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.

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.

References

1. Chatterjee, S.; Abadie, T.; Wang, M.; Matar, O. K.; Ruoff, R. S. *Repeatability and Reproducibility in the Chemical Vapor Deposition of 2D Films: A Physics-Driven Exploration of the Reactor Black Box*. Chemistry of Materials 2024, 36, 1290-1298.

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

1. epitaxial growth
2. heterostructures
3. interface engineering
4. van der Waals epitaxy
5. 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.

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:

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[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:

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[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.

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

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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)

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]

References:

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2. Popov, Mattinen et al., *JVSTA*, **43**, 030801 (2025).
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5. Hämäläinen, Mattinen et al., *Adv. Mater.*, **30**, 1703622 (2018).
6. Mattinen et al., *JVSTA*, **37**, 020921 (2019).
7. Mattinen et al., *Chem. Mater.* **15**, 5713 (2019).
8. Mattinen et al., *2D Mater.*, **7**, 011003 (2020).
9. Mattinen et al., *Adv. Mater. Interfaces*, **7**, 2001046 (2020).
10. Mattinen et al., *Chem. Mater.* **34**, 7280 (2022).
11. Mattinen et al., *ACS. Appl. Mater. Interfaces*, **15**, 35565 (2023).

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.

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.

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.

Author Index

Bold page numbers indicate presenter

Author Index