, such as chamber material, cathode electrode material, and pumping optimization, as well as the status of balancing the optimal design for both the high voltage and vacuum systems.

VT-ThP-4 Microreactor for Quantitative Reactivity Measurements and In Situ Infrared Spectroscopy on Single-Crystal Model Catalysts, *Adam Lagin, Johannes Filzmoser, Ulrike Diebold, Michael Schmid, Gareth Parkinson,* ***Jiri Pavelec***, TU Wien, Austria

Single-crystal model catalysts provide an ideal platform for elucidating reaction mechanisms and benchmarking computational models. Yet, accurately determining intrinsic reaction kinetics on low-surface-area single crystals at realistic pressures remains challenging [1]. Direct comparability with theory therefore requires tight control of gas-flow dynamics and exceptionally low background signals. Here, we present the design of a dedicated high-pressure reaction cell that addresses key limitations of conventional “pressure-gap” approaches through rigorous vacuum engineering and flow optimisation.

A defining feature of the microreactor design is operation in the molecular-flow regime within the narrow cell gap at pressures around 1 mbar. In this regime, quantitative turnover frequency (TOF) measurements can be obtained without the complex fluid-dynamic modelling or diffusion corrections typically required at higher pressures. The system retains the capability for operation up to atmospheric pressure (~1 bar). Trace product formation is detected by coupling the exhaust to a high-sensitivity mass spectrometer equipped with liquid-helium cryogenic pumping. In parallel, molecules on the catalyst surface are monitored using a home-built in situ IRAS setup optimised for the low reflectivity of metal oxides [2].

O-ring-free sealing is achieved by mating two optically flat surfaces [3]: the single-crystal sample and an IR-transparent diamond window. This “hard-seal” concept suppresses background contamination during high-pressure experiments. The design is prepared for full integration with standard UHV surface-science infrastructure. This enables controlled surface preparation and post-reaction characterisation by X-ray photoelectron spectroscopy, low-energy ion scattering, and scanning tunnelling microscopy facilitating direct correlation of atomic-scale structure with quantitative reactivity.

Essential aspects of the design have been supported by modelling, mainly in COMSOL Multiphysics, including vacuum-flow studies, heat transport, mechanical and optical simulations, as well as coupled multiphysics calculations. These studies guided critical design choices and will be showcased in this contribution.

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VT-ThP-5 New Developments in the Use of Fixed Length Optical Cavities as a Photonic Pressure Standard, ***Thomas Howard***, *Thinh Bui, Jacob Ricker, Kevin Douglass, Jay Hendricks,* NIST-Gaithersburg

The Fixed Length Optical Cavity (FLOC) is an optical pressure standard based on gas refractometry. Three different FLOC technologiesare being developed at NIST to cover a wide pressure range from micropascal to megapascal. Typical FLOC instruments determine pressure by measuring the shift in the beat note frequency between two separate lasers coupled to a dual cavity system. Recent advances allow the use of only a single laser source, reducing cost and complexity while maintaining the high (part-per-million level) precision and accuracy of the typical two laser system. Results and comparisons to previous FLOC pressure measurements will be discussed here.

VT-ThP-6 The Vacuum System Design for the Extreme Photonics Applications Centre (EPAC), ***Keith Middleman***, Science & Technology Facilities Council - STFC, UK

The EPAC facility currently under construction at the STFC Rutherford Appleton Laboratory is a new UK national facility that provides a unique opportunity to develop laser driven accelerator research, enabling a plasma wakefield accelerator facility with multi-GeV electron beams and spatially coherent x-ray and gamma-ray beams for cutting-edge experiments in plasma physics, laboratory astrophysics and condensed matter and material science.

This paper describes the design of the vacuum systems for Experimental Area 1 of the EPAC facility where high intensity lasers interact with a high density of gas molecules to ignite a plasma. The EPAC facility will run in the High Vacuum (HV) range with a typical operating pressure of 10^{-6} – 10^{-7} mbar. However, at the interaction point where the plasma is ignited there will be a gas injection nozzle that will provide the required gas density. It is anticipated that the expected gas pressure at the interaction point could be in the range of 10^{0} – 10^{2} mbar.

The vacuum design is presented showing what has been done to minimise the spread of the localised high-pressure gas from the target location into the laser delivery beamline. This is essential to avoid laser breakdown and non-linear effects occurring before the laser reaches its peak intensity at the focus. The differential pumping configuration will be explained and there will be an overview of the gas dynamics work done across the pressure regimes from transitional flow to molecular flow.

The outcome of this work is a vacuum system capable of the demands put upon it from localised gas densities to the performance of the laser optics in delivering the required laser intensities. It is anticipated that this new UK user facility will open in late 2026.

Actinides and Rare Earths
Room 320 - Session AC-FrM

Actinides and Rare Earths Science

Moderators: Dr. Krzysztof Gofryk, Idaho National Laboratory, **Prof. Dr. Ladislav Havela**, Charles University, Czech Republic, **Dr. Paul Roussel**, AWE, **Dr. David Shuh**, Lawrence Berkeley National Laboratory

8:15am **AC-FrM-1 Environmental Radioactivity at the Department of Energy's Hanford Site: Sources and Sinks**, ***Carolyn Pearce***, Pacific Northwest National Laboratory; *Jay LaVerne,* University of Notre Dame; *Hilary Emerson, Amanda Lawter, James James Szecsody, Rob Mackley, Xin Zhang, Zheming Wang, Kevin Rosso, Gregory Schenter,* Pacific Northwest National Laboratory; *Linda Young,* Argonne National Laboratory; *Thomas Orlando,* Georgia Institute of Technology; *Aurora Clark,* University of Utah; *Xiaosong Li,* University of Washington; *Lynn Francesconi,* Hunter College, City University of New York **INVITED**

Plutonium production for the U.S. weapons program at the Department of Energy's Hanford Site created one of the world's largest environmental remediation challenges. Cleanup of 200 million liters of radioactive and chemically complex waste stored in 177 underground tanks will take decades and cost billions of dollars. Addressing the sources and sinks of environmental radioactivity requires: (i) characterization of radioactive tank waste chemistry and (ii) understanding contaminant transport and reactivity in the subsurface. The Ion Dynamics in Radioactive Environments and Materials (IDREAM) Energy Frontier Research Center provides mechanistic insights into precipitation and dissolution processes central to Hanford tank waste treatment. Hanford sludge contains water-insoluble aluminum oxides/ hydroxides that influence waste processing. Atomic force microscopy (AFM) showed that gibbsite dissolution in alkaline solutions proceeds through release of aluminate dimers rather than classical monomer detachment mechanisms. Gibbsite can also selectively adsorb or incorporate rare earth elements in tank waste. IDREAM developed an AFM integrated with an X-ray source to directly observe radiolytically driven interfacial reactions with unprecedented spatial resolution. These studies revealed how ionizing radiation, adsorbed water, and surface impurities alter mineral reactivity under highly alkaline conditions. Adsorbed carboxylates or chromium on boehmite nanoplates significantly slowed dissolution despite incomplete surface coverage. In parallel with tank waste retrieval, legacy disposal to cribs and trenches during plutonium separations operations produced vadose zone contamination and groundwater plumes that continue to impact the environment. Key groundwater contaminants include technetium-99, present as highly mobile pertechnetate (TcO_4^-), and uranium. Current remediation strategies include treatment of perched water zones and permeable reactive barriers. Technologies under evaluation include tin apatite particles, sulfur-modified iron particles, bismuth subnitrate particles, calcium polysulfide, and polyphosphate amendments. Proposed immobilization mechanisms include reduction, adsorption, incorporation into mineral phases, and in situ precipitation/coating reactions. Their effectiveness for sequestration of Tc-99 and uranium was evaluated through batch and column studies using Hanford sediments. Advances in understanding radioactive waste chemistry, radiolytic interfacial processes, and contaminant immobilization mechanisms are critical for reducing environmental risks associated with Hanford waste retrieval, treatment, and disposal.

8:45am **AC-FrM-3 Reaching the Monolayer Limit in a van der Waals Actinide Magnet**, ***Priscila Rosa***, Colorado State University **INVITED**

The discovery of local-moment magnetism in van der Waals (vdW) semiconductors down to the single-layer limit has led to a paradigm shift in the understanding of two-dimensional (2D) magnets and unleashed their potential for applications in microelectronic and optoelectronic devices. The incorporation of strong electronic and magnetic correlations in 2D vdW metals remains a sought-after platform not only to enable control of emergent quantum phases, such as superconductivity, but also to achieve more theoretically tractable microscopic models of complex materials. To date, however, there is limited success in the discovery of such metallic vdW platforms, and *f*-electron monolayers remain out of reach. In this talk, I will discuss experimental and theoretical studies of β-UTe_3, an actinide ferromagnet that can be exfoliated to the monolayer limit. A sizable electronic specific heat coefficient provides the hallmark of strong correlations. Remarkably, β-UTe_3 remains ferromagnetic in the half-unit-cell limit with an enhanced ordering temperature of 35 K, a factor of two larger than its bulk counterpart. Time permitting, I will also share recent spectroscopic insights into this system. Our work establishes β-UTe_3 as a novel materials platform for investigating and modeling correlated behavior in the monolayer limit and opens numerous avenues for quantum control with, e.g., strain engineering.

9:15am **AC-FrM-5 Theory of High-Resolution X-Ray Absorption and Resonant Inelastic X-Ray Scattering: Focus on Intermediate Valency**, ***Jindrich Kolorenc***, Institute of Physics (FZU), Czech Academy of Sciences, Prague, Czechia **INVITED**

I will discuss modeling of the high-energy-resolution x-ray absorption and the resonant inelastic x-ray scattering in actinide compounds by means of the charge-transfer multiplet theory, that is, using the Anderson impurity model constructed on the basis of first-principles electronic-structure calculations. As one of the applications, I will analyze uranium L_3 and M_4 x-ray absorption spectra taken on UPd_2Cd_{20}. These spectra indicate that the uranium 5f shell undergoes valence fluctuations in this compound [1].

The regime of valence fluctuations, known from intermetallics based on the anomalous rare-earth elements (such as Ce, Yb, Sm, Eu), has not yet been identified by microscopic techniques in any uranium compound. It was only suggested in a few of them on the basis of thermodynamic properties (such as the magnetic susceptibility) and on their similarity to the properties of the rare-earth valence fluctuators [2]. Such arguments, however, are hardly unequivocal. The x-ray absorption spectroscopy certainly provides a more direct probe of the 5f-shell behavior. Although UPd_2Cd_{20} has only one type of uranium site in its primitive cell, the absorption spectra obtained in the high-energy-resolution fluorescence-detection (HERFD) mode display two edges, each of which can be associated with a different valence state, $5f^2$ and $5f^3$. The shape of the L_3 spectrum is well approximated by two shifted copies of the uranium 6d density of states obtained in density-functional calculations, the shape of the M_4 spectrum is well approximated by a combination of UCl_3 ($5f^3$) and UCl_4 ($5f^2$) spectra reported previously [3]. This points to the $5f^2 \leftrightarrow 5f^3$ fluctuations on a timescale longer than the characteristic time of the spectroscopy technique. Unlike 4f systems, in which such fluctuations typically lead to a destruction of magnetism due to one of the involved $4f^n$ configurations being non-magnetic [4], the $5f^2$ and $5f^3$ states are both magnetic, allowing for a magnetic ordering in the fluctuating state—UPd_2Cd_{20}, in particular, is antiferromagnetic.

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9:45am **AC-FrM-7 Electronic Structure Studies of Tetravalent Actinides by Solid State NMR Spectroscopy**, ***Herman Cho***, *Khyati Anand,* Pacific Northwest National Laboratory; *Sejun Park,* Los Alamos National Laboratory; *Khusboo Rana, Eric Walter,* Pacific Northwest National Laboratory **INVITED**

The magnetic properties of tetravalent actinide centers differ markedly within the actinide row and with isoelectronic counterparts from the lanthanide row. Notable examples include the temperature independent paramagnetism of PuO_2,[1,2] exotic forms of multipolar order in UO_2 and NpO_2,[3,4] and the existence of multiple magnetic transitions in UF_4 and NpF_4.[5] These studies have provided definitive evidence that the assignment of the valence electrons of actinides to 5f orbitals oversimplifies the underlying electronic structure. With magnetic resonance spectroscopic techniques we have shown that local magnetic and electric fields at ligand sites and the metal itself can be measured in the solid state with better than part per thousand resolution. We apply this approach in systematic studies of electronic structure in an isomorphous series of An(IV) compounds including the tetrafluorides (Fig. 1)[6,7] and the dioxides (Fig. 2).[8] Plutonium, which is positioned in the 5f row between the light actinides -- characterized by itinerant valence electrons -- and higher *Z* elements that have valence electrons found to be in localized (atom-like) states, presents examples of both types of behavior.

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10:30am **AC-FrM-10 High-Resolution X-ray Spectroscopic Studies on Protactinium and Actinium**, ***Jacob Branson**, Bianca Schacherl, Kiara Maurer, Tim Prüßmann, Kathy Dardenne,* Karlsruhe Institute of Technology, Institute for Nuclear Waste Disposal, Germany*; Rikard Malmbeck, Olaf Walter,* European Commission, Joint Research Center, Karlsruhe, Germany*; Tonya Vitova,* Karlsruhe Institute of Technology, Institute for Nuclear Waste Disposal, Germany **INVITED**

Despite occurring in nature, the chemistry of protactinium remains relatively unstudied due to its low abundance, radioactivity, and difficulty of isolation. However, existing studies on protactinium reveal chemical behavior and electronic structure that is unique even amongst the actinides, and this behavior has been attributed to the relatively large radial extent of the Pa 5f orbitals in tandem with their similar energy to the Pa 6d orbitals. In this work, the nature of the involvement of the Pa 5f and 6d orbitals is probed using high-resolution X-ray spectroscopy (HR-XANES) and resonant inelastic X-ray scattering (RIXS) experiments at the Pa $M_{3,4}$-edges, which have been demonstrated to be valuable probes of actinide electronic structure. For these studies, K_2PaF_7 and $Pa_2O_5{\cdot}xH_2O$ were synthesized in the solid state and characterized using Pa L_3-edge EXAFS. The Pa $M_{3,4}$-edge HR-XANES and RIXS experiments on these samples were conducted using two different scattering geometries and reveal dramatic differences in Pa 5f and 6d molecular orbital energetics and bond covalency between these coordination environments. We relate these differences to the competing influences of orbital energy and orbital overlap. These results form a basis of understanding for the electronic structure and chemistry of more complex Pa systems and demonstrate the high potential of the Pa 5f and 6d orbitals to participate in bonding interactions. The first experimental results on Ac M_3-edge HR-XANES of Ac-DOTA, relevant for understanding the bonding properties of Ac in radiopharmaceuticals, will also be presented and discussed. All experiments were conducted at the ACT end station of the CAT-ACT beamline at the KIT Light Source in Karlsruhe, Germany.

11:00am **AC-FrM-12 Manufacturing to Performance: Advanced Characterization of Nuclear Fuels**, ***Robert Harrison**, Jonathan Morgan,* University of Manchester, UK*; Angus Wylie,* Massachusetts Institute of Technology*; Samira Bostanchi, Chris Green, David Pearmain,* Lucideon, UK*; Dave Goddard,* UKNNL, UK*; Mike Short,* Massachusetts Institute of Technology **INVITED**

Development of novel manufacturing techniques and advanced nuclear fuel materials offers significant economic and safety benefits for current and future reactor systems. However, linking processing to in-pile performance requires correlative advanced characterisation across multiple length scales. This work presents two case studies demonstrating this approach.

Firstly, field-assisted sintering (FAS) techniques, including spark plasma sintering (SPS) and flash sintering (FS), are being developed for UO_2 and mixed uranium–plutonium oxide (MOx) fuels. These methods significantly reduce sintering temperatures and processing times compared to conventional routes. However, understanding the impact of these rapid sintering processes on microstructure and chemical homogeneity—particularly plutonium distribution—is critical for fuel performance and reprocessability. A bespoke uranium-active FS system has been optimised (873-1173 K), achieving >95% theoretical density and ~5µm grain sizes, representing ~50% reductions in temperature and cycle time for UO_2. Extension to MOx surrogate systems (CeO_2-doped UO_2) revealed significant heterogeneity, including Ce-rich inclusions and degraded pellet quality. To resolve this, a correlative characterisation framework combining XRD, SEM-EDS, EPMA and Raman microscopy is employed to probe phase composition, chemical distribution and local defect chemistry. This multi-modal approach provides insight into the formation of heterogeneous regions and their relationship to processing conditions and pellet quality.

Secondly, uranium nitride (UN) is studied as an advanced and accident tolerant fuel. Ion irradiation (Ar, up to 100 DPA at 573 K) is used as a surrogate for neutron damage. Post-irradiation examination integrates XRD and TEM-EELS to characterise defect evolution, including dislocation loops, lattice swelling and gas bubble formation with Transient grating spectroscopy (TGS) to measure near-surface thermal diffusivity. This revealed a significant reduction of thermal conductivity at doses >10 DPA, directly correlated with nanoscale defect populations. In-situ annealing using TGS and TEM shows recovery of thermal transport above ~773 K, linked to point defect recombination. Overall, this work demonstrates how correlative, multi-technique characterisation links manufacturing, defect evolution and functional performance, supporting predictive understanding and accelerated development of advanced nuclear fuels.

11:30am **AC-FrM-14 Cooperative Phenomena in Locally Non-Centrosymmetric Heavy-Systems and Raman Effect in Cecosi**, ***Gertrud Zwicknagl**,* TU Braunschweig, Germany

Heavy-fermion systems with magnetic ions in non-centrosymmetric sites have gained high attention during the past years. A prominent example is CeRh2As2 which exhibits a complex phase diagram with many unusual phases [1,2]. Theoretical discussions mainly focused on the role of the Rashba effect, i. e., on the consequences of local inversion symmetry breaking on the spins of the heavy quasiparticles [3].

In the present contribution, I will discuss consequences of local inversion symmetry breaking on the orbital degrees of freedom, i. e., the possible hybridization of orbitals with different parities. The inter-site interaction resulting from local Ce 4f-Ce 5d hybridization and d-d- hopping can lead to new cooperative phenomena like the lattice instability in CeCoSi [4].

I will discuss the consequences of these cooperative phenomena for the Raman spectra of CeCoSi [5].

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[2] D. Hafner et al, Phys. Rev. **X 12**, 011023 (2022)

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[4] Takeshi Matsumura et al., Phys. Rev. **B 113**, 014415 (2026)

[5] Owen Moulding et al., arXiv: 2505.03249

11:45am **AC-FrM-15 Statistical Enhancement of Fissile Isotope Discrimination via Superposition of Fission-Track Clusters**, *Rami Babayew, Yaacov Yehuda-Zada,* Nuclear Research Center Negev, Israel*; Galit Bar,* Soreq Nuclear Research Center, Israel*; Noam Elgad,* Nuclear Research Center Negev, Israel*; Danny Dayan,* Ben Gurion University Be'er Sheva, Israel*; Jan Lorincik,* Centre Řež, Czech Republic*; Itzhak Orion,* Ben Gurion University Be'er Sheva, Israel*; Shay Dadon,* Nuclear Research Center Negev, Israel*; Aryeh Weiss,* Bar Ilan University, Israel*; Galit Katarivas Levy, **Itzhak Halevy**,* Ben Gurion University Be'er Sheva, Israel

Accurate fissile isotope identification using Fission Track Analysis (FTA) is fundamentally limited by stochastic variations in individual fission-fragment trajectories and by the finite statistics obtainable from single-cluster measurements. While recent advances in automated image processing and synthetic-data-driven reconstruction have improved the robustness of FTA, isotopic discrimination between fissile materials with similar fission-fragment distributions remains challenging.

In this work, we propose a novel statistical enhancement framework based on superposition of reconstructed fission-track clusters originating from the same fissile grain. The method combines multiple realizations of track topologies into a unified statistical representation, effectively increasing counting statistics without increasing detector area or irradiation complexity.

Monte Carlo simulations using Geant4 were performed for ^{235}U, ^{233}U, and ^{229}Th embedded in aerogel-assisted LEXAN® solid-state nuclear track detectors (SSNTDs). Synthetic microscope images were generated and processed using an automated reconstruction pipeline to extract track morphology, cluster centroids, and Real Flight Path (RFP) distributions.

Statistical analysis demonstrated that the proposed superposition framework reduces stochastic uncertainty approximately according to: $\sigma_{eff} = 1/\sqrt{N}$

where N is the number of superposed cluster realizations. For example, superposition of N = 9 realizations improves discrimination between ^{235}U and ^{229}Th from ~3σ to ~9σ, and between ^{235}U and ^{233}U from ~1σ to ~3σ, consistent with the expected $\sqrt{N}$ scaling. More distinct isotope pairs

exhibited even stronger enhancement, exceeding 5σ significance for modest superposition levels.

The proposed methodology transforms FTA from a primarily single-event morphological analysis into an ensemble-based statistical fingerprinting technique. This approach provides a scalable pathway toward improved isotopic sensitivity, automated nuclear forensic analysis, and enhanced safeguards verification, particularly for isotopes with partially overlapping fission-fragment signatures.

Future work will focus on experimental validation under neutron irradiation conditions and implementation of physics-informed alignment algorithms for real detector datasets.

AI/ML/Autonomous Experimentation for Thin Films Processing
Room 317 - Session AIML1-FrM

Materials Design and Autonomous Discovery

Moderators: Eden Goodwin, Carleton University, Canada, **Prof. Stephanie Law**, Pennsylvania State University

8:15am **AIML1-FrM-1 Accelerating Discovery and Design for Thin Film Polymer Self-Assembly through Machine Learning**, ***Gregory Doerk,*** Brookhaven National Laboratory **INVITED**

Thin film polymer self-assembly is a powerful approach to create nanoscale patterns across large areas with low cost for diverse applications in electronics and materials science. The confluence of compositional and architectural variation, entropic and surface energy constraints arising from thin film confinement, and process-dependent assembly pathways yields of panoply of nanoscale morphologies of which only a fraction can be discovered, catalogued, and engineered through manual experimentation. This talk will elaborate examples where artificial intelligence and machine learning (AI/ML) can accelerate thin film polymer self-assembly research. We describe the application of Gaussian process regression to automate x-ray scattering characterization for the discovery of new morphologies in template-directed self-assembly of block copolymer blends. We then illustrate the application of an active learning approach that incorporates foundation model-supported “few shot” image classification for determining processing-morphology relationships in spray-deposited block copolymer/homopolymer blend films using minimal quantities of data. Complementary in situ x-ray scattering measurements during spraying provide key mechanistic insights into trends in self-assembled structural organization across the process design space.

8:45am **AIML1-FrM-3 Autonomous Discovery of PFAS-Free Low Surface Energy Thin Films**, ***Stanley Lo,*** *Abraham Herzog-Arbeitman, Alan Aspuru-Guzik, Helen Tran, Nipun Gupta, Harrison Mills,* University of Toronto, Canada

Per- and polyfluoroalkyl substances (PFAS) have long dominated low-surface-energy coatings due to their exceptional water and oil repellency. However, regulatory pressure and environmental persistence concerns have created urgent demand for fluorine-free alternatives. Rational design of such materials requires systematic exploration of polymer composition–wettability relationships, a challenge ideally suited to autonomous experimentation.

We present a self-driving laboratory for accelerated discovery of PFAS-free polymer thin films with low surface energy. The platform integrates a continuous-flow reactor, an automated fraction collector for composition-resolved sample handling, a spin coater for reproducible thin-film deposition, and a multi-liquid dynamic contact angle goniometer for comprehensive wettability characterization. Closed-loop control enables autonomous navigation of copolymer composition space.

The chemical system employs ring-opening metathesis polymerization (ROMP) of norbornene-based monomers to produce statistical polynorbornene copolymers. Monomer design is grounded in the Hansen solubility parameter (HSP) framework, which decomposes intermolecular interactions into three orthogonal dimensions: dispersion (δD), polarity (δP), and hydrogen bonding (δH). Three monomers were synthesized with side groups systematically representing each dimension: an apolar aliphatic chain (low δP, low δH), a polar non-protic group (high δP), and a polar hydrogen-bonding group (high δH). ROMP copolymerization of these monomers yields materials with continuously tunable surface chemistry across the HSP space.

Dynamic contact angle measurements using multiple probe liquids (water, ethylene glycol, and hexadecane) enable surface free energy decomposition and discrimination between hydrophobic and oleophobic character. The platform iteratively selects compositions, deposits films, measures wettability, and updates a surrogate model to identify low-surface-energy optima without fluorinated components.

This work establishes a generalizable, data-driven framework for discovering sustainable high-performance surface coatings and provides mechanistic insight into how monomer polarity and hydrogen-bonding capacity govern macroscopic wettability.

AI/ML/Autonomous Experimentation for Thin Films Processing
Room 317 - Session AIML2-FrM

AI/ML in Semiconductor Processing & Manufacturing

Moderators: Prof. Dane de Quilettes, Princeton University, **Ms. Zahra Nasiri**, University of Alabama at Birmingham

9:00am **AIML2-FrM-4 Process Informatics Framework for Optimizing Thin-Film Deposition in Advanced Semiconductor Manufacturing**, ***Shota Oda,*** *Seitaro Sanai, Takeshi Hashishin, Ichiro Akai, Takeshi Momose,* Kumamoto University, Japan

We developed a framework based on physics-informed process informatics for supercritical fluid deposition (SCFD) that enables efficient optimization of high deposition rates and conformality in high-aspect-ratio (HAR) structures. As semiconductor devices transition toward three-dimensional integration, high-throughput conformal deposition in HAR features such as through-silicon vias is increasingly required. SCFD, which involves chemical reactions of metal organics in supercritical CO_2($scCO_2$) to allow thin film deposition, is promising because the high diffusivity and solubility of precursors in $scCO_2$ enable concentrated precursor transport deep into microstructures. However, fluid properties and reaction kinetics are highly sensitive to process conditions, and their relationships with deposition behavior have not been quantitatively established. Consequently, conventional process development has relied largely on empirical trial-and-error.

To address this issue, we propose a causal decomposition framework that separates process-condition from physicochemical-response effects, introducing physicochemical parameters as intermediate variables between process conditions and deposition outcomes. Specifically, the SCFD process is mapped onto a causal chain: process conditions → physicochemical parameters → deposition outcomes. The physicochemical parameters are linked to deposition outcomes through mass balance analysis of precursors in HAR features, clarifying their relationship with deposition rate and conformality. To model the relationship between process conditions and physicochemical parameters, we applied Physics-Informed Bayesian Optimization (PIBO). In PIBO, a prior physical model is incorporated as the mean function of Gaussian process regression. The predictive model is sequentially updated using newly acquired data to recommend subsequent process conditions in a closed-loop manner. In this contribution, PIBO was evaluated through sequential sampling from synthetic process-response surfaces designed to emulate SCFD behavior and compared with conventional Bayesian Optimization.

Rather than relying solely on data-driven learning, the proposed framework integrates physically describable behavior with data-driven residual learning. This hybrid approach enables optimal deposition conditions to be derived from sparse datasets while maintaining physical consistency and extrapolation reliability, and can be extended to different target structures without re-optimizing the entire process from scratch. This framework provides a scalable and physically interpretable strategy for optimizing next-generation semiconductor thin-film deposition processes.

9:15am **AIML2-FrM-5 Physics-Informed AI for Semiconductor Equipment Status Estimation and Process Quality Prediction: Equipment Manufacturer's Perspective**, ***Hyunho Yun,*** *Yongjo Kim, Dain Ham, Yun Hyeong Lee, Seon Hye Kim, Young Hoon Kim, Da Gyung Lee, Yoonsun Lee, Hanbee Lee, Hyemin Song, Youjin Jeong, Hongyeon Kim,* Wonik IPS, Republic of Korea

The rapid expansion of AI services has significantly increased demand for advanced semiconductor chips, accelerating the need for equipment strategies that maximize yield, process stability, and tool availability. In fabs, even a single instance of unscheduled downtime can cause substantial

losses in production throughput. However, conventional rule-based process management systems such as Fault Detection and Classification (FDC) and Statistical Process Control (SPC) have inherent limitations. They require extensive manual effort to define process-specific rules across diverse process conditions and hardware configurations. In addition, high-cost of metrology equipment typically limits wafer sampling to approximately 1% of mass production wafers, making real-time quality assurance difficult.

To address these challenges, Wonik IPS has developed an intelligent monitoring framework that combines AI-based equipment health diagnosis with wafer quality prediction. The core of the framework is a Condition-Based Maintenance (CBM) model. In deposition equipment, complex physical interactions among sensors often make direct analysis of raw sensor data unreliable. Wonik's CBM model overcomes this limitation by integrating process log data with a sensor relationship network that captures process role and physical location of each sensor, thereby enabling equipment health diagnosis from the system level down to individual components. Unlike conventional Time-Based Maintenance (TBM), CBM provides a more effective approach for maintaining optimal equipment conditions by reducing downtime and enabling early fault diagnosis.

Wafer quality prediction is further enhanced by integrating CBM-based equipment health information with real-time Virtual Metrology (VM). Wonik's VM solution adopts a hybrid architecture that combines a neural network optimized for subtle pattern recognition and a physics-based model capable of robust inference based on physical principles. Using process log data collected from Wonik's deposition equipment, GEMINI HQ, thickness prediction results demonstrated strong performance even under data-constrained conditions, achieving average error rates of approximately 1% for the neural network model and 5% for the physics-based model.

Going forward, Wonik plans to integrate CBM and VM into a unified predictive framework to further advance autonomous process control. By combining equipment data, health diagnosis, and recipe conditions, this data-driven optimization strategy is expected to enhance real-time monitoring across all process stages and contribute to the development of an intelligent semiconductor equipment ecosystem.

9:30am **AIML2-FrM-6 Multi-Objective Optimization of the Operational Durability of Meniscus-coated Perovskite Solar Cells***, **Eric Oberholtz**, Jongbeom Kim, Maimur Hossain, Ayush Tiwary, Lucas Mar, Yube Ostos, Divenaa Madan, David Fenning,* University of California San Diego

Perovskite solar cells are strong contenders for commercialization of renewable photovoltaics, but making the leap from lab-scale fabrication to commercial devices requires switching to industrial-scale thin film fabrication techniques such as meniscus coating while maintaining high quality thin films. Transitioning from spin coating to meniscus coating introduces a highly complex, multi-variate parameter space we must navigate while balancing thin film quality alongside operational stability of the finished devices. To bridge the lab-to-fab gap, we integrate MEITNER (Meniscus Integration for Thin film Nano Electronics Robot)- an autonomous platform for meniscus depositions- within our robotic experimentation ecosystem paired with a multi-objective Bayesian optimization framework. This framework explores the multi-dimensional parameter space comprised of fabrication and chemistry design choices aimed to maximize (1) the initial quality of the perovskite thin film, (2) the initial performance of the pristine perovskite devices, and (3) the operational stability under accelerated degradation of the thin film devices. Our workflow accelerates the discovery of promising candidates for industrially relevant fabrication of operationally durable semiconductor thin film devices.

AI/ML/Autonomous Experimentation for Thin Films Processing

Room 317 - Session AIML3-FrM

Connecting Datasets, Models, and Characterization

Moderators: Ms. Molly McDonough, Pennsylvania State University, **Dr. Amanda Sanchez**, Universidad Anahuac

9:45am **AIML3-FrM-7 In the Design of Thin Charge-Transport Films for Perovskite Solar Cells, Predictions from Machine Learning and Physics Only Partially Overlap***, Joseph Oti, Elvis Twumasi,* SUNY Polytechnic Institute*; Nana Derkyi,* SUNY Polytechnic Institute, Ghana*; Tabiri Asumadu, Desmond Klenam, Bernice Abraham,* SUNY Polytechnic Institute*; Rodica Neamtu, **Nancy Burnham**,* Worcester Polytechnic Institute*; Iulian Gheraisou, Winston Soboyejo,* SUNY Polytechnic Institute

We present a hybrid machine learning (ML) and physics-based computational modeling framework that informs experimentally realizable thin charge-transport-layers for perovskite solar cells (PSCs). Using supervised ML models, 12294 previously published curated datapoints predicted device efficiency. Ten high-efficiency descriptor combinations with greater than 21% power conversion efficiency were mapped into SCAPS-1D (a physics-based simulation software) employing a $FASnI_3$ absorber to assess their physical plausibility. In contrast with the ML predictions, the SCAPS configurations yielded PCEs in the range of 0.03–22.7%. Discrepancies between ML and SCAPS predictions arose from interfacial recombination, optical losses, and physical constraints not explicitly encoded in the ML dataset, describing a tightly focused set of fabrication parameters. Thus, the complementary use of both machine learning and physical simulations offers a time- and material-saving scalable pathway for the development and fabrication of low-cost photovoltaic devices.

10:00am **AIML3-FrM-8 Closed-Loop Ai Workflow for Literature-Guided Perovskite Thin-Film Discovery***, **Jordan Marshall**,* University of Tennessee Knoxville

In this project, we are developing an AI-assisted thin-film materials discovery workflow for halide perovskite solar cells. The goal is to make materials discovery more connected, adaptive, and efficient by bringing together steps that are often handled separately: literature knowledge, predictive modeling, robotic synthesis, and high-throughput characterization. Instead of treating these as independent parts of the research process, the workflow is being designed so that information from one stage can help guide the next. A large part of this work has focused on building a literature-mining agent for perovskite solar-cell papers. The perovskite literature contains a large amount of useful information, including device structures, perovskite compositions, processing conditions, interface layers, power conversion efficiencies, and stability measurements. However, this information is often reported in different ways across papers, which makes it difficult to use directly for machine-learning studies. The literature agent is designed to read papers, extract the relevant information, and organize it into a structured format compatible with the Perovskite Database. The workflow also aims to preserve where the information came from, separate evidence from model-ready features, flag incomplete records, and identify possible duplicate device entries. This makes the dataset update process more transparent and easier to check. The updated dataset can then be used to train sequential machine-learning models for device performance and stability. First, power conversion efficiency is predicted from design, processing, interface, and device-context features while avoiding target leakage from already measured performance values. Stability is then modeled using a similar feature space. We compare design-only stability prediction, stability prediction using model-predicted PCE, and post-fabrication prediction using measured initial device performance. This structure helps separate early design guidance from later experimental decision-making. This work is an important step toward a closed-loop discovery platform for perovskite and related semiconductor thin films. Literature knowledge can update the database, models can suggest promising directions, robotic synthesis can test those ideas, and high-throughput characterization can provide new information that feeds back into the system. While the workflow is still being developed, it provides a practical foundation for more efficient and autonomous thin-film experimentation.

10:30am **AIML3-FrM-10 Multimodal AI Meets Materials Characterization**, ***Linda Hung***, *Weike Ye, Jithendaraa Subramanian, Daniel Schweigert, Amalya Johnson, Flora Chen,* Toyota Research Institute **INVITED**

Many large-scale materials AI models rely on atomic-resolution crystal structure as a required input. Such models leverage the availability of large computational datasets but can be difficult to apply to experimental workflows. We present multimodal models that are instead built on inputs more commonly available in the lab, such as XRD and composition, and show benchmarks on use cases including noisy XRD and incomplete composition. We then discuss what it takes to build the datasets these models need, and share progress toward that goal.

11:00am **AIML3-FrM-12 Building Informative Materials Datasets Beyond Targeted Objectives**, ***Rafael Espinosa Castañeda***, University of Toronto, Canada, Mexico; *Jason Hattrick-Simpers,* University of Toronto, Canada

Materials science data collection can be expensive, making the reuse and long-term utility ofdatasets critically important for future discovery campaigns. In practice, researchers prioritize a subsetof properties due to research interests. However, ignoring a subset of outcomes in data collectioncampaigns potentially generates datasets poorly suited for future learning tasks. Here, we present a framework for dataset construction that maximizes informativeness for target properties of interest while preserving performance on untargeted ones. Our approach uses diversity-aware selection to ensure broad coverage of the materials space. In noisy experimental dataset construction, we find that without our diversity-aware framework, prediction performance on untargeted properties can degrade by up to sim40% relative to random sampling, whereas applying our framework yields improvements of up to 10\%. For targeted properties, performance can degrade with respect to random sampling by up to 12.5% without diversity, while our framework achieves gains of up to sim25%. Incorporating diversity into dataset construction not only preserves informativenessfor the targeted properties, but also improves materials coverage for potential future objectives. As aresult, the constructed datasets remain broadly informative across considered and unconsidered outcomes,ensuring unbiased quality entries and mitigating cold-start limitations in subsequent modeling anddiscovery campaigns.

AI/ML/Autonomous Experimentation for Thin Films Processing

Room 317 - Session AIML4-FrM

Panel: Funding Agencies

Moderators: Andreas Werbrouck, Ghent University, Belgium, **Prof. Matthias Young**, University of Missouri

11:15am **AIML4-FrM-13 Panel: Funding Agencies**

Advanced Microelectronic Materials and Devices Mini-Symposium

Room 318 - Session AM1+EM+TF-FrM

Materials Discovery and Synthesis

Moderators: Prof. Michelle Paquette, University of Missouri-Kansas City, **Prof. Dr. Haozhe "Harry" Wang**, Duke University

8:15am **AM1+EM+TF-FrM-1 Machine Learning for Electronic Materials Discovery and Synthesis**, ***Christopher Hinkle***, University of Notre Dame **INVITED**

Recent advances in AI applied to high-throughput materials discovery, synthesis, and processing offer a pathway to accelerated breakthroughs and scaled optimization of advanced electronic materials for data-intensive computation. We will discuss our recent work using high-throughput techniques and ML-aided characterization to synthesize new materials and optimize them in an accelerated manor.

8:45am **AM1+EM+TF-FrM-3 Exploration of Limiting Factors for c-BN Growth by Ion-Beam Assisted Molecular Beam Epitaxy**, ***Tyler Erickson***, *Matthew Hardy, Eric Jin, Andrew Lang, James Hart, Peter Litwin, David Boris, Scott Walton, Neeraj Nepal, Douglas Katzer, Virginia Wheeler,* US Naval Research Laboratory

Cubic boron nitride (c-BN) is a prospective barrier material for high power density electronics due to its high breakdown field of 15 MV/cm and thermal conductivity of 13 W/(cm·K). The low lattice mismatch between c-BN and diamond (~1.3%) provides a direct avenue for pursuing molecular beam epitaxy (MBE) growth of c-BN/diamond heterostructures. The hexagonal phase of boron nitride (h-BN) is the thermodynamically favorable phase over c-BN, promoting h-BN formation for standard growth conditions. The formation of c-BN requires altering the energy dynamics of the growth, such as the addition of a plasma-based Ar^+ ion source during the growth. This introduction of an Ar^+ ion source has led to successful c-BN growths with high phase purity at the cost of overall growth rate. Here, we investigate methods to improve c-BN crystal quality and growth rate using ion assisted MBE on diamond (100) substrates. We prepared diamond substrates with acid cleans and ethanol rinses in air before degassing in vacuo. Substrates are then transferred to the growth chamber and exposed to high temperature annealing to remove residual surface oxides prior to c-BN deposition. Deposition is performed using a boron e-beam evaporator, plasma-based active N source, and plasma-based Ar+ ion source. The boron flux is shuttered at regular intervals during the growth while the N and Ar^+ ion fluxes are constant. This modulation prevents the formation and continued build-up of polycrystalline h-BN in the samples. Systematic variations of the surface preparation, boron flux, nitrogen flowrate and substrate temperature are performed. The c-BN phase purity and thickness are then investigated with Fourier transmission infrared (FTIR) spectroscopy, high-resolution transmission electron microscopy (TEM) and optical profilometry. X-ray photoemission spectroscopy (XPS) measurements give additional insight into the band alignment based on surface preparation. FTIR measurements show a large reduction in the longitudinal c-BN mode (≈1312 cm^{-1}) with reduced B flux, N flow and increase in substrate temperature. The TEM measurements indicate a large dependence of the film thickness uniformity and overall growth rate on the substrate preparation, with thickness variations on the order of the total thickness for hydrogenated substrates. XPS measurements show a change in valence band offset with respect to the diamond substrate of -0.1 ± 0.1 eV for the oxygen terminated surface to -0.5 ± 0.1 eV for hydrogen terminated surface.

9:00am **AM1+EM+TF-FrM-4 Tuning the Physicochemical Properties of Polymer-like a-C:H Thin Films via Ultraviolet C (UV-C) Irradiation**, ***Seonhee Jang***, *Kenneth Lathrum, Jhonatan Romero,* University of Louisiana

Hydrogenated amorphous carbon (a-C:H) thin films represent a versatile class of materials characterized by a unique combination of desirable physical and chemical properties, leading to their adoption across a wide range of industrial applications. The fundamental properties of a-C:H films are governed by two primary factors: their total hydrogen content and the specific hybridization state of the constituent carbon atoms. Based on these parameters, a-C:H materials are generally categorized into four distinct groups: diamond-like, tetrahedral, graphite-like, and polymer-like. Among these, polymer-like a-C:H films have received comparatively limited attention within the research community because they lack the extreme hardness or high thermal stability of their counterparts.

A key advantage of polymer-like a-C:H materials is their exceptional property tunability through post-processing techniques. Specifically, curing via ultraviolet C (UV-C, 200-280 nm) radiation has proven to be a highly effective method for modifying their characteristics. When these films are irradiated under ambient conditions, the interaction between UV-C light and atmospheric molecules generates oxygen radicals and ozone (O_3). Simultaneously, the high-energy photons facilitate the removal of hydrogen atoms from the film surface, creating a high density of dangling bonds.

In this study, polymer-like a-C:H films were synthesized on silicon (Si) substrates using plasma-enhanced chemical vapor deposition (PECVD) with a cyclohexane precursor. The deposition was performed with plasma power varied between 20 and 80 W. Subsequent UV-C irradiation at a wavelength of 275 nm was applied to the samples, utilizing irradiances of 0.0022 and 0.0466 W/cm^2 for durations of 1 and 4 hours.

Experimental results indicated that UV-C treatment led to a reduction in film thickness. However, the films maintained their optically transparent and topological smoothness. Surface analysis revealed a substantial increase in wettability, while the optical bandgap values showed a clear downward trend following UV-C irradiation. Fourier transform infrared (FTIR) spectroscopy confirmed the underlying chemical changes: a reduction in CH_x peak intensity indicated hydrogen removal, while an increase in C=O peak intensity, implying oxygen incorporation and structural rearrangement. It is proposed that unbound carbon and hydrogen atoms present within the as-deposited film reacted to form C=O and O–H bonds, respectively, during the UV-C curing process. This study demonstrates that UV-C irradiation serves as a critical mechanism for

precisely tuning the composition and functional properties of polymer-like a-C:H films.

9:15am **AM1+EM+TF-FrM-5 Aerosol–Assisted CVD of NbN Using Novel Thermally Stable Niobium Imido Single–Source Precursors**, ***Narender Kumar***, *Nariman Neekzad, Hao Hung Chen, Tatsuya Kasai, Lisa McElwee White,* University of Florida

Transition–metal nitrides are attracting intense interest for next–generation electronic and superconducting technologies because of their exceptional thermal stability, chemical inertness, and tunable electronic properties. Niobium nitride (NbN) combines a relatively high superconducting critical temperature (≈ 16 K) with a large critical current density, enabling its use in superconducting nanowire single–photon detectors and as an ultrathin Cu diffusion barrier in CMOS interconnects. However, achieving high-quality NbN thin films with precise stoichiometry and conformal coverage at the nanoscale remains a persistent challenge. We report a new class of thermally robust, clean–decomposing niobium imido–based single–source precursors designed for low–temperature aerosol–assisted chemical vapor deposition (AACVD). The strong Nb–N imido bond ensures delivery of the correct metal–nitrogen stoichiometry. The precursors were fully characterized by multinuclear NMR spectroscopy, single–crystal X–ray diffraction, and thermogravimetric analysis, confirming their structural integrity and favorable thermal behavior. Preliminary AACVD experiments demonstrate efficient precursor transport and the formation of NbN thin films, which were analyzed using SEM and XRD.

9:30am **AM1+EM+TF-FrM-6 Ta Doping in MBE Grown WSe_2 2D Semiconductor**, ***Daniel Stokes***, *Stephen McDonnell,* University of Virginia; *David Lawrence,* James Madison University

Two-dimensional (2D) transition metal dichalcogenides (TMDCs) present a range of novel and tunable electronic properties. 2D TMDC semiconductors have potential applications in highly scaled devices owing to their direct electronic bandgap in the single-layer limit and their surface free of dangling bonds. To incorporate 2D TMDC semiconductors into devices, they must be able to be synthesized with high purity and controllably electronically doped. We present results on Ta doping during molecular beam epitaxy (MBE) growth of WSe_2 thin films grown on sapphire substrate. The electrical characteristics of the films indicate that we can controllably introduce Ta dopant atoms during synthesis to tune the resistivity, charge carrier concentration, and charge carrier mobility of WSe_2.

9:45am **AM1+EM+TF-FrM-7 Multilinear Regression Modeling of SiO_2 PECVD Deposition Based on Full Factorial Experiments**, *Tarun Maredla, Rohit Surikuchi, David Barth,* ***Lucas Barreto,*** University of Pennsylvania

Silicon dioxide is a fundamental material in microelectronics, MEMS, optical coatings, and several other technological areas. In many of these applications, SiO_2 must be deposited as a thin film with controlled optical and physical properties. Plasma Enhanced Chemical Vapor Deposition, PECVD, is widely used for this purpose because it enables high-throughput deposition, good process control, and relatively low deposition temperatures. However, PECVD offers a broad and flexible set of deposition conditions, and these parameters are often strongly coupled. Therefore, process optimization based on a One Variable at a Time, OVAT, approach may neglect important interactions between deposition parameters.

In this work, we present a replicated full factorial experimental design study of the SiO_2 PECVD deposition process. Silane, SiH_4, and nitrous oxide, N_2O, are used as the main precursors, and the deposited film properties are measured by ellipsometry. Four process factors are investigated: deposition temperature, chamber pressure, RF power, and silane flow. Two responses are evaluated: refractive index and deposition rate. A multilinear regression model is used to describe the dependence of the responses on the process factors and their interactions. Analysis of variance, ANOVA, is applied to validate the model and assess its predictive capability. The results show that the regression model provides an excellent estimate of the measured responses. Based on coefficient p-values, the most influential process parameters and statistically significant interaction terms are identified, providing a systematic framework for optimizing SiO_2 PECVD thin film deposition.

The results indicate that deposition temperature strongly affects the SiO_2 refractive index, while it has no statistically significant impact on deposition rate within the investigated factor range. In contrast, the remaining factors contribute significantly to one or both responses. In addition, second-order interaction terms are essential for accurately describing the experimental results, since excluding them leads to poor model performance. This confirms that the deposition parameters are coupled and must be considered jointly for an adequate description of the process. Therefore, an OVAT approach may neglect critical factor effects and interactions during process modeling and optimization. The proposed methodology provides a detailed and accurate description of SiO_2 PECVD deposition within the investigated process window and can be used to guide process optimization toward desired film properties.

10:00am **AM1+EM+TF-FrM-8 Transition Metal-Doped Sodium Niobate Thin Films: Microstructure, Ferroelectric Phase Stabilization, and Implications for Plasma-Assisted Catalysis**, ***Shanza Baig***, *Muhammad Abdullah, Vagif Mammadzada, Baharak Sajjadi,* University of Oklahoma

Non-thermal plasma catalysis offers a practical route to activate stable molecules such as methane and carbon dioxide without the high temperatures required by conventional thermal processes. A key challenge, however, is that most existing catalysts are not designed for plasma environments, where energetic electrons, strong electric fields, and non-equilibrium reactive species control the surface chemistry. Ferroelectric materials are attractive in this context because their spontaneous polarization can concentrate local electric fields, increase electron density at active sites, and strengthen plasma-surface interactions relevant to molecular activation. Sodium niobate ($NaNbO_3$) is a perovskite oxide with a well-known antiferroelectric-ferroelectric phase competition that is sensitive to composition and microstructure. In bulk form, $NaNbO_3$ is predominantly antiferroelectric at room temperature, but B-site doping and thin-film strain have been shown to shift the phase balance toward ferroelectric ordering and improve polarization switching. Thin-film geometries are particularly useful here, as they introduce lattice strain and modify grain structure in ways that are difficult to achieve in bulk ceramics. In this study, $NaNbO_3$ thin films were doped with 1 mol% Fe, Ni, and Cu at the B-site to understand how each transition metal influences grain growth, microstructure, and ferroelectric response. Fe, Ni, and Cu were selected because they vary in ionic radius and valence state and are therefore likely to distort the NbO_6 octahedra differently, introduce different defect types, and shift the polarization response in distinct ways. The intent was to determine whether these dopant-driven structural changes, alongside the strain naturally present in thin films, are sufficient to push the material toward a stable ferroelectric phase with reliable polarization switching. Stronger ferroelectric behavior in these films should enhance local field concentration and encourage microdischarge formation under plasma conditions, which directly affects plasma intensity and the efficiency of electron-driven activation. The broader aim of this work is to clarify how dopant chemistry and thin-film microstructure together control polarization behavior in $NaNbO_3$, and to use that understanding to guide the development of ferroelectric catalysts for greenhouse gas conversion.

Advanced Microelectronic Materials and Devices Mini-Symposium
Room 318 - Session AM2+EM+TF-FrM

Devices II

Moderators: Dr. Samantha Jaszewski, Sandia National Labs, **Somil Rathi**, Arizona State University

10:30am **AM2+EM+TF-FrM-10 Development of Metallic Gate Stacks at Atomic Scale : Application to Advanced FD-SOI Transistors**, ***Elouan Le Cun***, *Julien Patouillard, Rémy Gassilloud, Mathieu Bernard, Zdenek Chalupa, Krunoslav Romanjek, Wissem Baik, William Vandendaele, Elhadji-Alhousseyni Diallo, Tadeu Mota Frutuoso, Pauline Hauchecorne, Virginie Loup, Théo Cabaret, Frédérique Glowacki, Mouaad Yassine Aliouat, Elise Arnoux, Gennie Garnier, Marie-Claire Cyrille, Olivier Renault, Claire Fenouillet-Béranger,* CEA-LETI, France

Fully-Depleted Silicon On Insulator (FDSOI) planar technology - an alternative to FinFET (3D field effect transistors) - address technologies involving very high energy efficiency, ultralow power consumption and cost reduction. 10 nm FD-SOI transistor requires complex metal on insulator (MOS) gate stacks. The MOS structure is composed of doped titanium nitride layers as metal gates, and SiON/HfON as gate-dielectric[1]. SiON is also called gate interlayer (IL). Thinning TiN layers results in better MOS performances. This is due to a known phenomenon called IL scavenging, where TiN acts as an oxygen reducer of the IL, which in turn reduces the IL thickness[2]. The targeted TiN thickness in the 10 nm-node FDSOI is closed to 2 nm, and the required equivalent oxide thickness (the electrical thickness of the IL/HfON insulator stack) is below 0,8 nm. As the layers

thicknesses reach the nm-scale, it introduces new challenges regarding the electrical behavior of the MOSFET due to the heterogeneity of the materials in the gate stacks.

To address those challenges, the developments of an ultra-thin 2 nm metallic gate stack with sub-stoichiometric titanium nitride ($TiN_{x<1}$) are required. CEA-Leti has acquired a PVD deposition tool by co-sputtering to deposit complex metallic layers on 300 mm silicon wafers with an atomic-scale thickness control.

This study examines TiN_x ultra-thin films with thicknesses below 5 nm. TiN_x structural, optical and electrical properties are evaluated by X-Ray Reflectivity (XRR), stress measurements, sheet resistance measurements, spectroscopic ellipsometry, X-Ray Photoelectron Spectroscopy (XPS) and X-Ray Diffraction (XRD). TiN_x layer composition is investigated by Elastic Recoil Detection Analysis (ERDA) and X-Ray Fluorescence (XRF) analysis. Those layers have been integrated on simplified electrical devices to evaluate their impact on transistor key performance parameters (EOT, Vt, Jg, ...).

This work was carried out in the framework of the FAMES Pilot Line of the Chips JU and the Platform for Nanocharacterisation (PFNC) funded by Horizon Europe grant 101182279, ANR NextGen project ANR-22-NEXTG-001, ANR programs “Recherche Technologique de Base” and "France 2030 - ANR-22-PEEL-0014".

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[2] T. Ando et al., Ultimate Scaling of High-κ Gate Dielectrics: Higher-κ or Interfacial Layer Scavenging, Materials 2012, 5, 478-500

10:45am **AM2+EM+TF-FrM-11 Towards Ordered Growth of Complex Oxide Thin Films for Memristive Devices**, ***Michael Mitchell***, *Xianchao Dong, Shweta Joshi, Tianshu Li, Gina Adam,* George Washington University

We present progress towards the ordered growth of the entropy-stabilized oxide, $(MgNiCoCuZn)_{0.2}O$, via reactive magnetron sputtering for the fabrication of memristive devices. To produce this film, the authors leveraged a custom-designed AJA ATC system with off-axis capabilities to reduce deposited atom kinetic energy and improve film crystallinity. The proposed methodology uses co-sputtering of multiple metal alloy targets in an oxygen-rich environment. Depositions are conducted at multiple substrate temperatures to identify phase transition temperatures. In addition to 100-oriented silicon, substrates composed of materials with improved lattice matching to literature values of $(MgNiCoCuZn)_{0.2}O$ are employed, and the relationship between substrate material and phase transition temperature is investigated. Various microscopic and spectroscopic characterization techniques, including Atomic Force Microscopy (AFM) and Energy Dispersive X-ray Spectroscopy (EDS), etc., were used to determine the film growth rate and stoichiometry. Molecular Dynamics simulations, with interatomic interactions provided by fine-tunned machine learning models, are employed to study the relationship between phase transition temperature and substrate composition. The computational findings for the influence of substrate composition and deposition stoichiometry on the phase transition temperature are then compared with the experimental results. The pathways for integration of the resulting film into memristive devices are also discussed.

11:00am **AM2+EM+TF-FrM-12 Electron beam lithography enabled nano EC-RAM development and fabrication**, ***Stefan Theodoru***, *Garry Rubloff,* UMD College Park*; Marshall Schroeder,* DEVCOM ARL

The exponential increase of computing demand is currently only being met with <10% improvement of computational power density per chip generation. Improvements in energy consumption have not kept pace with either industry demand or grid capacity. Electrochemical random-access memory (EC-RAM) is well postured to fulfill this demand, boasting six orders of magnitude modeled energy consumption lower than CMOS technology. EC-RAM models predict downscaling energy consumption based on micron scale devices which should at the nano scale deliver atto J cost per computation compared to the current pico J state of the art. Further boons to EC-RAM include its intrinsic non-volatility, analog states, and co-located compute and memory centers. This makes EC-RAM ideal for use in neural network computation. Scaling studies to prove these modeled results have not yet been conducted in the sub 100nm regime however, leaving a large gap between EC-RAM’s modeled capabilities, and what has been experimentally proven.

This presentation describes the process development done to fabricate Au, TiO_2, and LiPON EC-RAM devices and the results of their characterization. We use TiO_2 for its wide range of conductance states as a function of Li content. While LiPON is both well known to the research group, and provides a source of Li provided during the LiPON deposition. Process development was needed to develop sub 100nm feature separation/widths using electron beam lithography, as well as to allow for nanolithography of the reactive LiPON film (Fig.2). Devices built for performance use the vertical architecture, see Fig.1, which minimizes the ion diffusion pathway. Devices built to allow for characterization using Raman and Plume SEM use the lateral architecture, see Fig.3. Both architectures have channels defined by the width of the source/drain and their separation, and have asymmetric and symmetric variants which allow us to test the impact of having a Li reservoir on device performance. The most important parameters for defining EC-RAM performance are state change speed, retention, and cycle life of the device. State change speed is the time it takes to intercalate enough Li^+ ions into the channel that the conductivity, as read by a bias across source and drain, changes to encode a unique conductance state. Retention is defined as the time that a written state endures with no applied gate voltage. The analysis of these characterization results and process development elucidate ideal EC-RAM architecture and fabrication methodology.

11:15am **AM2+EM+TF-FrM-13 Limitations of Layered Dielectrics**, ***Peter Dickens***, *Brianna Klein, Andrew Binder,* Sandia National Laboratories, USA

Next-generation power conversion systems increasingly rely on SiC power MOSFETs to minimize switching losses and maximize power density. Conventional SiO_2 gate dielectrics limits maximizing the gate capacitance and drive current, making higher-k dielectrics attractive to improve switching characteristics.However, to date, severe defect densities at the direct high-k/SiC interface has prevented strict high-k adoption.Consequently, recent work has focused on utilizing a dielectric bilayer with SiO_2 serving as the interface dielectric with SiC to enable low defect densities and a high-k stacked on top in an attempt to gain the “best of both worlds”.Despite some reported successes, there remain critical gaps discussing what fundamental advantages or limitations exist from this dielectric bilayer approach.

In this presentation, we present analysis of the available design space for layered dielectrics in SiC-based MOSFETs.Our analysis operates under three fundamental assumptions related to applied gate bias, avoidance of time-dependent-dielectric-breakdown (TDDB), and the requirement to be high-k (effective dielectric permittivity greater than the permittivity of the semiconductor).We show that when these assumptions are applied then the available design space for layered dielectrics is quite limited and calls into question advantages of a layered approach.

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Atomic Scale Processing Mini-Symposium
Room 316 - Session AP1+EL+PS+TF-FrM

Thermal and Plasma-Enhanced ALD

Moderators: Dr. Sagar Udyavara, LAM Research, **Dr. Virginia Wheeler**, U.S. Naval Research Laboratory

8:15am **AP1+EL+PS+TF-FrM-1 Analyzing Plasma-Enhanced ALD of III-Nitrides via Experimental and Theoretical Studies**, *Steven Allaby, Heba Saleh, Fatih Bayansal,* ***Necmi Biyikli***, University of Connecticut **INVITED**

Research efforts on low-temperature (T < 300 °C) synthesis of crystalline III-nitride thin films using plasma-assisted ALD utilized various reactor configurations featuring different plasma sources. While our early III-nitride growth experiments using quartz-based ICP sources resulted in nanocrystalline/amorphous films with elevated oxygen impurities, shifting to stainless-steel based hollow-cathode plasma sources revealed highly (002) oriented polycrystalline III-nitride films on Si(100) and sapphire substrates. Upon further modification of the hollow-cathode plasma source

and reactor chamber design, we have achieved monocrystalline AlN, quasi-epitaxial GaN and (002) oriented InN films on sapphire substrates at a common growth temperature of 200 ℃.

The films were deposited using conventional metal-alkyl precursors (trimethylaluminum, triethylgallium, trimethylindium) and various nitrogen plasmas (N_2/H_2/Ar, N_2/H_2, N_2/Ar, and N_2-only) as metal precursor and nitrogen co-reactant, respectively. *In-situ* ellipsometry and optical emission spectroscopy (OES) were employed to monitor the surface ligand-exchange reactions, plasma surface interactions, and formed reaction byproducts in real-time. *Ex-situ* spectroscopic ellipsometry measurements revealed the film thickness variation, growth-per-cycle (GPC) and optical properties of the III-nitride films. When compared to reference films grown on Si(100) substrates, growth-per-cycle (GPC) values obtained for III-nitride films on c-plane sapphire substrates showed a notable increase. Moreover, a significant improvement of crystalline order has been observed for all binary nitride films grown on sapphire substrates, achieving or approaching epitaxial quality films. We attribute this significant improvement in crystal quality to the synergistic impact of customized HCP-ALD reactor, large-diameter third-generation hollow-cathode plasma source, and optimized growth conditions (plasma gas mixture, rf-power, pressure).

To gain further insight into how different plasma mixtures and radical species affect III-nitride film quality, we have carried out density functional theory (DFT) based simulations of both metal-organic and plasma half cycles. The computational studies revealed how different adsorbed metal-organic precursor surface groups interact with hydrogen and nitrogen radicals by depicting energetically favorable reaction routes. These results are compared and correlated with the experimental observations, deciphering the critical role of hydrogen radicals.

8:45am **AP1+EL+PS+TF-FrM-3 Optical Bandgap and Thermal Stability Driven High–κ Engineering of HfAlO Dielectrics on a 200 mm ALD Platform**, ***Partha Mukhopadhyay***, *Zuriel Caribe, Ivan Fletcher, Jim Fulford,* Tokyo Electron America, USA

This work demonstrates the tunable high–κ, optical, and thermal stability characteristics of hafnium aluminate ($Hf_xAl_{1-x}O$) thin films synthesized using a 200 mm high–volume batch atomic layer deposition (ALD) platform. Precise monolayer–level engineering of HfO_2/Al_2O_3 superlattice structures enables controlled Al incorporation, which systematically modulates the optical bandgap, dielectric constant, and electrical structure of the alloy. A key outcome is that increasing Al content systematically increases the optical bandgap of the alloy from 5.5 – 6.5 eV, accompanied by improved film density and structural uniformity, which directly influences the dielectric response and reliability of the material.

At lower Al content (~0.31), the alloy exhibits superior dielectric properties with κ > 22 and a capacitance density of 12.46 fF/μm^2, representing ~29% enhancement over HfO_2, attributed to suppressed oxygen vacancies and reduced trap density. With increasing Al composition, the widened bandgap increases barrier height, resulting in reduced leakage current and improved dielectric robustness. A higher Al fraction (~0.56) demonstrates a breakdown electric field of ~8 MV/cm, exceeding HfO_2 by over 3 MV/cm, while maintaining low leakage (~10^{-6} A/cm^2) even after 650 ℃ annealing. Notably, increasing Al content significantly enhances the thermal budget of the dielectric stack, stabilizing the amorphous phase and preventing dielectric degradation at elevated temperatures, while preserving relatively high κ values compared to pure Al_2O_3.

XPS analysis reveals systematic shifts of Hf4f and Al2p peaks toward higher binding energies with increasing Al concentration, indicating modified bonding characteristics and enhanced ionic contributions, consistent with bandgap widening and improved film stability. These electronic structure changes correlate with reduced surface charge transfer effects and improved dielectric integrity. Additionally, the films exhibit excellent capacitance linearity over applied voltage and stable frequency response, making them highly suitable for RF applications.

The 200 mm batch ALD platform ensures excellent uniformity, repeatability, and scalability for compositionally engineered dielectrics. Overall, this study highlights that Al–content–driven optical bandgap tuning, coupled with improved thermal stability and enhanced breakdown strength, provides a powerful route to customize high–κ behavior in HfAlO. This enables optimized performance trade–offs between capacitance density, leakage, and reliability, making HfAlO a compelling material system for advanced MIM capacitors in BEOL, RF, and memory technologies.

9:00am **AP1+EL+PS+TF-FrM-4 Atomic Layer Deposition Metal and Barrier Layers Enabling Next Generation Interconnects**, *Matthew Weimer, Sara Harris,* Forge Nano; *Thomas Moffat,* NIST-Gaithersburg; *Dane Lindblad,* Forge Nano; *Daniel Josell,* NIST-Gaithersburg; ***Arrelaine Dameron***, Forge Nano

Device miniaturization continues to push the technological boundaries of manufacturing processes and integrated circuit (IC) manufacturing must keep pace to meet the design requirements for next-gen transistors. Back end of line (BOEL) fabrication poses several challenges to chip scaling: most notoriously the copper bottleneck in which thick barrier layers and resistance capacitance (RC) delays limit functional interconnect pitch to 21 nanometers [1]. To overcome this critical barrier, low resistivity, conformal metal films have been studied for hybrid metallization; decreasing interconnect resistance and reducing barrier layer thicknesses. As interconnect pitch decreases line-of-sight PVD copper barrier/seed layers experience pinch off and void formation [2]. This work explores the use of ruthenium (Ru) and lower resistivity thermal ALD iridium (Ir) thin films for copper seed layers to enable next generation interconnects. Thermal ALD Ir and Ru deposited at 250 ℃ both demonstrate conformal deposition on 10:1 aspect ratio through glass vias (TGVs) and show void free copper fill using a cyclic pulsed electrochemical deposition process. Deposited in partnership with ALD SiO2 and TiN layers, this completes a metal barrier seed solution for TSVs. As expected, the primary difference between the Ir and Ru is electrical resistivity. Seed film resistivity as deposited on TGVs was measured using four-point probe; a 10 nm Ru film measured 41 μΩ·cm and a 10 nm Ir film measured 16 μΩ·cm. Successful copper electrochemical deposition (ECD) at various ECD potentials, was completed with 10 nm of Ir with (resistivity 16 μΩ·cm) and 20 nm of Ru (resistivity 22 μΩ·cm) with the full layer stack for these film shown in Figure 1. Reduction in required layer thickness combined with improved electrical properties and demonstrated conformality can serve as crucial steps forward for advanced interconnects and BEOL architecture. Additionally, this work compares Ir film quality as deposited at 250 ℃ and 300 ℃. Ir deposited at 300 ℃ exhibits improved environmental stability when compared to 250 ℃ Ir as measured with 4-point probe after aging in atmosphere over several months. 300 ℃ Ir also shows a shortened nucleation delay, and optical constants (n and k) more closely aligned to bulk Ir values, as measured with spectroscopic ellipsometry. Ir film characterization for both temperatures including XPS, XRR, XRD and AFM is ongoing, and will be presented

9:15am **AP1+EL+PS+TF-FrM-5 Tuning the Mechanical Properties of Silica Aerogels Using Atomic Layer Deposition**, ***Victor Vogt***, *Ali Madanchi, Katherine Rybkin, Andrés Miranda Mañón, Andrej Lenert, M.D. Thouless, Neil Dasgupta,* University of Michigan

Silica aerogels are a key material used in aerospace, catalysis, and energy applications due to their ultralow density and thermal conductivity as well as high solar transparency. Specifically, they show promise as an emerging transparent insulating material in concentrating solar thermal energy generation.[1] In our recent work we have shown that atomic layer deposition (ALD) can be used to improve the thermal stability of silica aerogels at high temperatures of up to 800 ℃.[2,3] This was attributed to the ability of ALD to conformally modify the pore structure of the aerogels and form a more thermally stable phase at the surface. However, silica aerogels also suffer from low strength and fracture toughness, restricting their potential applications and making practical implementation difficult due to the risk of brittle fracture in assembly or operation.

In this study, we utilize sub-nanometer ALD treatments to conformally modify silica aerogels with aspect ratios > 100,000:1. We demonstrate a monotonic increase in stiffness with increasing number of ALD cycles, resulting in a ~30-fold increase in elastic modulus after 3 cycles of Al_2O_3 (nominal ~4 Å thickness). This result is investigated using finite element modeling (FEM) of the aerogel nanostructure, which reveals the key factors which drive the large increase in elastic modulus. Furthermore, we show that ALD increases the fracture toughness of the aerogels, resulting in a ~7-fold increase in fracture toughness after 3 ALD cycles. Due to the ultra-thin and conformal nature of the ALD layer, the porous nanostructure is maintained, allowing the aerogels to maintain high solar transparency and low thermal conductivity. This method enables a pathway to broader applications for silica aerogels through improving their mechanical durability while maintaining the favorable properties of low thermal conductivity and high optical transparency over a range of operating temperatures.

References:

[1] McEnaney, K., Weinstein, L., Kraemer, D., Ghasemi, H. & Chen, G. Aerogel-based solar thermal receivers. *Nano Energy* **40**, 180–186 (2017).

[2] A.J. Gayle, Z.J. Berquist, Y. Chen, A.J. Hill, J.Y. Hoffman, A.R. Bielinski, A. Lenert, and N.P. Dasgupta, Tunable Atomic Layer Deposition into Ultra-High-Aspect-Ratio (>60000:1) Aerogel Monoliths Enabled by Transport Modeling, *Chem. Mater.* **33** (14), 5572-5583 (2021).

[3] Z.J. Berquist, A.J. Gayle, N.P. Dasgupta, and A. Lenert, Transparent Refractory Aerogels for Efficient Spectral Control in High-Temperature Solar Power Generation. *Adv. Funct. Mater.* **32**, 2108774 (2022).

9:30am **AP1+EL+PS+TF-FrM-6 Multilayer FUV Coatings Using ALD-Grown LaF_3 and ZrF_4, *John Hennessy,*** Jet Propulsion Laboratory

We report on the targeted development of atomic layer deposition processes for high-refractive-index metal fluorides, specifically focusing on lanthanum fluoride and zirconium fluoride. The primary objective is to integrate these ALD-deposited materials into multilayer optical coatings designed for demanding far-ultraviolet (FUV) applications. By successfully combining ALD processes for lanthanum and zirconium fluorides with established processes for lower-index materials, we enable the fabrication of specialized optical components that are critical to various NASA applications. As a demonstration of this ALD capability, a 16-layer AlF_3/LaF_3 mirror was fabricated and shown to achieve an average reflectance exceeding 90% within a band centered around 140 nm. Finally, we discuss the prospects for increasing coating complexity and further optimizing FUV performance.

9:45am **AP1+EL+PS+TF-FrM-7 Controlling the Crystallinity of V_2O_5 Deposited by Plasma-Enhanced Atomic Layer Deposition*, Scott Walton,*** *Peter Litwin, Neeraj Nepal, Maria Sales, David Boris, Michael Johnson, Mackenzie Meyer, Virginia Wheeler,* Naval Research Laboratory

Plasma-enhanced atomic layer deposition (PEALD) is a low temperature, conformal, layer-by-layer deposition technique that is based on a pair of self-terminating and self-limiting gas-surface half-reactions, in which at least one half-reaction involves species from a plasma. This approach to ALD generally offers the benefit of substantially reduced growth temperatures and greater flexibility in tailoring the gas-phase chemistry to produce amorphous, crystalline, and epitaxial films of varying types and characteristics. Importantly, by carefully controlling the plasma properties, it has been shown that the degree of crystallinity and phase selection is possible.

In this work, we demonstrate the ability to manage the crystallinity of V_2O_5 through careful control of the plasma characteristics during growth in a Kurt J. Lesker 150 LX PEALD system. We employ both plasma diagnostics and material characterization techniques to understand the process-to-structure-property relationship while varying the input power, operating pressure, and gas flow ratio. Optical emission spectroscopy (OES) and Langmuir probe measurements are used to characterize the production and delivery of energetic and reactive species to the growing film surface, while x-ray photoelectron spectroscopy (XPS) and Raman spectroscopy are used to characterize the physico-chemical properties of the V_2O_5 films. We find that by varying the operating pressure in the system during the plasma process, the films can be selectively deposited in an amorphous or crystalline state. We link the transition from amorphous to crystalline material to the energy flux density delivered to the material surface during deposition and derive an estimate of the critical energy flux density necessary for crystallization. Lastly, we discuss these results more broadly and the applicability of these findings to other material systems. This work is supported by the Naval Research Laboratory base program.

10:00am **AP1+EL+PS+TF-FrM-8 Epitaxial Growth of VN on Si_3N_4(0001)/Si(111) Using Molecular Beam Epitaxy*, Nuri Oncel,*** *Mehmet Ozdogan, Carlos Munoz, Deniz Cakir,* University of North Dakota*; Randy Duma,* Quantum Design*; Rajendra Dulal,* University of North Dakota

We report on the epitaxial growth of VN thin films on β-Si_3N_4 (0001)/Si(111) substrates using molecular beam epitaxy. The growth process and resulting film properties were systematically investigated using in-situ reflection high-energy electron diffraction (RHEED) and ex-situ scanning/transmission electron microscopy (S/TEM), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), energy-dispersive spectroscopy (EDS), and electrical transport measurements. RHEED and cross-sectional TEM analyses confirm the formation of epitaxial VN(111) films, with growth proceeding via a Volmer–Weber Island mechanism followed by coalescence. Increasing nitrogen flux during deposition significantly improves film continuity, stoichiometry, and crystalline quality. Structural characterization reveals an azimuthally aligned epitaxial relationship without the expected in-plane rotational reconstruction, indicating that interfacial bonding and strain relaxation dominate over simple lattice-mismatch considerations. XPS and EDS measurements confirm near-stoichiometric VN composition with reduced oxygen incorporation at higher nitrogen flux. Electrical measurements demonstrate ohmic transport across the VN/Si_3N_4/Si heterostructure, suggesting efficient carrier transport through the ultrathin dielectric layer via tunneling or defect-assisted conduction. Low-temperature transport measurements reveal a suppressed superconducting transition temperature relative to bulk and oxide-supported VN films, attributed to compressive strain and structural disorder. These results establish Si3N4(0001)/Si(111) as a viable platform for integrating epitaxial VN with semiconductor technology and provide insight into nitride–nitride heteroepitaxy and interface-driven property modulation.

Atomic Scale Processing Mini-Symposium
Room 316 - Session AP2+EL+PS+TF-FrM

Enabling Atomic Scale Processing (ALD/ALE) by leveraging new Precursors and Surface Reactions

Moderators: Prof. Austin Minnich, California Institute of Technology, **Dr. Angel Yanguas-Gil**, Argonne National Laboratory

10:30am **AP2+EL+PS+TF-FrM-10 Plasma-Enhanced ALD of SiO_2 with an Alternative Precursor: From Mechanistic Insight to Area-Selective Deposition*, James Jensen,*** *Jay Swarup, James Engstrom,* Cornell University

Silicon dioxide (SiO_2) is and has been an extremely important thin film material in microelectronics and related fields.The great majority of approaches to atomic layer deposition (ALD) of SiO_2 involve the use of plasma since, for example, the Si-H bond is resistant to reaction with molecules such as H_2O and O_2.We have examined the use of an alternative Si precursor, which we refer to as di-isopropylamido trisilylamine [DiPA(TSA)], employing an O_2 plasma as the co-reactant. The precursor contains only Si-N and Si-H bonds.We have investigated the process using *in situ* real time quartz crystal microbalance (QCM) techniques in a custom-built hot-wall reactor, which provides detailed insight into the half-reactions, and the presence of nucleation delay.We find that ALD with DiPA(TSA) occurs over a large temperature window, spanning a range of T = 120 – 285°C.The thickness deposited per cycle decreases with increasing temperature, from 4.7 Å-cycle^{-1} at T = 120°C to 2.9 Å-cycle^{-1} at T = 285°C.These rather large rates of growth from ALD reflect the silicon content in the precursor (three atoms per molecule).From QCM a nearly complete loss of the di-isopropylamido ligand is implicated in the precursor half reaction.The deposited thin films have been characterized using *ex situ* X-ray photoelectron spectroscopy (XPS), X-ray reflectivity (XRR), spectroscopic ellipsometry (SE) and atomic force microscopy (AFM).From XPS we find that the thin films are near stoichiometric (O:Si ~ 1.9) over the entire range of temperatures, while the expected impurities (e.g., C, N) are < 1%.From XRR we find that the thin film density increases from 2.24 g-cm^{-3} at T = 120 °C, to 2.38 g-cm^{-3} at T = 285 °C, which can be compared to the values for amorphous silica (2.20), and quartz (2.65).From AFM we find that the thin films are continuous and smooth exhibiting an average roughness of 0.54 nm at T = 120 °C (19 nm thick film), and 0.30 nm at T = 285 °C (13 nm thick film).Finally, we have conducted a preliminary set of studies concerning blocking PE-ALD growth of SiO_2 on Al_2O_3 using acetylacetone (Hacac) and we find the deposition can be blocked for at least 10 cycles, over the temperature range T = 120-285 °C.

10:45am **AP2+EL+PS+TF-FrM-11 Temperature-Dependent Growth Behavior of Aluminum Oxide Using Dimethylaluminum Isopropoxide and Water*, Azeez O. Musa,*** University of Missouri-Columbia*; Hemant Kumar, Campbell Sweet,* University of Missouri, Columbia*; Justin R. Walensky,* University of Missouri-Columbia*; Matthias J. Young,* University of Missouri, Columbia

Area-selective atomic layer deposition (AS-ALD) requires precursors with controlled surface reactivity to enable selective film growth on targeted regions while minimizing unwanted nucleation on non-growth surfaces. Dimethylaluminum isopropoxide (DMAI) has emerged as a promising alternative to trimethylaluminum (TMA) for AS-ALD applications due to its reduced reactivity and non-pyrophoric nature. However, experimental mechanistic studies of DMAI/H_2O ALD and the influence of deposition temperature on growth behavior remain limited. In this work, the temperature-dependent growth characteristics of Al_2O_3 ALD using DMAI and H_2O were investigated using in situ quartz crystal microbalance (QCM) measurements together with ex situ X-ray photoelectron spectroscopy

(XPS), Fourier-transform infrared spectroscopy (FTIR), and spectroscopic ellipsometry. DMAI was synthesized from aluminum isopropoxide and trimethylaluminum in 79% yield and >95% purity, with product formation confirmed by ^{1}H NMR spectroscopy. Real-time QCM measurements were used to examine precursor adsorption, ligand removal behavior, saturation conditions, and mass gain per cycle (MGPC) between 100 and 200 °C. Al_2O_3 growth at 100 °C exhibited a lower MGPC (~19 ng cm^{-2} cycle^{-1}) and less stable saturation behavior compared to films deposited between 150 and 200 °C, where the average MGPC remained approximately constant at ~29 ng cm^{-2} cycle^{-1}. Single-cycle QCM analysis further revealed distinct differences in surface reaction behavior between low- and intermediate-temperature growth regimes. These findings provide experimental insight into DMAI/H_2O ALD surface chemistry and establish growth conditions relevant to the development of DMAI-based AS-ALD processes.

11:00am **AP2+EL+PS+TF-FrM-12 Void-free Thermal ALD BaTiO3 Thin Films Prepared by Removing Water Dose after Ba Precursor**, ***Jiayi Chen***, Georgia Institute of Technology, China; *Mark Losego,* Georgia Institute of Technology, USA; *Asif Khan,* Georgia Institute of Technology

This talk will discuss our efforts to develop a robust atomic layer deposition process (ALD) to create ferroelectric $BaTiO_3$ (BTO) thin films using Bis-(1,2,4 triisopropylcyclopentadienyl)-Barium and Titanium Isopropoxide precursors.Ferroelectric materials are potential candidates for future low voltage RAM and NAND memory because of their reversible two polarization states under low external electric field. While the CMOS compatible gate dielectric materials HfO_2 and $Hf_{0.5}Zr_{0.5}O_2$ are ferroelectric, they have high coercive fields that make it difficult to lower switching voltages below 1 V. Therefore, perovskite ferroelectric materials, like $BaTiO_3$ are desirable to use for these applications because their coercive voltages can be an order of magnitude lower, approaching 0.1 V.However, these ferroelectric films must be deposited by ALD to match the conformality and small thickness requirements desired for RAM and NAND memory. While reports exist for ALD processes of these materials, most if not all those reports use ALD recipe of “A metal precursor – oxidant – B metal precursor – oxidant”. This talk will present our finding that high quality BTO films can still be deposited with recipe in the form of “H_2O – Ba – Ti” or “H_2O – Ba – Ba – Ti”. A hypothetical ALD chemistry mechanism is proposed. These reactions can happen at 280 °C, but not 220 °C. Inverting the precursor sequence, such that H_2O – Ti – Ba, does not work. XRD confirms the formation of BTO crystal lattices through these novel recipes. One benefit of these recipes is getting void-free BTO films after annealing, whereas our previous studies show that conventional ALD recipes produce BTO films with voids because of the evaporation of H_2O during annealing. 40 nm BTO film deposited with this dehydration recipe shows high dielectric constant of 72 with low dielectric loss at the magnitude of 10^{-3}.

11:15am **AP2+EL+PS+TF-FrM-13 Optimizing Molybdenum Pentachloride Delivery for Vapor Deposition Processes**, ***James Maslar***, *Vladimir Khromchenko, Berc Kalanyan,* NIST-Gaithersburg

Molybdenum metal has favorable properties for ultrathin layers compared to metals such as copper and tungsten and, therefore, has attracted much recent interest as a potential material for interconnects and gate metallization. A common method for forming ultrathin metal layers in high volume manufacturing is vapor deposition. For vapor deposition of molybdenum metal layers, molybdenum pentachloride is a common precursor. However, molybdenum pentachloride is a solid and can be difficult to reproducibly deliver from the precursor canister to the deposition surface in a tool, depending on delivery conditions and canister design. Also of concern is the presence of molybdenum oxychloride impurity species in the canister, and whether the oxychlorides are being generated during delivery or are present in the supplied material. The primary goal of this study was to characterize the process space for pulsed delivery of molybdenum pentachloride with respect to overall mass carryover, pulse-to-pulse stability, and impurity evolution. The approach used in this study was to quantify the amount of molybdenum pentachloride and molybdenum oxychlorides in an argon carrier gas as a function of carrier gas flow rate, system pressure, canister temperature, and canister design. Quantification was based on direct absorption measurements in the ultraviolet-visible and infrared spectral regions. The results of this study should facilitate the identification of process conditions that optimize molybdenum pentachloride for different applications.

11:30am **AP2+EL+PS+TF-FrM-14 Atomic Layer Modulation of Ru-Ir Alloy Thin Films for Low-Resistivity Interconnect Applications**, ***Yoonseo Choi***, *Wonjoong Kim, Byungchan Lee, Minhyeok Lee, Han-Bo-Ram Lee,* Incheon National University, Republic of Korea

As semiconductor devices continue to scale down, Ru and Ir have attracted attention as promising candidates to replace Cu interconnects because their short mean free path and low bulk resistivity lead to a low figure-of-merit (FOM). However, ALD-grown single Ru and Ir thin films suffer from increased resistivity at thicknesses comparable to their mean free path due to enhanced electron scattering, particularly surface scattering, and film discontinuity. In this study, a Ru-Ir system was designed and fabricated by atomic layer modulation (ALM) to mitigate the thickness-dependent resistivity. ALM sequentially exposes different precursors to the surface with purge steps between each precursor exposure, followed by co-counter reactant exposure, enabling multicomponent thin films growth within a single atomic-layer cycle. In particular, the ratio of each element is controlled by the surface reactivity, adsorption behavior, and steric hindrance effects of the precursors, making ALM advantageous for forming compositionally uniform Ru-Ir alloy thin films even at reduced thicknesses. In this work, Ru-Ir alloy thin films were deposited at 250 °C by sequentially pulsing tricarbonyl(trimethylenemethane)ruthenium (Ru(TMM)$(CO)_3$) and tricarbonyl (1,2,3-η)-1,2,3-tri(tert-butyl)-cyclopropenyl iridium ($C_{18}H_{27}IrO_3$) as Ru and Ir precursors, respectively, with O_2 as the counter reactant. To design the process and understand the composition-control mechanism, density functional theory (DFT) and Monte Carlo (MC) simulations were used to analyze precursor surface reactions and their effects on film composition. In addition, a deep-learning-based framework (IDEAL) was used to explore candidate compositions and crystal structures for Ru-Ir alloy films. X-ray diffraction (XRD) and transmission electron microscopy (TEM) analyses confirmed that ALM-grown Ru-Ir films formed a solid solution without distinct phase separation. The electrical properties varied depending on the alloy composition; while single Ru and Ir films showed resistivity above 40 μΩ·cm at 7 nm, Ir-rich Ru-Ir films exhibited a relatively low resistivity of 37.6 μΩ·cm at 5 nm. The high crystallinity of the Ir-rich Ru-Ir films was also consistent with the IDEAL framework prediction. These results demonstrate that ALM-based Ru-Ir alloy thin films can overcome the thickness-scaling limitations of single-component Ru and Ir thin films and have potential as next-generation interconnect materials for replacing Cu.

11:45am **AP2+EL+PS+TF-FrM-15 Pulsed Thermal Etching of Amorphous TiO_2 Thin Films Using $MoCl_5$**, ***Hyuenwoo Yang***, National Institute for Science and Technology (NIST); *James Maslar, Berc Kalanyan,* NIST-Gaithersburg

Gas-phase pulsed etching has emerged as a promising approach for advanced thin-film processing, enabling controlled and potentially low-damage material removal with advantages in process integration over conventional continuous etching methods. Despite growing interest in pulsed etching, including atomic layer etching (ALE), the thermal etching chemistry of metal halides—particularly $MoCl_5$—remains largely unexplored for oxide materials. In this work, we investigate the pulsed thermal etching of amorphous TiO_2 thin films by $MoCl_5$ in a warm-walled viscous-flow reactor. Thickness changes were monitored in real time by in-situ spectroscopic ellipsometry during repeated $MoCl_5$/Ar cycles, while delivered precursor dose and impurity content were monitored upstream using a non-dispersive UV–vis gas analyzer.

Amorphous TiO_2 films on Si/native SiO_2 exhibited clear thickness loss under repeated $MoCl_5$ exposure, with etching behavior that depended strongly on substrate temperature, $MoCl_5$ source temperature, and Ar purge duration. Increasing the $MoCl_5$ source temperature increased the measured UV–vis absorbance signal and produced a corresponding increase in TiO_2 etch rate, indicating that precursor delivery is a key parameter controlling the etching behavior. A substrate-temperature-dependent process window was also observed: etching was strongly suppressed at 150 °C and 350 °C, while the highest etch rate was observed near 250 °C. Temperature-switching experiments further showed that the low-temperature suppression was reversible upon heating to 250 °C, whereas exposure at 350 °C led to an etch-inactive state that did not recover after returning to 250 °C.

To our knowledge, this is the first report of TiO_2 etching using pulsed $MoCl_5$ chemistry. This work establishes an initial process window for $MoCl_5$-based thermal oxide etching and identifies precursor dose, substrate temperature, delivery history, and purge duration as important variables governing pulsed TiO_2 etching.

Advances in Battery Engineering, Interface Design, and Characterization Mini-Symposium
Room 319 - Session BT+AS+CA+TF-FrM

Solid-State Batteries

Moderators: Prof. Alexander Kozen, University of Vermont, **Prof. Chuan-Fu Lin**, Catholic University of America

8:15am **BT+AS+CA+TF-FrM-1 Grain Structure Control of Evaporated Li Metal Films for Optimized Solid State Batteries**, ***Andrew Westover***, *Peyton Carden,* Oak Ridge National Laboratory, USA **INVITED**

Lithium metal is a critical anode material for next-generation, high-energy batteries. To realize these batteries, the lithium metal must be between thick, depending on the cathode chemistry. Furthermore, lithium metal must have controlled surface chemistry and high purity for optimal performance. Thermal evaporation is one of the most effective methods for producing thin lithium metal films that meet these criteria. In this work, we present our efforts to understand how to produce lithium metal films as thin as , and we explore the ability to fabricate lithium metal thin films with controlled microstructures. We have developed a process to modify the as-deposited lithium metal grain size in evaporated films from . Using these thin films with standard liquid electrolytes, localized high-concentration electrolytes, and solid electrolytes lead to significant differences in the cycling performance of lithium metal films. This work demonstrates the critical importance of microstructure control for realizing next-generation, high-energy lithium metal batteries.

This work was funded by the United States Department of Energy Transportation Technology Office Battery Materials Research Program and German-US Collaboration on Energy Storage under Simon Thompson and Tien Duong.

8:45am **BT+AS+CA+TF-FrM-3 Unravelling the Mechanism of Al2O3 Atomic Layer Deposition on Li_6PS_5Cl for All-Solid-State Batteries**, *Kyobin Park, Donghyeon Kang, Taewoo Kim, Vepa Rozyyev, Anil Mane, Hacksung Kim, Francisco Vargas, Zachary Hood, Peter Zapol, Justin Connell,* ***Jeffrey Elam***, Argonne National Laboratory

Sulfide superionic conductors with the argyrodite structure (e.g., Li_6PS_5Cl, LPSCl) are extremely promising for all solid-state batteries, but poor atmospheric stability and high interfacial reactivity limit their widespread adoption. Coating LPSCl powders with ultrathin, metal oxide coatings using atomic layer deposition (ALD) mitigates these problems, protecting LPSCl against atmospheric degradation[1] and reducing reactivity with Li metal, yielding more stable cycling[2]. Despite significant promise, the ALD mechanism is unknown, hampering the development of new coating chemistries.

In this study, we elucidate the mechanism for Al_2O_3 ALD on LPSCl using trimethyl aluminum (TMA) and H_2O by combining *in situ* Fourier transform infrared spectroscopy measurements and *ex situ* solid-state magic angle spinning nuclear magnetic resonance, UV Raman spectroscopy, and X-ray photoelectron spectroscopy measurements with density functional theory calculations. We determine that ALD Al_2O_3 nucleates promptly via TMA reaction with native -OH, -SH, and PS_3-OH groups to form transient C-Al-O(S) species that are rapidly hydrolyzed during the subsequent H_2O exposure. This reversible transformation maintains surface nucleophilicity and prevents sulfide decomposition. The resulting layer-by-layer growth leads to highly conformal Al_2O_3 coatings on LPSCl.

This detailed understanding of ALD surface reactions provides critical insights guiding the selection of future ALD chemistries with greater enhancement in cycling performance.

1. *Acs Materials Letters* **2024,** 6, (12), 5409-5417.
1. *Advanced Materials* **2023,** 35, (21), 13.

9:00am **BT+AS+CA+TF-FrM-4 Engineered Cathode Chemomechanics Enables Ultra-Low Stack Pressure Solid-State Batteries**, ***Paul Braun***, University of Illinois Urbana-Champaign

In solid-state batteries, stresses resulting from electrode material chemomechanics are strongly coupled to solid electrolyte-electrode interface failures. Such failures are significant barriers to realization of practical Li metal solid-state batteries. While high external pressures can reduce these failures, the required pressures are impractical, and thus a different approach to reducing interface failures is required. We show that control of cathode chemomechanical stress provides an important path for realization of solid-state batteries which operate at commercially relevant low (e.g., <1 MPa) stack pressures. Using a series of cathodes with different chemomechanics we provide experimental evidence of the role of electrode chemomechanics in solid-state battery failure. Our model systems reveal that electrode chemomechanics significantly alter Li metal plating and stripping behavior at low stack pressure. We utilize these learnings to build long cycle-life solid-state batteries with practical areal capacity (5 mAh/cm^2) operating under a 1 MPa stack pressure and at room temperature. Our findings highlight the importance of controlling positive electrode chemomechanics to realize low stack pressure solid-state batteries.

9:15am **BT+AS+CA+TF-FrM-5 Pulsed Laser Deposition of Solid Electrolytes: How Limited Thermal-Budget Processing Relates to Li-ion Conductivity**, *Nicola Perry,* University of Illinois*; En Ju Cho, Kai-Wei Lan,* ***Nicola Perry***, University of Illinois Urbana-Champaign **INVITED**

Near-room-temperature, thin-film deposition of air-sensitive Li-ion conductors can enable multilayer solid electrolytes and coatings for high-energy-density batteries and microdevices, compatible with thermally sensitive components. We investigate the capabilities of pulsed laser deposition for fabrication of high-quality layers of low-voltage- and high-voltage-stable solid-electrolyte compositions, including low-melting antiperovskite hydroxyhalides and higher-melting nasicon-structured oxides that contain glass-forming elements. The influence of growth parameters such as temperature, pressure, and laser fluence on stoichiometry, density, roughness, crystallinity, and conductivity is explored. Grazing-incidence nuclear reaction analysis paired with Rutherford backscattering spectrometry provides insight into light-element stoichiometry (e.g. Li, Cl, P) and the expected loss of Li (e.g.) with increasing temperature (given its volatility) and growth pressure (given its mass that enables scattering). Strategies to control stoichiometry of multiple light elements and deposition rates, through composite targets and sequential multi-target deposition, are demonstrated. X-ray reflectometry, grazing-incidence diffraction, and ellipsometry shape the understanding of structural dependence on growth parameters. We also examine the benefit of integrated impedance spectroscopy in the PLD chamber during and after growth to provide insights into transport behavior in a clean (air-free) environment as a function of temperature. We find most compositions benefit from vacuum deposition, but while the antiperovskite hydroxyhalides form single-phase, highly conductive films at room temperature, with phase decomposition and conductivity degradation above ~60 C, the nasicon-structured electrolytes benefit from post-deposition anneals to improve crystallinity and conductivity.

9:45am **BT+AS+CA+TF-FrM-7 Open-Circuit Energy Band Alignment at NMC/LLZTO and LLZTO/Li Interfaces for Solid-State Microbattery Applications**, ***Austine Amisi***, *Raquel-Garza Hernandez, Fabian Ambriz-Vargas,* Centro de Investigaciones en Óptica, Mexico

Stable electrode/electrolyte interfaces are critical for the electrochemical performance and long-term reliability of solid-state microbatteries. This work reconstructs the open-circuit energy band diagram of an all-solid-state $LiNi_xMn_yCo_zO_2$ (NMC)/$Li_7La_3Zr_{2-x}Ta_xO_{12}$ (LLZTO)/Li microbattery stack through band alignment analysis of the NMC/LLZTO cathode–electrolyte and LLZTO/Li electrolyte–anode heterojunctions. Thin-film bilayers were fabricated by RF magnetron sputtering and thermal evaporation. Valence and conduction band offsets (VBOs and CBOs) were experimentally determined using the Kraut method through conventional and angle-resolved X-ray photoelectron spectroscopy (XPS/ARXPS). A VBO of +3.13 ± 0.1 eV and a CBO of −6.00 ± 0.1 eV were measured at the NMC/LLZTO interface, with a large CBO that suggests the formation of an electronically insulating interface that suppresses electrolyte decomposition at the cathode during charging. In contrast, a VBO of +1.92 ± 0.1 eV and a near-zero CBO of +0.08 ± 0.1 eV were determined at the LLZTO/Li heterojunction, indicating an electronically conductive interface that promotes electron accumulation and facilitates LLZTO degradation upon contact with the anode. An electrochemical potential window of 6.00 ± 0.1 eV and an open-circuit voltage of 3.29 ± 0.1 eV were obtained from the reconstructed full-stack band diagram. These results establish a direct link between interfacial band alignment and potential degradation mechanisms and provide critical design guidelines for advancing the operational stability of LLZTO-based solid-state microbatteries.

10:00am **BT+AS+CA+TF-FrM-8 LiPON-Enabled Reduction of V2O5 during Fabrication of Thin-Film Ionic Devices**, ***Leopoldo Tapia-Aracayo***, *David Stewart, Gary Rubloff,* University of Maryland College Park

Vanadium (V) Oxide (V_2O_5) is a well-researched layered oxide with high capacity (375 mAh/g), often cited for its applications in energy storage, electrochromic, and neuromorphic applications. In the field of thin-film ionic devices, we can sputter Lithium Phosphorus Oxynitride (LiPON) on top

of crystalline V_2O_5, creating our electrolyte/electrode stack. This sequence simplifies the fabrication of thin-film ionic batteries as sputtering LiPON can insert Lithium up to 2 Li^+ per V_2O_5. We wanted to address the roughness of the LiPON/V_2O_5 interface by altering the fabrication steps to form a smooth interface, but unintentionally reduced the V_2O_5 to a VO_2 phase.

This smooth interface was achieved by sputtering amorphous V_2O_5 thin films in Ar/O_2 environment, then coated with LiPON, and subjected to post-deposition annealing in N_2 gas environment at 300 ◦C. The N_2 gas environment for the post-deposition annealing would crystallize the V_2O_5 and preserve the LiPON composition. We tracked the formation of a VO_2 phase, which was not observed for N_2 annealed V_2O_5 without LiPON, which remains VO_2 free. We used electrochemical cycling to probe the presence and evolution of the VO_2 phase, illustrating VO_2 reaction peaks instead of characteristic crystalline V_2O_5 peaks in the 2.2 V – 4.0 V vs Li+/Li window. (Seen in Figure 1). We will discuss how this behavior may be caused by LiPON-enabled reduction pathways at the buried interface. We confirm this reduction is limited to the interface as analysis via Raman identifies lithiated V_2O_5 phases. Systematic variation of LiPON sputtering parameters and annealing conditions, while holding LiPON thickness constant, reveal processing regimes that drive VO_2 formation versus preserving V_2O_{-5}. Ultimately, preserving the morphological benefits of a smooth LiPON/ V_2O_5 interface while constraining VO_2 formation, providing guidance for designing desired application-specific vanadium-oxide phases.

Chemical Analysis and Imaging at Interfaces
Room 321 - Session CA1-FrM

Chemical Analysis and Imaging at Interfaces Oral Session I

Moderators: Dr. Andrei Kolmakov, National Institute of Standards and Technology (NIST), **Gabriel Parker**, Oak Ridge National Laboratory

8:15am **CA1-FrM-1 Semiconductor Manufacturing Metrology*, Alexander Liddle,*** Canon Nanotechnologies Inc. **INVITED**

The old adage from optics that, if it can be measured, it can be made, is nowhere more true than for semiconductor manufacturing.Leading-edge devices contain nanoscale features, and require sub-nanometer dimensional, compositional, and interfacial control over length scales up to the diameter of a 300 mm wafer.Every step of the fabrication process, from deposition, to lithography, to etch, depends on sophisticated metrology, often in-line and at speed, to achieve the level of precision and accuracy needed to flawlessly produce the billions of transistors that make up today's high-performance integrated circuits.In this talk, I will provide a high-level overview of some of the outstanding measurement challenges that must be overcome in order to maintain the semiconductor industry's extraordinary progress in manipulating and controlling matter at the atomic scale.In particular, I will focus on the metrology needed to enable the transition to highly three-dimensional structures, such as gate-all-around (GAA) transistors, high-capacity NAND flash memory, and hybrid-bonded high-bandwidth memory.

8:45am **CA1-FrM-3 High Performance Computing and Artificial Intelligence Enabled Materials Characterization and Experimental Automation*, Mathew Cherukara,*** Argonne National Laboratory **INVITED**

The capabilities provided by next generation light sources along with the development of new characterization techniques and detector advances are revolutionizing materials characterization (metrology) by providing the ability to perform scale-bridging, multi-modal materials characterization under *in-situ* and *operando* conditions. For example, providing the ability to image in 3D large fields of view (~mm^3) at high resolution (<10 nm), while simultaneously acquiring information about structure, strain, elemental composition, oxidation state, photovoltaic response etc.

However, these novel capabilities dramatically increase the complexity and volume of data generated. Conventional data processing and analysis methods become infeasible in the face of such large and varied data streams. The use of AI/ML methods is becoming indispensable for real-time analysis, data abstraction and decision making at advanced, high-data rate instruments. I will describe how high-performance computing (HPC) along with AI on edge devices enables real-time data analysis and self-driving experiments, creating the next generation of AI-powered materials characterization tools.

As instrument and analysis workflows increase in complexity, large language models (LLM) have the potential to assist and enhance the productivity of scientists. I will describe early experiments with AI-powered scientific co-pilots that can provide assistance through every stage of an experiment; planning, execution, analysis and even instrument operation.

9:15am **CA1-FrM-5 Challenges in Real-Time Plasma-Surface Diagnostics*, Vincent Donnelly,*** University of Houston **INVITED**

An array of quantitative surface diagnostic methods has been used over the past 65 years to gain detailed insights into the physics and chemistry of surfaces. These include Auger electron spectroscopy (AES), x-ray photoelectron spectroscopy (XPS), low-energy electron diffraction and similar methods. These techniques required high- or ultrahigh vacuum to detect electrons without collisions with background gas, as well as to keep surfaces clean of unwanted contaminants. Similar constraints are imposed by mass spectrometry methods such as temperature programmed desorption (TPD) and secondary ion mass spectrometry (SIMS). When the gas pressure exceeds a level where the collision mean-free-path becomes comparable to a characteristic distance (e.g. 1 mTorr at ~5 cm), the primary information carried by the electron energy, and neutral or ion desorption product is degraded or lost. The problem is exacerbated in a plasma, where large electron and ion densities, electric fields and magnetic fields dilute and distort the surface analysis signals. Despite these issues, considerable advances have been made in the application of conventional surface analysis methods for real-time probing of plasma-surface interactions. This talk will review some of this work from our laboratory and elsewhere, where AES, XPS and TPD/SIMS-like desorption spectroscopy have been used to obtain information such as adsorbate coverages, reactive sticking coefficients, surface catalyzed reactions, and primary desorption products, all while operating a plasma. Examples will include operando XPS, spinning wall AES and desorption mass spectroscopy, ion-desorption optical emission spectroscopy and laser-desorption spectroscopy.

9:45am **CA1-FrM-7 Gaede Langmuir Award Talk: Investigation of Solid-Solid and Solid-Liquid Interfaces under Electrical Potential via XPS and EIS*, Sefik Süzer*[1],** ÜNİVERSİTELER MAH, Turkey **INVITED**

X-ray Photoelectron Spectroscopy (XPS) and Electrochemical Impedance Spectroscopy (EIS) are well established analytical tools for interrogating surface and interface chemistry of mostly solid materials and their interfaces. Herein, we report using both techniques together, our observations on slow dynamics of devices with Semi-Conducting n- and/or p-doped Si Electrodes, having also ~3-4 nm oxide layer on top, separated by a Porous Polyethylene Membrane (PEM) soaked by an Ionic-Liquid as the electrolyte. As such, the device has two different interfaces: (i) Ionic Liquid / Silicon, and (ii) Silicon / Silicon Oxide. Using XPS, time dependent shifts of well-separated Si2p peaks of the semi-metallic (Si^0) as well as the oxide (Si^{X+}), together with O1s peak have been recorded under external electrical bias, to reflect the local electrical potential developments. For the electrolyte (Ionic Liquid), C1s, O1s and F1s peaks have been used to record the electrical potential developments at different locations. Complementary Electrochemical Impedance Spectroscopic measurements have also been recorded on the very same device within the XPS instrument before and after XPS measurements to follow the various changes, in addition to similar measurements under ambient conditions. Electrochemical findings, regarding the two interfaces, obtained from measurements of these two powerful spectroscopic techniques will be presented and discussed.

Chemical Analysis and Imaging at Interfaces
Room 321 - Session CA2-FrM

Chemical Analysis and Imaging at Interfaces Oral Session II

Moderators: Carles Corbella, NIST-Gaithersburg, **Xiao-Ying Yu**, ORNL

10:15am **CA2-FrM-9 in Situ Molecular Imaging of Ion Clusters Reveals the Acid Gas Capture Capacity and Mechanism of Water-Lean Ionic Liquids*, Xiao-Ying Yu,*** Oak Ridge National Laboratory*; Difan Zhang,* Oak Ridge Natinal Laboratory*; Zihua Zhu,* Pacific Northwest National Laboratory*; Gabriel Parker, Roger Rousseau,* Oak Ridge Natinal Laboratory

Water-lean solvents are a promising technology for capturing acid gases like carbon dioxide (CO_2).In situ liquid time-of-flight secondary ionization mass spectroscopy (ToF-SIMS) is used to study a representative solvent N-(2-ethoxyethyl)-3-morpholinopropan-1-amine (2-EEMPA) with different CO_2 loadings to reveal the complex solvent structure upon CO_2 capture.Characteristic peaks of 2-EEMPA, such as m/z^- 215 $C_{11}H_{23}N_2O_2^-$ (deprotonated 2-EEMPA) and m/z^+ 217 $C_{11}H_{25}N_2O_2^+$ (protonated 2-EEMPA),

[1] **Gaede-Langmuir Award Winner**

are detected due to acid gas uptake.Also, solvent molecules and carboxylate ion pairs, such as *m/z*⁻ 259 $C_{12}H_{23}N_2O_4^-$ [(deprotonated 2-EEMPA$\cdots CO_2$)] and *m/z*⁺ 261 $C_{12}H_{25}N_2O_4^+$ (protonated 2-EEMPA$\cdots CO_2$), are observed.Interestingly, more than one CO_2 molecule can be captured per each solvent molecule as evidenced in SIMS mass spectra, for example, *m/z*⁻ 321 $C_{13}H_{25}N_2O_7$ [(deprotonated 2-EEMPA)$\cdots 2CO_2\cdots H_2O$], *m/z*⁺ 305 $C_{13}H_{25}N_2O_4^+$ [(protonated 2-EEMPA)$\cdots 2CO_2$], *m/z*⁻ 389 $C_{17}H_{29}N_2O_8$ [(deprotonated 2-EEMPA)$\cdots 3CO_2\cdots 3CH_2$], and *m/z*⁺ 373 $C_{16}H_{25}N_2O_8^+$ [(protonated 2-EEMPA)$\cdots 3CO_2\cdots 2C$].However, the monomer of 2-EEMPA and CO_2 seems to be most prevalent.Furthermore, solvent clusters are detected in loaded solvents, for instance *m/z*⁺ 433 $C_{22}H_{49}N_4O_4^+$ [(2-EEMPA)$_2\cdots$H] and *m/z*⁺ 646 [(2-EEMPA)$_3$-2H], while capturing CO_2 at different amounts.Relative abundance of cluster ions provides a semi-qualitative venue to assess the free energies gas capture energetics, indicating the relative stability trend within the same solvent system, previously impossible.These observed ion clusters are verified with molecular modeling, where dimer, trimer, and cluster ions are validated for their presence either due to weak molecular interactions or hydrogen bonds.In situ molecular imaging of ionic liquids and molecular modeling reveals that the acid gas capture mechanism by ionic liquids includes both physical adsorption and chemical bonding with multiple reaction pathways, engaging cluster formation and alteration of solvent structures.

10:30am **CA2-FrM-10 Modulating Active Site for Water Electrolysis**, ***Sen Zhang***, University of Virginia **INVITED**

This presentation focuses on modulating active sites for oxygen evolution reaction (OER) through precise control of single atom/cluster sites and nanocrystal surfaces and interfaces. Emphasis is placed on the use of in situ and operando spectroscopic techniques, including X-ray absorption spectroscopy (XAS), Raman spectroscopy, and surface sensitive IR, to directly probe dynamic surface reconstruction, oxidation state evolution, and formation of catalytically active species under working conditions. These real-time insights reveal how applied potential induces active-phase transformations and how tuning active site coordination environment can optimize adsorption energetics and reaction intermediates. By correlating spectroscopic signatures with electrochemical performance, we establish robust structure–activity relationships that guide rational active-site engineering for highly efficient and durable OER electrocatalysts.

10:45am **CA2-FrM-11 Synthesis and in Situ Characterization of Simulated Hanford Tank Waste Models in Aqueous Solution**, ***Tobias Misicko***, Oak Ridge National Laboratory, USA; *Mackenzie Savage,* University of Virginia; *Gabriel Parker, John Lasseter,* Oak Ridge National Laboratory, USA; *Kaleigh Louque, Yang Xiao,* Louisiana Tech University; *Xiao-Ying Yu,* Oak Ridge National Laboratory, USA

The nuclear waste stored at the US Department of Energy's Hanford Site as an environmental remediation facility presents many major challenges. Mainly, the remediation of aluminum-containing tank waste generated from the separation of aluminum cladding of spent fuel rods requires processing and its complex dissolution chemistry is still not well understood. These wastes typically consist of three aluminum oxide/oxy-hydroxide species, namely gibbsite (γ-Al(OH)$_3$),[1] boehmite (α-AlOOH),[2] and bayerite (α-Al(OH)$_3$).[3] Targeted remediation of these solids is complicated by their dissolution and stability in solution as well as a wide range of particle sizes. Physical property information on the tank waste is scarce due to computational simulation limits and the radioactivity of the waste preventing laboratory handling. Herein we report a versatile hydrothermal synthesis technique enabling tunable and scalable production of gibbsite, boehmite, and bayerite in submicrometer for use as simulant materials for in situ analysis and related experimental investigations. Synthesized samples were characterized ex situ using X-ray Diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), time-of-flight secondary ion mass spectrometry (ToF-SIMS), and physisorption to verify structural and chemical properties. *In situ* particle analysis and imaging were subsequently investigated using the System for Analysis at the Liquid-Vacuum Interface (SALVI) microfluidic platform, which enabled probing of the vacuum-liquid interface with SEM and ToF-SIMS.[4] The insights gained from this work are expected to inform the development of remediation approaches and formulate remediation methodologies that are safe for both site personnel and the environment.

References:

[1] Page, J.S., *et al.*, *Journal of Hazardous Materials,* 384 (**2020**) 121318

[2] Peterson, R.A., *et al., Separation Science and Technology,* 42 (**2007**) 1719-1730

[3] Herting, D.L., *et al., US DOE Office of Environmental Management,* (**2002**), OSTI ID: 808264

[4] Yang, L., *et al., Lab on a Chip*, 11 (**2011**), 2481-2484

11:00am **CA2-FrM-12 Accessing Surfaces and Interfaces in the Modern Scientific Era: An Overview of Important Instrumentation Advances**, ***Andrew Yost***, Scienta-Omicron Inc.; *Patrick Lömker, Takahiro Hashimoto,* Scienta-Omicron AB, Sweden; *Jürgen Köble, Andreas Janzen,* Scienta-Omicron GmbH, Germany; *Patrik Karlsson,* Scienta-Omicron AB, Sweden; *Daniel Beaton,* Scienta-Omicron Inc. **INVITED**

Scientific progress has repeatedly been driven by advances in experimental capability, with many of the most transformative discoveries in physics, chemistry, and materials science arising not solely from new theoretical understanding, but from the development of instrumentation capable of probing nature with greater sensitivity, spatial resolution, temporal resolution, and analytical precision. The ability to observe previously inaccessible phenomena frequently creates entirely new areas of research and enables scientists to ask questions that were once beyond experimental reach. In many cases, breakthroughs in instrumentation have reshaped our understanding of matter at fundamental length and energy scales while simultaneously enabling technological developments that extend far beyond the laboratory environment.

In this talk, we take a brief look at several major advancements in scientific instrumentation spanning the past several decades through the present day and examine how these developments have transformed modern surface science research. The progression of increasingly sophisticated measurement tools has enabled researchers to move from macroscopic characterization toward atomic-scale and electronic-scale investigations, allowing direct access to the structural, chemical, and electronic properties of materials and interfaces.

Particular focus will be placed on techniques that have had substantial impact across both fundamental research and industrial applications. Topics will include angle-resolved photoemission spectroscopy (ARPES), which has provided unprecedented insight into electronic band structures and many-body interactions; scanning probe microscopy (SPM), which has enabled real-space imaging and manipulation at near-atomic and atomic length scales; x-ray photoemission spectroscopy (XPS), which has become an essential tool for understanding surface chemistry and composition; and time-of-flight photoemission electron microscopy (ToF-PEEM), which combines spectroscopic and imaging capabilities to reveal spatially resolved electronic and chemical information.

Both academia and industry have benefited significantly from these developments, which have contributed to technologies that influence everyday life, including semiconductor devices, energy systems, catalysis, advanced materials, and nanotechnology. By examining the historical progression of these techniques and their broader impact, this talk aims to illustrate the central role that instrumentation innovation continues to play in enabling scientific discovery and driving future technological advancement.

11:30am **CA2-FrM-14 Studying Electrified Catalysis at the Laboratory and at Synchrotron End Stations**, ***Patrick Lömker***, Scienta Omicron, Sweden; *Andrew Yost, Daniel Beaton, Xin Zhang,* Scienta Omicron

Catalysts are central to the transition from fossil-based to renewable energy systems, with both thermal and electrocatalysis playing key roles in enabling carbon-neutral production of chemicals and fuels. However, their investigation presents significant technical challenges. This contribution discusses advanced sample environments for Dip+Pull methodologies and cell-based electrocatalytic systems.

In Dip+Pull catalysis, recent developments emphasize improved usability and experimental efficiency. Sample cell designs have evolved from in-line electrode configurations to on-axis arrangements, thereby reducing electrolyte transport distances. This approach has been successfully applied to a range of systems, including CO reduction catalysis and studies of battery materials and their degradation mechanisms.

The second part focuses on electrochemical cell geometries, particularly configurations in which the catalyst acts as a barrier between the liquid phase and the vacuum environment. Such setups enable the investigation of membrane transport properties and the operando surface states of platinum catalysts and their intermediates under oxygen reduction reaction conditions.

A unifying aspect of both approaches is the investigation of the electrochemical double layer, which plays a critical role in governing

catalytic activity and interfacial processes. Its characterization under these experimental conditions is discussed in detail.

11:45am **CA2-FrM-15 Energy Flux from Non-Thermal Discharges Measured via Nanocalorimetry: Toward Plasma Standard Development***, **Carles Corbella,*** National Institute of Standards and Technology (NIST)/ University of Maryland, College Park*; Aritra Sil, Berc Kalanyan, James Maslar,* National Institute of Standards and Technology (NIST)*; Lakshmi Ravi Narayan,* National Institute of Standards and Technology (NIST)/ University of Maryland, College Park*; William Osborn, Feng Yi, Andrei Kolmakov,* National Institute of Standards and Technology (NIST)

The use of rapid thermal probes to characterize plasma processes has been under development for a few decades. Despite a growing interest in quantifying the energy fluxes from low-temperature discharges used for surface processing, the decoupling of the elementary contributions from the different plasma species remains a challenge. Primary heat fluxes carried by ions, electrons, photons, and neutrals, are usually convoluted with secondary fluxes from chemical reactions, phase transitions, and recombination processes in calorimetry measurements. Nanocalorimeter sensors, which in our design consist of a Pt thin film microresistor lithographically defined on a free-standing, ultrathin SiN_x membrane with a thermal mass down to nJ/K, constitute an alternative solution to obtain instantaneous energy fluxes given their sensitivity, selectivity, and short response time. In this presentation, the potential application of nanocalorimetry to elucidate and control fundamental surface plasma-induced processes is motivated by the current needs of the coatings industry, where substrate temperature is a critical parameter. Here, we will discuss nanocalorimetric methods to discriminate the individual thermal fluxes from plasma species, such as the use of catalytic coatings to detect plasma radicals, the application of DC bias voltages to select impinging charged particles, and the exploration of interactions with light using optical filters. The presented prototype has been tested under hydrogen, helium, argon, and oxygen RF glow discharges operated in both inductive and capacitive modes. The energy flux, including the dominant participation of energetic ions in Ar plasma, ranges from 10 W/m^2 up to 1700 W/m^2. The experiments were performed in a dedicated research setup equipped with a Langmuir probe, retarding field energy analyzer, optical emission spectroscopy, and quadrupole mass spectrometry, to support and validate the nanocalorimetry measurements. The main objective is to develop plasma energy flux metrology as a standard plasma diagnostics tool that quantifies the thermal effect on plasma-exposed materials across different plasma sources and applications. The relevance of this emerging metrology to the plasma-materials community is justified by the nanocalorimeters' real-time and sensitive performance, robustness, and integrability to other metrology platforms.

Advanced Packaging
Room 304 - Session PK+MS-FrM
Advanced Packaging Oral Session

Moderators: Dr. Mohanalingam Kathaperumal, Georgia Institute of Technology, USA, **Dr. John Lannon**, Micross, **Dr. Prahalad Murali**, AMD

8:15am **PK+MS-FrM-1 Advances Packaging Approaches for Chiplet Solutions***, **Tanja Braun,*** Fraunhofer IZM, Germany **INVITED**

The economic advantages of silicon scaling according to Moore's Law have gone, as today, only a limited number of foundries can afford the manufacturing of high-end nodes. Now, heterogeneous integration in combination with advanced packaging are the path to achieve economic advantages and also to enable new applications. Many options for the package including silicon interposers, Fan-out on substrate, bridge solutions and variations of 3D stacking approaches are seen as possible solutions. However, performance of current applications requires still more transistors per system, but industry also needs a new, more economical system packaging approach. Chiplets are considered the main solution to address this challenge.

Besides all the design aspects, packaging of Chiplet-based systems also holds quite some challenges and requires advanced packaging approaches. The presentation will summarize different advanced packaging solutions as Flip Chip on organic, silicon or fan-out interposer and discuss key challenges as e.g. warpage and possible mitigation solutions. In summary the entire packaging approach from chip to system board has to be considered.

8:45am **PK+MS-FrM-3 Advanced Packaging Enables the Future of the Semiconductor Industry***, **Charles Woychik,*** NHanced Semiconductors, Inc.

The semiconductor industry has long relied on Dennard scaling and Moore's Law to drive advancements in performance and cost efficiency. Dennard scaling asserts that as transistors shrink, power density remains constant, allowing for faster clock speeds and more transistors per unit area without increased power consumption. Moore's Law predicts the doubling of transistors on a chip approximately every two years, leading to exponential growth in computing power. However, as these principles reach their physical and economic limits, the industry faces escalating challenges. Shrinking transistors further is becoming increasingly difficult and expensive due to quantum effects, power leakage, and escalating fabrication costs. Consequently, advanced packaging (AP) technologies have emerged as pivotal in continuing the trajectory of semiconductor innovation.

AP refers to techniques that integrate multiple semiconductor chips into a single package, enhancing performance, power efficiency, and functionality without solely relying on further transistor miniaturization. Methods such as 3D stacking, system-in-package (SiP), and heterogeneous integration (HI) allow for the combination of different types of chips—each optimized for specific functions—into compact, efficient systems. This approach not only mitigates the limitations of traditional scaling but also enables enhanced connectivity, reduced latency, and improved thermal management. By leveraging advanced packaging, the semiconductor industry can continue to innovate, meeting the growing demands for higher performance and efficiency in applications such as artificial intelligence, high-performance computing, and telecommunications. In this presentation, an overview of our 3 families of Si and glass interposers will be presented along with our hybrid bonding capabilities to achieve the aggressive future demands for AI generative computing.Examples will be presented that use these core AP/HI technologies to achieve the aggressive requirements for AI generative computing.

9:00am **PK+MS-FrM-4 Heterogeneous Integration Enabled by Fanout Wafer Level Packaging Prototyping Facility and Activities at Arizona State University***, **Hongbin Yu,*** Arizona State University

Advanced packaging and integration have received increasing attention as computing and communication systems have become more sophisticated and ubiquitous, from CPU/GPU integration with HBM for AI application to III-V power and communication chips integrated with Si COMS chips. Fanout wafer level packaging (FOWLP) has become a versatile and capable technology that enables such heterogenous integration (HI). At Arizona State University, a 300 mm FOWLP prototyping line is being established that is aimed for facilitation advanced packaging research and development as well as demonstration. Examples from Southwest Advanced Prototyping (SWAP) Hub and Department of Commerce funding advanced substrate program SHILED will be discussed.

9:15am **PK+MS-FrM-5 Maskless Lithography for Wafer and Panel-Level Advanced Packaging: Enabling Adaptive Patterning Beyond Reticle Limits***, **Jonas Wiedenmann,*** Heidelberg Instruments Mikrotechnik GmbH, Mittelgewannweg 27, 69123 Heidelberg, Germany **INVITED**

The continued evolution of advanced semiconductor packaging is driven by increasing demands for higher data rates and bandwidth in artificial intelligence- and high performance computing-oriented devices. As a result, package sizes are growing while line and space requirements are becoming more stringent. Traditional mask-based lithography approaches face fundamental limitations as substrate dimensions exceed reticle boundaries. At the same time, warpage, distortion, and non-uniform topography introduce additional challenges for pattern fidelity and manufacturing yield.

Maskless lithography has emerged as a promising enabling technology for next-generation advanced packaging, particularly for panel-level and large-format applications. By eliminating the need for masks and enabling direct-write patterning, maskless approaches offer unique advantages in flexibility, scalability, and cost efficiency. In particular, adaptive patterning strategies—enabled by real-time design data corrections—provide new pathways for compensating substrate distortion, local warpage, and process-induced variations.

This presentation will provide an overview of maskless lithography in the context of advanced packaging applications, including redistribution layers (RDL) and substrate patterning. Key capabilities such as high-resolution patterning down to the 1–2 µm line/space regime, as well as seamless patterning across large areas through stitching, will be discussed.

The second part of the talk will focus on grayscale lithography and its applications in co-packaged optics. A key challenge in this domain is the

fabrication of large-area flat optical elements. Using a newly developed grayscale process, it will be demonstrated how such structures can be realized without introducing unwanted step artifacts. Additional applications of direct laser writing for co-packaged optical systems will also be addressed.

9:45am **PK+MS-FrM-7 Development of a Domestic Fan-Out Wafer-Level Packaging Platform for Advanced Heterogeneous Integration***, **James Will**,* SkyWater Technology

Advanced packaging has become a critical enabler for heterogeneous integration in applications spanning defense and aerospace, telecommunications, high-performance computing, and artificial intelligence. While substantial investments are being made to strengthen domestic semiconductor manufacturing, advanced packaging capabilities remain limited within the United States. To address this gap, SkyWater Technology is establishing a domestic fan-out wafer-level packaging (FOWLP) manufacturing capability to support secure, scalable integration of advanced semiconductor devices.

This work presents the development of key process modules required for implementation of a 300 mm FOWLP platform capable of integrating multiple die within high-density chip-scale packages (CSP) and multi-chip modules (MCM). The process flow leverages adaptive patterning technology to compensate for die placement variation and enable fine-pitch redistribution layer (RDL) interconnects for heterogeneous integration beyond conventional reticle limitations.

Results from process module development and integration activities are presented, including die placement and molding processes, wafer reconstitution, dielectric deposition and patterning, copper redistribution layer fabrication, and process characterization supporting fine-line interconnect formation. Particular emphasis is placed on achieving high-yield pattern fidelity, overlay control, and electrical continuity across large-area reconstituted wafers. Development efforts supporting fine-pitch interconnect architectures, including line/space dimensions approaching 1.5 µm and die I/O pitch down to 20 µm, are discussed along with associated metrology and defectivity reduction strategies.

The presentation will further describe process integration challenges encountered during establishment of a domestic FOWLP manufacturing line and the approaches used to improve manufacturability, scalability, and reliability. Early electrical, physical, and reliability characterization data from engineering test structures and package demonstrators will be reviewed. In addition, development activities supporting future expansion to dual-side fan-out architectures, including through-mold vertical interconnect technologies for enhanced power delivery and signal integrity, will be discussed.

These results demonstrate progress toward establishing a trusted domestic FOWLP capability and provide insight into the process technologies required to enable next-generation heterogeneous integration solutions for national security and other critical applications.

10:00am **PK+MS-FrM-8 SCAPEx: Status of Onshoring Secure 300mm Wafer Bumping and TSV Wafer Finishing***, **Rex Anderson**, John Lannon,* Micross Advanced Interconnect Technology LLC

The Reshore Ecosystem for Secure Heterogeneous Advanced Packaged Electronics (RESHAPE) program is tasked with ensuring the defense industrial base (DIB) has access to a secure, domestic advanced packaging, assembly, and test capability. As part of that program, the Micross Advanced Interconnect Technology business unit in North Carolina has been funded to establish 300mm wafer bumping and 300mm wafer preparation (wafer finishing) capabilities in its post-CMOS wafer processing facility. This paper will provide an overview of the RESHAPE program and the advanced packaging capabilities that are deployed and those that will be deployed at Micross as part the RESHAPE program.

10:30am **PK+MS-FrM-10 On-Shore Sustainable Organic IC Substrate (ICS) Fabrication***, **Michael Gleason**,* GreenSource Fabrication **INVITED**

GreenSource Fabrication's (GSF) proposal to the US government under the Defense Production Act Title III authorization was titled SOTA (**S**tate-of-the-Art) **O**nshore **A**dvanced **P**ackaging **P**roduction or SOAPP.With the help from funding provided by Federal and State resources, GSF is currently in the process of standing up a High-Density Build-Up (HDBU) facility focused on organic IC Substrate and Substrate-Like Printed Circuit Board (SLP) production.GSF's greenfield project includes world class processing tools, advanced automation and a patented generation III Aqua Regen Kinetics Zero Liquid Discharge (ZLD) wastewater treatment system.The facility will be open to serve both the DIB and commercial clients alike who have sustainable, high-mix, low to medium volume requirements which cannot be served well by larger offshore suppliers.Status and timeline of the project will be presented as well as project risks, demand, supply chain vulnerabilities, targeted technology offerings and future state.

11:00am **PK+MS-FrM-12 Impact of Formic Acid Distribution on Fluxless Reflow: Enhancing Process Uniformity and Performance***, **XINXUAN TAN**, Chen Fang, Zulal Tezcan, Purnima Narayanan, Zia Karim,* Yield Engineering System Inc.

Advanced fine-pitch fluxless solder reflow has become increasingly sensitive to both thermal and chemical process variations as bump pitch approaches 10µm and below. Previous studies demonstrated the correlation between reflow defects, process window optimization, and formic acid reduction mechanisms.

In this work, we investigate the impact of formic acid flow distribution and vapor transport on thermal uniformity and process stability in vacuum fluxless reflow processing for advanced AI chip and panel-level packaging applications. The study focuses on three critical process specifications: (1) the impact of formic acid on within-wafer (WiW) and panel-in-panel temperature uniformity, (2) process window stability, and (3) SnO/tin-formate byproduct residue control.

A vacuum fluxless reflow platform with dynamically controlled pure formic acid vapor delivery was utilized to study the interaction between gas flow distribution, thermal behavior, and byproduct transport. Process simulations were conducted to evaluate formic acid distribution, gas recirculation regions, temperature gradients, and tin-formate byproduct concentration behavior inside the process chamber. Experimental studies were performed using multiple combinations of formic acid flow, vapor distribution conditions, soak temperature, and reflow process parameters. Thermal uniformity was monitored using pyrometer and thermocouple measurements, while SEM, XPS, optical microscopy, and AOI inspections were used to characterize reflow quality, residue formation, and process window stability.

Results demonstrate that formic acid distribution directly impacts both reaction kinetics and local thermal behavior during soak and reflow processes. Higher formic acid flow improved oxide reduction efficiency but also increased localized thermal gradients and Sn-formate residue accumulation in gas recirculation regions. By optimizing formic acid flow distribution and vapor transport behavior, improved vapor mixing uniformity and byproduct removal capability were achieved while maintaining sufficient oxide reduction performance.

The optimized process demonstrated improved within-wafer and panel-in-panel temperature uniformity, expanded stable process window margins against under- and over-reflow conditions, and reduced SnO/tin-formate residue. High-yield defect-free microbump reflow performance was achieved for advanced AI chip and panel-level packaging applications.

This work demonstrates that balancing formic acid reduction chemistry, thermal uniformity, and byproduct transport is critical for enabling stable high-volume vacuum fluxless reflow manufacturing for next-generation advanced packaging technologies.

11:15am **PK+MS-FrM-13 Bilayer Liners for Through Glass Vias with PVD and ALD Deposited Seed Layer and Fully Copper Plated Vias***, **Meghna Narayanan**, Mohanalingam Kathaperumal, Mark Losego,* Georgia Institute of Technology, USA

As glass packaging gains traction for next generation heterogenous integration, through glass vias (TGVs) face a critical reliability challenge arising from the large mismatch in the coefficient of thermal expansion (CTE) between glass and copper. Thermally induced stresses generated during processing and operation can lead to crack initiation in the glass substrate and eventually cause copper delamination, with the severity of failure increasing with increase in copper thickness. Mitigating these thermos – mechanical reliability concerns thus, becomes essential for the successful deployment of glass – based packaging technologies.

This work explores a bilayer liner approach for stress mitigation in TGVs, by combining the advantages of inorganic and polymeric materials. While polymer liners offer low elastic modulus and improved stress buffering, they duffer from relatively higher CTE and limited adhesion to glass. To address these limitations, a hybrid bilayer consisting of silicon oxynitride (SiOxNy) and Parylene C is investigated. SiOxNy serves as the interfacial adhesion promoting inorganic layer due to its strong adhesion to glass (8 N/cm) and compatibility with subsequent polymer deposition, while Parylene C, with it lower adhesion strength (5.3 N/cm) provides mechanical compliance provides mechanical compliance for stress relaxation.

Conformal deposition of SiOxNy and Parylene C is achieved by PECCVD and CVD, respectively. Bilayer thicknesses are characterized using confocal fluorescence imaging, leveraging the distinct fluorescence responses of the two materials for independent thickness evaluation.

In parallel, this work investigates seed layer strategies for copper metallization in TGVs, comparing conventional sputtered titanium/copper seed layers with conformal platinum seed layers deposited by atomic layer deposition (ALD). As the aspect ratio of TGV increases, achieving uniform seed coverage becomes a significant challenge. Copper filling is performed through electroplating, and via fill quality is evaluated using non-destructive X-ray imaging.

This presentation will discuss the integration of hybrid liners with advanced seed layer approaches for reliable TGV metallization. Interface chemistry, morphology, and structural integrity will be examined using XPS, FIB cross section, Raman spectroscopy, while highly accelerated stress testing will be used to evaluate adhesion and failure behavior across the multilayer interfaces.

11:30am **PK+MS-FrM-14 Thin Film Characterization and Mechanisms EnablingExtreme Laser Lift-off (LLO)*, Joshua Peck,*** Tokyo Electron America Inc.,

Fusion and Hybrid permanent wafer bonding are essential for 3D high density packaging. To enable scaling for AI applications that require multiple hybrid bonds such as HBM (high bandwidth memory). Conventional thinning processes use deionized water for contact-dependent removal, which reduces wafer yield. To address this yield loss, Tokyo Electron has developed a laser lift-off (LLO) tool that reduces water consumption by 90%. LLO enables wafer separation of fusion or hybrid bonded wafers by inorganic dielectrics. Although full-wafer LLO is novel, it remains a relatively new technology. For effective carrier wafer separation, the properties of the films that enable lift off are characterized then related to defects that may occur without an optimization. Moreover, with an optimized release process the top carrier wafer may be reworked to enable multiple uses of the same carrier wafer.

To enable LLO and wafer reuse, the film properties have been characterized. This characterization covers how increasing laser energy affects wafer bow, how decreasing laser fluence reduces surface roughness, and the films' thermal response from 500-800°C. The challenges associated with carrier wafer integration after LLO will be addressed.

Keywords: laser lift-off, topology, AVS

[1][2]

Figure #1: As Laser pitch increases RMS roughness (Rq) exponential decreases do to low fluence.

Figure #2: Simulation of stress on engineered thin films during LLO

11:45am **PK+MS-FrM-15 Plasma Surface Engineering for Low Distortion Wafer Bonding*, Andrew Tuchman,*** *Christopher Netzband, Joshua Greklek, Nathan Ip, Ilseok Son,* Tokyo Electron America, Inc.

Low distortion wafer-to-wafer bonding is a critical technology for several advanced logic and memory architectures including backside power delivery network (BSPDN) and $4F^2$ DRAM. These process flows require a direct wafer bonding step to transfer a patterned device layer to a separate blanket carrier wafer with less than 5nm of pattern distortion after higher order lithography alignment and correction. In this work we explore the impact of the wafer bonding surface chemistry on the post-bond distortion of SiO_2 bonding dielectrics. A nitrogen-based RF surface activation plasma was used to modify the SiO_2 surface prior to bonding with several plasma conditions. A direct correlation was made between surface nitrogen concentration as measured by XPS and post-bond distortion, with higher nitrogen concentration providing lower post-bond wafer warpage and distortion. Higher surface nitrogen content replaces the hydrophilic -(OH) and dangling Si bonds on the surface, reducing the adhesion energy during bonding and lowering the post-bond warpage. Additionally, the surface nitrogen concentration on the SiO_2 bonding dielectric could be controlled through several plasma parameters. However, the final bond strength was also directly reduced at higher surface nitrogen concentrations, creating a tradeoff between lower distortion and bond strength. By tailoring the plasma conditions to maximize the surface nitrogen concentration, the post-bond distortion was reduced by 27% compared to baseline conditions. Finally, machine learning algorithms were used to determine the optimal plasma parameters for high surface nitrogen concentration with minimized variation across the full wafer. These results highlight the importance of surface-plasma engineering in low distortion bonding flows.

Plasma Science and Technology
Room 315 - Session PS-FrM

Novel Chemistries and Materials in Plasma Processing

Moderators: Prof. Kenji Ishikawa, Nagoya University, Japan, **Dr. Thorsten Lill**, Lam Research Corporation

8:15am **PS-FrM-1 Low Energy Remote Plasma and Non-Plasma Methods for Highly Selective Etching of Advanced Nanodevices*, Mark Kawaguchi,*** LAM Research **INVITED**

In the pursuit of higher performance semiconductors, device length scales continue to shrink down to nanometer dimensions with emerging chip designs increasingly dependent on 3D structures to maintain scaling. Memory manufacturers have already deployed 3D NAND devices with ongoing development for 3D DRAM devices. Advanced logic manufacturers have already deployed 3D FinFET devices and are beginning to deploy more complex GAA (Gate-All-Around) 3D devices as well. Building 3D structures has increased the need for more sophisticated selective etching. As these selective etches have become critical to the formation of the device, atomic precision material loss is required with low contrast materials. We review exemplary materials systems where insufficient selectivity control necessitates innovative approaches such as remote-plasma radicals with atomic layer passivation & ultra-low residual ions as well as plasma-less low energy thermal chemical etching.

Dummy polysilicon removal requires full removal of the polysilicon with minimal film loss to dielectric films such as silicon oxide and silicon nitride. Remote-plasma radical etch removes the polysilicon, but it is desirable to improve film damage control due to higher energy reactants reaching the surface. The first approach applies atomic layer passivation to modify the top monolayer of an oxide encapsulation layer. Epitaxial film damage is improved by hindering diffusion of halogen radicals through the encapsulating film. The second approach reduces the higher energy reactant flux to the surface. We characterize the intensity of higher energy reactants by measuring the residual ion flux to the wafer surface.By modifying flow geometry above the wafer, the residual ion flux is reduced over 2 orders of magnitude, in the range of nA/cm^2, and results in improved material loss.

GAA device integration relies on depositing and subsequently removing SiGe layers to form Si-nanowires or nanosheets. Besides the bulk SiGe etch, we highlight strict film loss requirements that require highly selective native oxide removal prior to removing SiGe layers. We describe a thermal chemical etching approach that applies wet etch mechanisms in a vacuum environment. Etch rates are tunable over a wide range from 2-200 A/min as well as high selectivity to both silicon and silicon nitride materials. In addition, we have applied a Langmuir-Hinshelwood surface kinetics model to extract steady state reactant surface coverage.We find that the surface coverage is sub-monolayer, and over a broad surface coverage range, localized etching characteristics are well-behaved as measured by AFM roughness.

8:45am **PS-FrM-3 A Novel Si Etch Chemistry for CFET Fin Definition*, Yifeng Zhou,*** *Hiroto Ohtake,* Applied Materials, Inc.

CFET channel design requires upper ~75% fin etch profile to be straight and smooth, in addition to the traditional requirements for profile loading, etch depth loading, line edge roughness, and mask selectivity. New etch chemistry and process structure are necessary to meet those challenges as the conventional Cl2- and SF6-based fin etch chemistries ran out of steam.

This study introduces a cyclical process featuring a BCl3/NF3 based etching step and a CH4/SO2 based passivation step that provides straight and smooth upper 85% profile, with minimal profile and depth loading among various pattern pitches.

Profile control: NF3 is the main etchant and BCl3 provides effective passivation for Si and SiGe sidewalls. HBr can provide more passivation, via re-deposition of less volatile SiBrx etch products. NF3:BCl3 and NF3:HBr gas flow ratios are the main knobs for profile control.

Si/SiGe scalloping: Scalloping results from relatively higher lateral etch rate of SiGe compared to that of Si. While SO2/CH4 passivation step helps reduce scalloping by forming Ge-S bonds, standalone H2 trim steps eliminates scalloping by trimming Si faster than SiGe.

Profile loading: iso/dense profile loading roots from sidewall passivation delta between spaces with difference widths. Directional breakthrough step removes more passivation from more sloped sidewalls to allow for more taper correction in subsequent etch steps.

Depth loading: SO2/CH4 passivation step deposits thicker carbon polymer on wider trenches, negating the higher etch rate from higher neutral fluxes.

9:00am **PS-FrM-4 Creation and Recovery of Defects in Lead Zirconate Titanate Thin-Films introduced by Inductively Coupled Plasma Reactive Ion Etching**, ***Madeleine Petschnigg***, *Marco Deluca,* Silicon Austria Labs GmbH, Austria*; Susan Trolier-McKinstry,* The Pennsylvania State University

Due to their excellent actuation performance, with an $|e_{31,f}|$ coefficient of about 15 Cm^{-2}, lead zirconate titanate (PZT) based thin-films are widely adopted for actuator type piezoelectric micro electromechanical systems (piezoMEMS), including inkjet printer heads[1–4], micro speakers[5,6], micro coolers[7,8] and auto focus devices[9,10].In the fabrication of piezoMEMS devices, accurate patterning of the active layer plays a key role. By combining physical and chemical mechanisms, inductively coupled plasma reactive ion etching (ICP-RIE) allows the fabrication of highly anisotropic profiles at high etch rates while maintaining a high selectivity against masking and stop-layer materials.

Plasma assisted dry etching techniques, like ICP-RIE, however, can degrade the patterned PZT and alter its dielectric and piezoelectric properties, which manifests itself in a decreased permittivity, and/or a decreased remanent polarization [11–14]. Degradation is a concern not only when the PZT surface is directly exposed to etching conditions, but alsothrough the introduction and migration of defects at etched side walls [14,15].Potential sources for degradation include changes in surface chemistry due to selective etching or contamination, crystallographic damage due to bombardment, and potential liberation of hydrogen from organic resist masks.Althoughthe electromechanical properties may be recovered by annealing treatments [11,16,17]at 500°C and above, a comprehensive study of the required temperature and time for recovery has yet to be done.

This work aims to uncover the primary mechanism responsible for the degradation of PZT during ICP-RIE patterning, including the effect of pre- and post-etch electrode deposition as well as the presence of hydrogen-containing gases during the plasma etch. Based on this, a targeted recovery treatment procedure will be defined, and the patterning process flow optimized.

Nb-doped PZT films will be deposited by sputtering on Pt-coated Si wafers and patterned by ICP-RIE. The electric properties as well as the aging behavior of pristine samples will be compared to samples right after the etch and after recovery. The potential incorporation of hydrogen will be assessed by Raman spectroscopy. Thermally stimulated depolarization current (TSDC) measurements and charge-based deep level transient spectroscopy (Q–DLTS) will provide insight on the difference in the films defect chemistry.

9:15am **PS-FrM-5 Plasma-Surface Interactions of Polyurea Deposited on SiO2 and SiNx with HF Plasmas**, ***Wallis Scholl***, Colorado School of Mines*; Mingmei Wang, Thorsten Lill, Wenyu Zhang, Louis Kim, Harmeet Singh,* Lam Research Corp*; Sumit Agarwal,* Colorado School of Mines

Fluorocarbon plasmas have been traditionally used to etch SiO_2 and SiN_x during semiconductor processing. Because fluorocarbon radicals inherently lower the etch rate by depositing a polymer on the SiO_2 or SiN_x surface, the industry is transitioning to C-free reactive plasmas, such as HF. As a result, new techniques are needed to enhance surface passivation and etch selectivity during HF plasma etching. During etching of high aspect-ratio (HAR) features, sidewall passivation is needed to preserve the profile. Molecular layer deposition (MLD) is a technique for depositing organic and hybrid organic-inorganic films. We studied the HF plasma interactions after a polyurea film deposited by MLD on top of SiO_2 or SiN_x. We have shown in previous work that MLD polyurea film deposited on top of SiO_2 or SiN_x can protect the underlying material from etching. During HF plasma etching of blanket films on a planar substrate, the polyurea film acted as a sacrificial layer and prevented SiO_2 or SiN_x etch while the polyurea was present. When the polyurea was completely consumed by reaction, the SiO_2 or SiN_x film was etched at its baseline etch rate (see Figure 1). The presence of polyurea also delayed the formation of ammonium fluorosilicate on the SiN_x surface, which is known to form on the surface in the presence of HF, and SiF_4 and NH_3 generated as etch products.

In this work, we also deposited polyurea onto 65:1 aspect ratio holes in SiO_2-SiN_x stacks, which were then exposed to an etching plasma to evaluate sidewall passivation. Scanning electron microscopy images show that the polyurea film reduced the diameter throughout the entire depth, showing both the conformality of the MLD film as well as successful passivation of the sidewalls. Subsequent etching of these features preserved the critical dimension compared to etching without the polyurea film (see Figure 2). Further, *in situ* infrared spectroscopy was used to monitor polyurea interactions with plasma species to better understand the etch mechanism. We exposed the films to a remote HF plasma and HF gas to mimic the conditions in HAR structures. While the radical species in the remote HF plasma gradually removed the polyurea film, it remained largely intact during exposure to HF gas. Fluorination of the polymer film was observed prior to its removal, suggesting that polyurea is removed as volatile hydrofluorocarbon fragments during HF plasma etching. Additionally, we show that during etching at a higher substrate temperature of 150 C, the presence of polyurea enhanced the SiO_2 etch rate: we attribute this to activation of HF through hydrogen-bonding interactions with the amines in the polyurea film.

9:30am **PS-FrM-6 Long-Term Influence of Fluorine Containing Plasmas and Gases on Sapphire (Single-Crystal Al2O3) and Ni-Based Alloy Surfaces**, ***Takuya Ishihara***, *Nozomi Kida, Hidenobu Tochigi, Keigo Iwamoto,* Azbil Corporation, Japan*; Kazuo Karahashi,* Nagoya University, Japan*; Satoshi Hamaguchi,* The University of Osaka, Japan

In semiconductor manufacturing processes such as dry etching or chemical vapor deposition, capacitance manometers are widely used as essential vacuum pressure sensors to monitor and control the pressures of process gases. These gauges must be corrosion-resistant against process gases such as halides and their radicals generated by the plasmas. The diaphragm material of the manometer is especially important because, if its surface is altered by such corrosive gases, the sensor would send imprecise output signals possibly with the zero-point drift or pressure sensitivity shift. The errors are caused by the changes in mechanical properties of the diaphragm arising from the formation of the modified surface layer. For this reason, Ni-based alloys or polycrystalline ceramics of aluminum oxide (Al_2O_3) are typically used as the diaphragm material of capacitance manometers. More recent capacitance manometers employ sapphire (single-crystal α-Al_2O_3) as their diaphragm material, which is of specific interest in this study [1]. Recent studies on the interactions of polycrystalline Al_2O_3 with fluorine-containing plasmas indicated the formation of aluminum fluoride layers on Al_2O_3 exposed to such plasmas [2,3,4,5,6]. We have reported the results of ion beam experiments to understand the surface modification mechanisms of Ni-based alloys and polycrystalline Al_2O_3 film by fluorine-containing plasmas [7,8]. In addition, Ni-based alloy samples were exposed to xenon difluoride (XeF_2) gases for 3 and 6 months and their fluorinated surfaces were analyzed [9]. In this study, we obtained 12 months XeF_2 exposure data of Ni-based alloys, in which fluorine continued to diffuse even after one year, unlike in sapphire.Furthermore, the differences in surface states between sapphire and nickel-based alloys upon exposure to XeF_2 or NF_2 remote plasma will also be reported.

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[8]H. Kang, *et al* Jpn. J. Appl. Phys. Vol. 64 Page: 046001(pp8) (2025)

[9] T. Ishihara, *et al*, the AVS 71st International Symposium & Exhibition (2025)

9:45am **PS-FrM-7 Investigations of Oxygen-Containing Plasma Etching of Diamond**, ***Justin Boles***, University of Houston*; Louis E. S. Hoffenberg, Jack S. Draney, David. B. Graves,* Princeton University*; Vincent M. Donnelly,* University of Houston

Plasma etching of single-crystal diamond is vital for the development of next-generation power electronics and quantum platforms based on nitrogen-vacancy complexes (NV-centers). Despite this, little has been reported on the fundamental etching mechanisms, including the roles of ions and neutrals. Here we report a detailed study of the etching of single-crystal diamond (100) in O_2/Ar magnetically-confined, inductively-coupled plasmas, using a combination of optical emission spectroscopy, ion flux measurements, etching rate measurements, and simulations. Fluxes of positive ions (O^+, O_2^+, Ar^+) to the (100) diamond surface were determined

from ion saturation current measurements and Langmuir probe measurements, while O and O_2 number densities were determined using optical emission actinometry. Optical emission spectroscopy was further employed to measure gas temperature (via N_2 rotational spectroscopy) and identify CO and CO_2 reaction products. Etch rates were measured via masking and optical profilometry as functions of ion energy and $\%O_2$ in Ar. In "pure" (98% or 100%) O_2 plasmas, with an O-to-O_2^+ flux ratio of about 25:1, the etch rate and product optical emission intensities obeyed a square root of ion energy dependence, with a threshold near 11 eV. The etching yield (C atoms-per-ion) was 7.5 at a mean ion energy (DC self-bias voltage plus plasma potential) of 215 eV. If CO were the only product, and since physical sputtering yields are much lower, O atoms must be playing a dominate role in etching at this energy. As the feed gas ratio was changed from pure O_2 to 20%O_2/Ar at constant pressure (10 mTorr), ICP power (300 W), and ion energy (215 eV), the total positive ion flux remained nearly constant (1-2 $X10^{16} cm^{-2}s^{-1}$) and the O-to-ion flux ratio actually increased to between 40:1 and 50:1, while the yield decreased monotonically to about 3.5 C-per-ion, still much larger than the sputtering yield of 0.16 C-per-Ar^+. The yields as a function of O-to-ion flux ratio and $\%O_2$ in Ar compare favorably with molecular dynamics simulations.

This work supported by the U.S. Department of Energy, Office of Science, Office of Fusion Energy Sciences under Award No. DE-SC0024537.

10:00am **PS-FrM-8 The Effect of Remote Ar Plasma Exposure on the Crystalline Structure of VO_2**, ***Peter Litwin***, *Neeraj Nepal,* U.S. Naval Research Laboratory*; Marc Currie,* US Naval Research Laboratory*; Andrew Lang, Luis Carrillo, David Boris, Michael Johnson, Scott Walton, Virginia Wheeler,* U.S. Naval Research Laboratory

The effect of chemically inert plasmas on the surface of thin film materials is of interest because it allows for an additional means to deliver energy to a material beyond increasing the material's temperature. This could be of use in cases where energy needs to be delivered to specific layers or interfaces in a heterostructure without subjecting the entire material stack to higher temperatures or to overcome energetic barriers, such as those associated with material crystallization (or amorphization) or the formation of metastable phases. However, plasmas make for a complex environment due to the various energy contributions from ions, electrons, excited species, and photons. Despite this complexity, an increased understanding of energy transfer by controlling the fluence and energy of ions at the plasma-surface interface opens additional avenues in material engineering. This may be particularly true for plasma-enhanced atomic layer deposition (PEALD) processes where thin films are cyclically exposed to plasmas during deposition and thus could benefit from an increased understanding of the interaction between plasmas and material surfaces.

In this work, we look at the impact of remote Ar plasmas on crystalline VO_2 thin films deposited by ALD as a function of plasma power and substrate bias. Thermal ALD of VO_2 was carried out at 150 °C using TEMAV and O_3 and subsequently crystallized in a dedicated thermal annealing vacuum system following a previously established process[1]. We find that the Raman signature of the equilibrium monoclinic phase of VO_2 (m-VO_2) decreases after exposing the sample to a remote Ar plasma beyond a minimum power or substrate bias threshold. Interestingly, this process is reversible, i.e., the signature of m-VO_2 can be recovered by exposing the sample to a subsequent Ar plasma of decreasing power or bias starting below the initial threshold required to reduce the m-VO_2 signature. These results suggest one of two possibilities: either amorphization of the film and subsequent recrystallization or selective stabilization of different VO_2 phases based on the plasma condition used. TEM analysis indicates the plasma-treated material is in fact highly crystalline despite the decreased signature of m-VO_2, which suggests the latter of the two explanations. This presentation will discuss the details of these experiments and, with the aid of in situ plasma diagnostics, attempt to elucidate the plasma parameters responsible for the behavior observed.

[1] J. Phys. Chem. C 2017, 121, 19341−19347

Surface Science

Room 305 - Session SS-FrM

Photo- and Electrochemical Energy Conversion

Moderators: Prof. Ashleigh Baber, James Madison University, **Matthew Montemore**, Tulane University

8:15am **SS-FrM-1 Real-Time Control of Interfacial Dynamics Enables Electrocatalytic C-H and C-C Bond Transformation and Fuel Formation**, ***Marcel Schreier***, University of Wisconsin-Madison **INVITED**

Producing fuels and chemicals using electricity has drawn considerable interest in recent decades. However, research in electrocatalysis, which allows us to link electricity to chemical transformations, remains strongly focused on the electricity-driven transformation of small inorganic molecules such as CO_2, H_2O, N_2, as well as oxygen containing molecules derived from biomass. Yet, comprehensive industrial electrification will require electrocatalytic methods that can promote the reactions that make up the core of the chemicals and fuels industry: n–alkane transformations.

In this presentation, I will show that using electricity to promote n-alkane transformations opens entirely novel avenues of reactivity with the potential to address long-standing challenges in reactivity and selectivity plaguing catalytic alkane chemistry. Specifically, I will show how our group combined fundamental understanding of the interfacial processes occurring in electrocatalytic reactionswith *in-situ* product analysis using electrochemical mass spectrometry, to gain independent control over the elementary steps of complex alkane transformation reactions in real-time. Using the real-time modulation of the electrode potential applied to an electrocatalyst, we were able to independently control the *adsorption* of n-alkanes to electrocatalyst surfaces, initiate the *transformation* of adsorbates while they are bound to the catalyst, and *selectively desorb* desired products, while leaving others bound. These methods allowed us to demonstrate the room-temperature fragmentation of ethane and butane into shorter chain fragments, achieve the dehydrogenation of n-alkanes at room temperature, open pathways towards the oxidation of n-alkanes in fuel cells, and achieve other industrially relevant hydrocarbon transformations at mild conditions. I will discuss the fundamental science behind these pathways and show how they may chart a path towards more targeted transformation of chemical compounds than is possible with current chemical technologies.

8:45am **SS-FrM-3 Exploring Non-Thiol DDQ Self-Assembly on Au(111) through Cyclic Voltammetry, AmbientSTM, and XPS**, ***Nazila Hamidi***, *Cara Plaisance, Alyssa Nanneman, Soumick Naskar, Sanwu Wang, Erin Iski,* University of Tulsa

Redox-active organic molecules on noble-metal surfaces provide model interfaces for studying molecular ordering, interfacial charge transfer, and surface-confined electrochemistry. In this study, the non-thiol adsorption and self-assembly of 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ), a strongly electron-accepting quinone, on Au(111) were investigated. Clean Au(111) substrates were immersed at room temperature in a saturated DDQ solution prepared in 0.1 M $HClO_4$ for selected immersion periods, allowing the time-dependent evolution of DDQ adsorption and surface assembly to be valuated. The resulting surfaces were characterized by Cyclic Voltammetry (CV) and ambient Scanning Tunneling Microscopy (STM), while X-ray Photoelectron Spectroscopy (XPS) is being used to evaluate surface composition. CVs showed reproducible DDQ-related redox features after immersion, indicating that electroactive DDQ species are retained at the Au interface after air exposure. The redox peak currents increase systematically with immersion time, consistent with progressive adsorption and increasing surface coverage. Scan-rate-dependent measurements support a surface-confined redox process, as the peak current scales linearly with scan rate rather than with the square root of scan rate. These results indicate that immersion time provides a direct way to tune the density of DDQ molecules on the Au(111) surface. Ambient STM was used to probe Au(111) after DDQ exposure. Compared with clean Au(111), DDQ-modified surfaces show clear changes in surface appearance, suggesting adsorbed molecular features and molecule-induced restructuring of the Au surface. The time-dependent STM observations indicate that DDQ adsorption evolves from early-stage surface modification toward more developed, linear assemblies at longer immersion times. Initial analysis suggests that the molecules tilt at elevated coverages, which allows the assemblies to be stabilized through possible pi-pi stacking and H-bonding. Because DDQ contains electron-withdrawing cyano groups and quinone carbonyl groups, adsorption may involve interactions between DDQ functional groups and Au surface atoms, including cyano-mediated

binding or adatom-assisted adsorption. Ongoing XPS analysis will clarify the chemical composition of the DDQ-modified Au(111) surfaces and identify changes in the local chemical environment associated with adsorption. Complementary density functional theory calculations are planned to support plausible adsorption geometries and DDQ–Au interaction pathways.

9:00am **SS-FrM-4 Substrate Electrochemical Inertness as a Prerequisite for Reliable Electrocatalytic Characterization: Cu-Doped CNT Films Assessed by SECCM**, ***Miguel Bernal***, *Dario Stacchiola,* Brookhaven National Laboratory

Substrate selection is a decisive factor in the accurate electrochemical evaluation of active materials, as the support itself can obscure or distort the measured response. An ideal substrate combines electrical conductivity with chemical and electrochemical inertness under experimental conditions, ensuring that all measured signals are unambiguously ascribed to the material under investigation. In practice, however, true electrochemical neutrality is rarely achieved, since most conductive supports introduce parasitic contributions arising from double-layer capacitance, surface phase transitions, or residual catalytic activity.

In this context, we present copper-doped multi-walled carbon nanotube (Cu-CNT) films synthesized via spray pyrolysis using α-pinene as a renewable carbon precursor and ferrocene as catalyst, followed by microwave-assisted treatment to promote uniform copper incorporation at the nanotube surface. Films were deposited onto ITO substrates and characterized using scanning electrochemical cell microscopy (SECCM) coupled with cyclic voltammetry, enabling spatially resolved mapping of local electrochemical activity across thousands of discrete surface sites.

Systematic SECCM mapping of bare ITO first established its electrochemical profile as a reference baseline. CNT/ITO surfaces exhibited featureless voltammetric profiles with negligible background current, confirming that the nanotube overlayer effectively cover the ITO surface and yields a well-defined, electrochemically featureless support interface. Cu-CNT/ITO surfaces displayed a well-resolved anodic feature attributable to surface copper oxidation, clearly distinguishable from ITO contributions, alongside characteristic hydrogen and oxygen evolution onset potentials. Strikingly, statistical analysis of spatially resolved voltammograms revealed exceptional surface homogeneity across the Cu-CNT film, with markedly lower site-to-site variability in peak potential and current density than typically observed for heterogeneous metal–carbon interfaces.

These results demonstrate that spray pyrolysis combined with microwave treatment produces Cu-CNT surfaces with uniform electroactive site distribution and reproducible interfacial behavior. The electrochemical cleanliness of the CNT support, confirmed through rigorous substrate mapping, positions Cu-CNT films as model platforms for mechanistic studies of copper-mediated electrocatalysis.

9:15am **SS-FrM-5 Atomic-Scale Investigation of Li/Ag(111) Interfaces: New Phases, Li-Ag Alloy Formation and Lithiophilicity**, ***Yuchen Niu***, *Janice Reutt-Robey,* University of Maryland, College Park

Bimetallic Li alloys are very promising for solid-state battery applications, particularly as thin film interlayer in next-generation Li metal anodes. Exceptional lithiophilicity and Li-transport properties derive from the structure and reversible formation of Li-Ag alloys across a range of compositions. However, atomic-scale knowledge of the structure and Li-transport dynamics of Li-Ag alloy surfaces is limited.

We present an atomically detailed investigation of the formation and evolution of surface and near surface $Li_xAg(111)$ alloys. Lithium is vapor deposited on a well-characterized Ag(111) single crystal substrate under UHV conditions. Lithium films, from sub-monolayer to multilayer thickness, spontaneously form surface alloys at room temperature. Surface alloys, in turn, support and stabilize lithium metallic islands, reflecting their lithiophilicity. The atomic-scale structures, energetics and evolution of Li-Ag surface alloys are mapped with scanning tunneling microscopy (STM), scanning tunneling spectroscopy (STS), low energy electron diffraction (LEED). Unreported Li-Ag phases are revealed, including a $Li_xAg(111)$ solid solution wetting layer (which supports Li islands) and local $Li_1Ag_1(111)$-($\sqrt{3}\times1$) and Li_xAg herringbone phases. Mechanisms of Li_xAg alloy formation, lithiophilicity, stability of $Li/Li_xAg(111)$ interface, and the growth mode of Li islands are discussed. We further explore electric-field driven Li transport, using the STM tip for both introducing a localized field and subsequent characterization tool. Together, these results bridge atomic-scale surface science and device-level interface engineering, offering mechanistic insights for next-generation Li-metal batteries.

9:30am **SS-FrM-6 Tracking Conducting Oxygen Ions in Solid Oxide Fuel CellElectrolytes by NAP-XPS**, *Po-Chiao Li,* National Synchrotron Radiation Research Center, Taiwan; ***Bo-Hong Liu***, National Sun Yat-sen University, Taiwan

Solid oxide fuel cells (SOFCs) are an important energy technology for stationary power generation, distributed energy systems, and integration into future hydrogen economies.[1] Yttria-stabilized zirconia (YSZ), which conducts oxygen ions O^{2-}, is the most common solid electrolyte. The high operating temperatures of 600–1000 °C is considered a drawback, as it results in heat lost, thermal stress, and materials degradation.[2] Fundamental understanding to the behavior of the conducting ion of the electrolyte is a key for the design and improvement of novel solid electrolytes. In this talk, I will present the study of YSZ-based SOFC model systems using Near-Ambient Pressure X-ray Photoelectron Spectroscopy (NAP-XPS). On a YSZ single crystal, we confirmed the presence of the thermal activated oxygen ion. The oxygen ion induces chemical shift in the Y 3d binding energy while marginal change is shown in the Zr 3p spectra. This evidences the local electronic environment modulation of yttrium during the oxygen ion conducting. We further elucidate the influence of gas environments, temperature, and the presence of electrode materials on the oxygen ion. The result provides basic understanding for designing advanced electrolytes with improved performance, durability, and lower-temperature operation.

Keywords:

Solid Oxide Fuel Cell (SOFC) Yttria-Stabilized Zirconia (YSZ)Oxygen Ion ConductivityNear-Ambient Pressure X-Ray Photoelectron Spectroscopy (NAP-XPS)(1) Shi, H.; Su, C.; Ran, R.; Cao, J.; Shao, Z. Electrolyte materials for intermediate-temperature solid oxide fuel cells. Progress in Natural Science: Materials International 2020, 30 (6), 764–774.(2) Kim, S. K.; Lee, H. J.; Moon, J. Y.; Jo, Y.-R.; Lee, J.; Park, J.-H.; Kim, S.-D.; Joo, J. H. Understanding the phase stability of yttria stabilized zirconia electrolyte under solid oxide electrolysis cell operation conditions. Journal of Materials Chemistry A 2024, 12 (14), 8319–8330.

9:45am **SS-FrM-7 Enhancing Hydrogen Evolution via Cation-Regulated Interfacial Proton Transfer on Single-Atom Catalysts**, ***Zhen Meng***, *Xiaofeng Feng,* University of Central Florida

Hydrogen evolution reaction (HER) in neutral electrolytes is typically limited by sluggish proton transfer at the electrode–electrolyte interface. Although electrolyte cations are recognized as key components of the electrochemical interface, how they regulate interfacial proton-transfer kinetics on single-atom catalysts remains unclear. Here, we investigate neutral HER on Fe-N-C and Co-N-C single-atom catalysts in Na^+- and NH_4^+-containing electrolytes to reveal how cations modulate proton-transfer processes. Compared with Na^+, NH_4^+ substantially enhances HER activity on both catalysts and increases the exchange current density by more than 20-fold,indicating accelerated intrinsic HER kinetics. The Tafel slopes in Na^+ and NH_4^+ electrolytes are comparable, suggesting that NH_4^+ increases the reaction rate without altering the apparent HER pathway. Rotating ring-disk electrode (RRDE) control experiments indicate that the activity enhancement cannot be explained by bulk buffering effects or suppression of local pH variation. Instead, computational studies and in situ spectroscopic characterization reveal that NH_4^+ accumulation within the electric double layer reorganizes interfacial water, enables a more continuous hydrogen-bond network, and lowers the barrier for interfacial proton transfer. These interfacial modifications facilitate more efficient proton delivery from bulk electrolyte to the catalytic active sites. This work identifies ammonium cations as active regulators of interfacial proton-transfer kinetics in neutral HER and establishes cation-controlled interface engineering as an effective strategy for tuning electrocatalytic activity on single-atom catalysts.

10:00am **SS-FrM-8 Translating Interfacial Ion Activity to Electrochemical Reactivity**, ***Samuel Johnstone***, *Seth Anderson, Evan Grothen, Matthew Gebbie,* University of Wisconsin - Madison

Electrochemical reactivity hinges on the local environment at electrode-electrolyte interfaces, where interactions between the charged electrode, reactive species, and electrolyte ions combine to dictate charge transfer. Of significant interest is how interfacial ion assembly can be leveraged to control reactivity, and many recent studies have worked to identify how particular ions can influence the rate and selectivity of reactions such as hydrogen/oxygen evolution and CO_2 reduction. Electrostatically, ions with the opposite charge as the electrode (counterions) are expected to have a large presence at the interface, while ions with the same charge (co-ions) are expected to have a minor presence. However, many reaction systems

utilize large polarizations and highly concentrated electrolytes, leading to correlated, charge-dense interfaces containing both counterions and co-ions. Therefore, it is important to consider the influence of both the counterion and the co-ion on reactivity and determine whether the combined effect of correlated ions differs from what would be expected from each ion individually. Here, we study the hydrogen evolution reaction in mixed salt electrolytes and show that counterions and co-ions act in tandem to significantly alter the interfacial water structure and influence the rate of reaction. We use a combination of interfacial techniques, including X-ray absorption spectroscopy and atomic force microscopy, to connect reactivity to changes in the structural and chemical makeup of the interface and again show that both ionic species together determine interfacial properties. Overall, our work provides fundamental insight into how correlated interfaces play a key role in modulating electrocatalytic reactions.

10:30am **SS-FrM-10 Caught in the Act: Correlating Chemical Transformations and Structural Evolution Under Reaction Conditions**, ***Slavomir Nemsak,*** Lawrence Berkeley National Laboratory **INVITED**

Understanding how catalysts behave under operating conditions remains a central challenge in surface science. This talk presents a multimodal platform combining ambient pressure X-ray photoelectron spectroscopy (AP-XPS) and grazing incidence X-ray scattering (AP-GIXS) at the APPEXS endstation of the Advanced Light Source, enabling simultaneous chemical and structural characterization at the same sample spot under identical conditions. Case studies include Ni nanoparticle exsolution from perovskite hosts, Ag-Cu bimetallic nanoparticles restructuring during photocatalytic CO_2 reduction, hydrogen storage in Pd-Ni nanoparticles, ligand oxidation on $NaYF_4$ nanoparticles, and nanopatterned ceria under H_2 and CO_2 atmospheres. Through this examples, we demonstrate how coupled chemical and morphological dynamics are revealed only through simultaneous measurement. Neither technique alone captures the full picture, but together they establish mechanistic links between surface chemistry and structural evolution that are directly relevant to catalyst design.

11:00am **SS-FrM-12 The Importance of Interfacial Water for Achieving Long-Range Ordered Assemblies**, ***Kevin Rosso,*** *Xiaoxu Li,* Pacific Northwest National Laboratory*; Tuan Ho,* Sandia National Laboratories, USA*; Duo Song, Sebastian Mergelsberg, Jianbin Zhou, Yining Wang, Narendra Adhikari, Nabajit Lahiri, Yatong Zhao,* Pacific Northwest National Laboratory*; Honghu Zhang,* Brookhaven National Laboratory*; Lili Liu,* Pacific Northwest National Laboratory*; Ruipeng Li,* Brookhaven National Laboratory*; Ping Chen, Mark Bowden, James De Yoreo, Zheming Wang, Carolyn Pearce, Xin Zhang,* Pacific Northwest National Laboratory

Self-assembly of nanocrystals by oriented attachment (OA) is a basis for growing larger crystals with defects organized along relict particle boundaries. A critical stage during OA events is the solvent separated state, in which the Angstrom-scale intervening water layers coating the particles provide the time in close proximity needed for interparticle torque acting across the gap to co-align particles.

This talk will feature new experimental and computational insights into how water structure on particle surfaces impacts particle interactions, using two illustrative systems.First, we examine the dispersion/aggregation of three morphologies of hematite nanocrystals in varied aqueous solutions using ex situ electron microscopy and in situ small-angle x-ray scattering. We demonstrate a unique tendency of (104) hematite nanoparticles to maintain a monodisperse state across a wide range of solution conditions not observed with (001)-and (116)-dominated particles, which instead form disordered aggregates. Density functional theory calculations reveal an inert, densely hydrogen-bonded first water layer on the (104) facet that favors interparticle dispersion.The finding clearly shows that facet-engineering is a route to controlling the hydration forces that influence the lifetime of the solvent-separated state.

Second, we demonstrate how macroscopic gibbsite mesocrystals emerge from nanoplates guided into staggered positions by directional sliding determined by intervening water layers. Electron microscopy and X-ray scattering reveal the monoclinic superlattice structure, based on nanoplate stacking with a uniform ≈50° stagger along the gibbsite [010] direction. In situ liquid-cell transmission electron microscopy captures preferential sliding along the gibbsite [010] direction, decelerating with increasing particle overlap. Molecular dynamics simulations reveal that this staggered arrangement corresponds to a global free-energy minimum, rather than full alignment. The simulations also confirm that with 1-2 intervening water layers, particle sliding along the [010] direction is energetically favored.The finding clearly shows the critical role of interfacial water for achieving long-range ordered assemblies.

Our collective insights highlight the central role that interfacial water plays in determining the residence time and energy landscape for interparticle configurational searching during aggregation, in turn determining the extent of order achieved and the corresponding properties of the aggregates themselves.

11:15am **SS-FrM-13 Surface Hydration and Antifouling Activity of Zwitterionic Polymers**, ***Zhan Chen,*** University of Michigan

Zwitterionic materials are well known for their outstanding antifouling properties and have been widely explored in biomedical applications, drug delivery systems, and marine coatings. These properties are generally attributed to the strong surface hydration they maintain. However, probing this hydration in situ is challenging because it occurs at the solid–liquid interface. To address this, we have employed sum frequency generation (SFG) vibrational spectroscopy to study the interfacial hydration of several zwitterionic polymers, including poly(carboxybetaine), poly(sulfobetaine), and poly(trimethylamine N-oxide). As a second-order nonlinear optical technique, SFG provides intrinsic surface sensitivity at the sub-monolayer level due to its selection rules.

Our findings reveal that strongly hydrogen-bonded water molecules dominate the polymer–water interface, giving rise to the robust hydration layer characteristic of these materials. pH-dependent measurements further show that the surface hydration of poly(carboxybetaine) varies with pH, whereas poly(sulfobetaine) remains largely unaffected. These trends closely align with their respective antifouling performances, reinforcing the idea that surface hydration plays a central role in governing antifouling behavior.

Additional SFG studies demonstrate that protein adsorption does not significantly disrupt the hydration layer of zwitterionic polymers, in contrast to polyethylene oxide, whose surface hydration can be compromised by proteins. This highlights a key advantage of zwitterionic systems. Interestingly, mussels tend to avoid settling on zwitterionic surfaces; however, when physically constrained to remain in contact, they can still achieve strong adhesion. SFG results suggest that, unlike on conventional fouling surfaces where mussels first dehydrate the interface, they instead exploit interfacial water and adhesive proteins to bind to zwitterionic materials.

We also found that dissolved salts can weaken surface hydration through charge screening effects, potentially reducing antifouling performance. Nevertheless, when the spatial separation between charges within the zwitterionic structure is small, hydration remains strong even under high-salt conditions. Poly(trimethylamine N-oxide), with its closely spaced charges, is particularly effective at resisting salt-induced screening and maintaining a robust hydration layer.

11:30am **SS-FrM-14 Energetics of Water and Methanol Adsorption on CO-Precovered Pt (111) Surfaces: Solvent - Adsorbate Interactions**, ***Arjan Saha,*** Washington State University*; Valeria Chesnyak,* Oregon State University*; Marcus Sharp,* Pacific Northwest National Laboratory*; Nida Janulaitis,* University of Washington*; Zbynek Novotny,* Pacific Northwest National Laboratory*; Charles T. Campbell,* University of Washington*; Líney Árnadóttir,* Oregon State University*; Zdenek Dohnálek,* Pacific Northwest National Laboratory

Carbon monoxide (CO) is among the most widely studied molecules in surface science, serving as a probe for surface structure, a reactant in catalytic processes, and a model adsorbate for investigating adsorbate–adsorbate interactions. Here we employ single-crystal adsorption calorimetry (SCAC) and sticking coefficient measurements to understand the influence of preadsorbed CO on the interaction of Pt(111) with prototypical solvents, methanol and water (D2O). At 100 K, the initial sticking probability of D2O on CO/Pt(111) is high (~0.9) and increases asymptotically to unity with increasing D2O coverage. The corresponding D2O heat of adsorption remains constant over submonolayer coverages and is identical to that of water multilayers. This suggests that D2O binds more weakly on the CO/Pt(111) as compared with bare Pt(111). Therefore, the measured heat arises mainly from D2O–D2O hydrogen bonding, as CO blocks the Pt sites. As the temperature increases from 100 to 130 K, the initial sticking probability decreases from ~0.9 to ~0.2. This indicates that isolated water monomers become unstable and desorb with high probability before they can find other waters by diffusion and be stabilized via cluster formation. With increasing D2O coverage, the sticking probability again increases asymptotically to unity, but only at coverage

well above 1 ML. This behavior indicates the formation of three-dimensional D2O clusters, demonstrating that the CO-covered Pt surface behaves as a non-wetting surface for water adsorption. Analogous studies for methanol on CO/Pt(111) reveal a similar trend in the heat of adsorption, indicating that methanol adsorption is also dominated by methanol–methanol hydrogen bonding rather than methanol–Pt interactions. These results show the impact of coadsorbed species on solvent binding and provide important insights into surface interactions relevant to electrodes and catalytic metal nanoparticles.

Vacuum Technology
Room 315 - Session VT-FrM

Vacuum Technology Pressure Measurement

Moderators: Dr. Julia Scherschligt, National Institute of Standards and Technology, **Mr. Charles Smith**, Oak Ridge National Laboratory

10:30am **VT-FrM-10 High Vacuum MEMS Devices – Advances in Vacuum Technology in Microscale**, ***Michał Krysztof***, *Tomasz Grzebyk, Piotr Szyszka, Paweł Urbański, Marcin Białas, Jakub Jendryka, Jan Sobków, Paweł Knapkiewicz, Jan Dziuban,* Wroclaw University of Science and Technology, Poland **INVITED**

High and ultra-high vacuum technologies have long been a cornerstone of advanced scientific instrumentation, including electron microscopes, mass spectrometers, and X-ray sources. Traditionally, such systems rely on large vacuum chambers and complex, multistage pumping infrastructures, which inherently limit their miniaturization, portability, and widespread deployment. Despite continuous optimization, the fundamental architecture of vacuum technology has remained largely unchanged for decades.

Recent advances in microelectromechanical systems (MEMS) enable a fundamentally different approach, in which vacuum is generated, maintained, and utilized directly at the microscale. A key breakthrough was achieved at Wroclaw University of Science and Technology with the development of a MEMS-compatible high-vacuum micropump [1]. Fabricated using standard silicon–glass MEMS processes, this integrated pump allows stable vacuum levels on the order of 10^{-7} mbar to be generated in millimeter-scale volumes, eliminating the need for external pumping systems.

This invited talk presents how the availability of such a miniature vacuum pump enabled the development of a family of fully integrated, ultra-compact vacuum devices (Fig. 1). Selected examples include MEMS-based field-emission X-ray sources [2], miniaturized gas analyzers [3] and quadrupole mass spectrometers [4], as well as other electron- and ion-based vacuum microsystems [5]. The technological aspects of integrating vacuum, electron-optical, and nanoelectronics components into sealed MEMS structures are discussed, together with their functional capabilities.

The presented results demonstrate that MEMS technology enables a paradigm shift in vacuum engineering—from large, centralized vacuum installations toward autonomous, application-specific microscale vacuum instruments. This approach opens new opportunities for vacuum technology in space science, materials research, environmental diagnostics, and distributed sensing systems.

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11:00am **VT-FrM-12 Cassini - A MEMS Pirani with Range of 9 Order of Magnitude**, ***Klaus Bergner***, *Kristian Kirsch, Lukas Reger, Andreas Truetzschler,* VACOM, Germany

Many key applications of vacuum technology—such as coating and thin-film processes, surface analysis, and semiconductor manufacturing processes—operate continuously between atmospheric pressure and approximately 10^{-6} mbar. To cover this range completely and with metrological reliability, three measurement principles are combined in practice: capacitive diaphragm sensors (CDG) for high pressure to low vacuum, thermal conductivity measurement (Pirani) for a broad medium vacuum range, and Bayard–Alpert ionization gauges (BAG) for high and ultra-high vacuum. However, the multisensor solution comes with engineering drawbacks: additional connection ports and dead volume, increased maintenance and calibration requirements, risks of errors in the overlap ranges, and higher system costs.

The Pirani sensor traditionally covers the largest single measurement range. Since Marcello Pirani, the principle has been based on the pressure-dependent heat transfer from a heated element to the gas. Classic wire Pirani sensors limit the expansion of the measurement range primarily due to control-related restrictions: To generate sufficient temperature differences at atmospheric pressure, high power levels would be required, which would thermally and mechanically overload the wire; at very low pressures, conservative control often results in a pressure-dependent signal excursion that is too small. Added to this are aging and drift, as well as long thermal time constants.

We present a new MEMS-based approach (Cassini) that specifically addresses these limitations. Central to this approach is pressure-adaptive control: different heating powers and temperatures are used depending on the pressure regime to consistently achieve a large pressure-dependent signal range. A combined control and evaluation method seamlessly links different modes across the various pressure regimes.

With Cassini, we demonstrate that a single, compact MEMS Pirani sensor can continuously cover nine orders of magnitude of pressure, from atmospheric pressure down to 1xE-6 mbar. Measurements in reference gases are calibrated against CDG and BAG standards and demonstrate consistent signal range, low hysteresis, and robust reproducibility.

11:15am **VT-FrM-13 AVS History Committee-Sponsored Talk: From Mercury Columns to Quantum-Based Standards: The Evolution of Vacuum and Pressure Metrology at NIST**, ***Jay Hendricks***, *Jacob Ricker, Kevin Douglass, Thinh Bui,* NIST

The pursuit of precision in measuring pressure and vacuum has been a cornerstone of scientific and industrial progress for over a century. This presentation provides a brief overview of the trajectory of pressure metrology, tracing its evolution from the early foundations at the National Bureau of Standards (NBS)—now the National Institute of Standards and Technology (NIST)—to the cutting-edge quantum-based innovations of the modern era.

The journey began in the early 20th century, shortly after the founding of the NBS in 1901. Initial efforts focused on establishing primary standards for atmospheric pressure, evolving through the 1920s and 1930s with the establishment of dedicated laboratories for vacuum research. Key historical milestones include the 1948 establishment of the Pressure Section, which formalized the development of primary standards and calibration services for government and industry. From the early use of mercury columns and the development of the McLeod gauge to the creation of altitude chambers for testing Liberty engines, NIST has consistently pushed the boundaries of how we measure the "extremes" of physical quantities.

Today, the Pressure and Vacuum Group at NIST remains a world leader, but the paradigm of measurement is shifting. The redefinition of the International System of Units (SI) has catalyzed a transition toward quantum-based metrology, enabling the realization of fundamental units through the laws of physics rather than physical artifacts. This talk will explore the technical breakthroughs driving this transition, specifically highlighting the Fixed Length Optical Cavity (FLOC) for pressure measurement and the Cold Atom Vacuum Standard (CAVS) for vacuum metrology. By leveraging quantum mechanics and photonics, these methods achieve unprecedented levels of accuracy and precision.

A theme of the presentation will be the intersection of vacuum science and miniaturization. The "NIST on a Chip" program exemplifies this trend, aiming to shrink complex metrology systems into field-deployable formats. This shift from laboratory-bound primary standards to compact, portable devices represents a fundamental change in the metrology ecosystem, allowing high-precision measurements to be conducted in real-world environments.

Finally, the talk will situate these advancements within the broader mission of the International Union for Vacuum Science, Technique and Application (IUVSTA), emphasizing how science transforms our ability to measure and understand the physical world.

11:30am **VT-FrM-14 Fast, Optimal Readout of a Tethered Optomechanical Pressure Sensor**, ***Daniel Barker***, *Stephen Chen, Yiliang Bao, John Lawall, Jason Gorman,* National Institute of Standards and Technology

We demonstrate a fast readout method for tethered optomechanical pressure sensors. The fast readout method allows mechanical ring-down measurement rates that exceed the total mechanical damping rate. We model the uncertainty of our ring-down measurements with the Cramér-Rao bound, including the effect of thermomechanical noise. Both our data and the Cramér-Rao bound indicate that measurement rates on the order of the mechanical damping rate produce the lowest uncertainty. At low pressures, using the optimal measurement rate allows 10× faster measurements or 3× lower uncertainty compared to allowing our sensor to ring down to the thermomechanical noise floor. Our results allow tethered optomechanical pressure sensors to operate at rates comparable to commercially available pressure gauges, removing an obstacle to adoption of optomechanical pressure sensors in industrial settings.

11:45am **VT-FrM-15 Recent Updates to the NIST Helium Leak Calibration Service**, ***Stephen Eckel***, *Daniel Barker, James Fedchak, Julia Scherschligt,* National Institute of Standards and Technology (NIST)

The NIST leak rate calibration service is responsible for calibrating helium leaks from roughly 10^{-13} mol/s to 10^{-6} mol/s. Traceability is established through NIST's primary vacuum flowmeters. These constant pressure flowmeters both generate and measure a flow rate of known gas and are traceable to measurements of pressure, temperature, volume displacement, and time. Over the last several years, major upgrades have been completed. In 2024, the vacuum leak system (VALES) — a system designed to hold the NIST working standards under vacuum and in a temperature-controlled environment— was completed. In late 2025, a fully automated flowmeter has been added to the system to allow all leaks to be calibrated against a flowmeter. In this talk, we will present the updated calibration service, discuss the associated uncertainties, and show initial results on the stability of the NIST leaks in the VALES.

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