Nanoscale Science and Technology
Room 320 - Session NS-MoM

Frontiers in Nanoscale Electron, Ion, and Scanning Probes I

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

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

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

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

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

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

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

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

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

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

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

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

Research sponsored in part by Division of Materials Science and Engineering, Basic Energy Sciences, Office of Science, US DOE at the Oak Ridge National Laboratory, and, at Clemson University by the State of South Carolina through funding for the Battelle Savannah River Alliance Workforce Development Program.

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

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

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

Unconventional superconductivity is central to emerging quantum technologies, including dissipationless electronics and topological quantum computing. Still, identifying the nature of unconventional superconducting states remains challenging because few experimental techniques can directly probe the superconducting order parameter. Here, we use scanning tunneling microscopy (STM) to perform multi-particle tunneling spectroscopy in atomic resolution and reveal the nature of unconventional superconductivity across a range of material systems. Multi-particle tunneling processes involving Cooper pairs—most notably Andreev

reflection and Josephson tunneling—provide direct spectroscopic access to superconductivity [1,2]. With atomic-scale spatial resolution, STM further uncovers local variations in these tunneling spectra, offering insight into the symmetry of the superconducting order parameter. Applying these techniques to Fe-based chalcogenides and epitaxial two-dimensional superconductors, we have identified clear signatures of unconventional superconductivity in both classes of materials [3,4].

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

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

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

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

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

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

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

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

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

Nanoscale Science and Technology
Room 320 - Session NS-MoA

Frontiers in Nanoscale Electron, Ion, and Scanning Probes II

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

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

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

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

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

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

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

1. R. Mittapally, J. W. Lim, P. Reddy, E. Meyhofer, B. Song. Quantifying the effect of nanofilms on near-field radiative heat transfer. *ACS Photonics,* 10 (8), 2474–2480 (2023)

2. S. Yan, Y. Luan, J. W. Lim, R. Mittapally, A. Reihani, Z. Wang, Y. Tsurimaki, S. Fan, P. Reddy, E. Meyhofer. Surface phonon polariton-mediated near-field radiative heat transfer at cryogenic temperatures. *Physical Review Letters*, 131 (19), 196302 (2023)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

1. T. Huff et. al., “Molecular tools for non-planar surface chemistry,” arXiv:2508.16798 [cond-mat.mtrl-sci] (2025), https://doi.org/10.48550/arXiv.2508.16798 (submitted for peer review).
2. T. McCallum, et. al., “(Hetero)adamantane synthesis: A triple alkylation reaction,” https://doi.org/10.26434/chemrxiv.15002728/v1 (submitted for peer review)
3. E. Barrera et. al., “Inverted-mode scanning tunneling microscopy for atomically precise fabrication,” arXiv:2512.24431 [cond-mat.mes-hall] (2025), https://doi.org/10.48550/arxiv.2512.24431 (submitted for peer review).

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

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

Nanoscale Science and Technology
Room 320 - Session NS-TuM

Multimodal Techniques in Surface and Interface Engineering at the Nanoscale

Moderators: Dr. Aubrey Hanbicki, Laboratory for Physical Sciences, **Prof. Deep Jariwala**, University of Pennsylvania

8:00am **NS-TuM-1 Foundation Models for 2D Materials Research*, Haozhe "Harry" Wang,*** Duke University **INVITED**

Foundation models are transforming the discovery, fabrication, and characterization of two-dimensional materials — moving the field toward autonomous laboratories in which AI plans, executes, and interprets experiments with minimal human guidance. In this talk, I will present three complementary advances from our group that together demonstrate a foundation model-native pipeline spanning synthesis, microscopy, and spectroscopic analysis of 2D materials.

First, I will introduce ATOMIC (Autonomous Technology for Optical Microscopy and Intelligent Classification), a foundation model-powered system for zero-shot autonomous microscopy of 2D semiconductors. Without any task-specific training, ATOMIC achieves 99.7% classification accuracy, showing that large vision models can autonomously navigate, image, and interpret nanoscale features at scale. Second, I will present SpectraNET, a curated benchmark of experimental spectroscopic data designed to bridge the gap between frontier AI capabilities and real-world materials characterization. SpectraNET provides standardized evaluation tasks for large language models applied to spectral analysis; through chain-of-thought prompting, we systematically improve inference performance while exposing the current boundaries of AI-driven spectral interpretation. Third, I will describe an LLM-guided chemical vapor deposition platform in which a reasoning-capable language model acts as an autonomous process controller for 2D material synthesis. Leveraging a structured recipe library and one-shot growth recommendations, the system achieves high-yield synthesis toward user-specified targets — dramatically reducing the experimental iteration traditionally required in nanomaterial fabrication.

Taken together, these efforts outline a concrete roadmap for AI-driven laboratories that close the loop from growth to characterization to discovery, accelerating the pace of 2D materials innovation.

8:30am **NS-TuM-3 Controlled Non-Volatile Modulation of Optical Dispersion in Monolayer Tungsten Disulfide via Ferroelectric Polarization Patterning*, Yuhong Cao,*** *Deep Jariwala,* University of Pennsylvania

The manipulation of optical properties, including reflection, refraction, polarization, phase, and frequency, has long been central to advancing photonic and optoelectronic technologies. However, existing electro-optical approaches rely on volatile mechanisms that require continuous power consumption. Here, we demonstrate strong, nonvolatile modulation of optical dispersion in monolayer tungsten disulfide (ML WS_2) using patterned ferroelectric domains in aluminum scandium nitride (AlScN). By locally poling ferroelectric domains into opposite states, we achieve substantial manipulation of the complex refractive index ($\Delta n > 0.7$, $\Delta k > 0.4$) and excitonic energy shifts (~50 meV) in ML WS_2, comparable to previous gate-tuning approaches while eliminating continuous power consumption. We introduce an asymmetric screening model that reveals how ferroelectric polarization induces carrier-density-dependent Coulomb screening, leading to distinct excitonic behaviors between electron- and hole-doped regions. Furthermore, we demonstrate a gate-free lateral p-n homojunction with a rectification ratio of 6×10^3, formed through spatial carrier redistribution. These findings establish ferroelectric/2D heterostructures as a powerful platform for nonvolatile optical dispersion engineering, enabling energy-efficient, reconfigurable photonic and optoelectronic devices.

8:45am **NS-TuM-4 Enhanced Ferroelectricity in Ultrathin Compositionally Graded AlScN*, Zekun Hu,*** *Haiwei Zhang, Rajeev Kumar, Yuhong Cao, Xiaolei Tong, Pedram Yousefian, Hyunmin Cho, Bongjun Choi, Chao-Chuan Chen, Yunfei He, Kefei Bao, Chloe Leblanc, Eric Stach, Roy Olsson, Deep Jariwala,* University of Pennsylvania

Ferroelectric $Al_{1-x}Sc_xN$ is a promising BEOL-compatible material platform for nonvolatile microelectronics because of its large polarization, wide bandgap, and compatibility with scalable nitride processing. However, aggressive thickness scaling remains limited by the coupled tradeoff among switchability, leakage, dielectric breakdown, ferroelectric stability, and control of the as-grown polarization state. Here, we report the first experimental demonstration of enhanced ferroelectricity in a 20 nm gradient AlN/AlScN/AlN heterostructure. By incorporating AlN interfaces together with compositional grading across the film thickness, the heterostructure modifies the polarization and dielectric response while preserving robust ferroelectric switching in the ultrathin regime. The gradient composition is directly verified by transmission electron microscopy, and, importantly, the heterostructure enables deterministic control of the as-grown polarization state on the same substrate, providing a distinct advantage for scalable integration and comparative device fabrication. Compared with uniform AlScN controls of similar thickness, the gradient heterostructure exhibits a 21.2% higher breakdown field, a 52.2% increase in coercive field, ~10% higher remanent polarization, a 17% lower permittivity, and approximately 40× higher resistivity, while maintaining comparable endurance. The combination of reduced permittivity, enhanced dielectric strength, strengthened polarization response, controlled polarization state, and strongly suppressed leakage suggests that gradient engineering with AlN interfaces improves field control and ferroelectric stability in ultrathin wurtzite nitrides. Importantly, this heterostructure design also enables scaling to a 5 nm AlN/AlScN/AlN sandwich structure containing only a 2 nm $Al_{0.64}Sc_{0.36}N$ ferroelectric layer, whereas a directly deposited 5 nm $Al_{0.64}Sc_{0.36}N$ film does not exhibit functional ferroelectric switching. These results establish a direct correlation between heterostructure design and ferroelectric performance, demonstrating that compositional grading and interfacial engineering together provide an effective route to stabilize and enhance ferroelectricity at reduced thickness. This strategy provides a pathway for further scaling of AlScN-based ferroelectric films, which may enable lower-voltage operation and higher-density integration in future nitride-based memory.

9:00am **NS-TuM-5 Functionalization-Driven Surface Assembly of Hexavanadate Molecular Memristors*, Dejia Kong,*** *Daniel Mejia Rodriguez, Amity Anderson, Wenjin Cao, Shuai Zhang,* Pacific Northwest National Laboratory*; Eric Z. Liu,* University of California at Santa Barbara*; Jonas Lorenz, Kirill Monakhov,* Leibniz Institute of Surface Engineering (IOM), Germany*; Venkateshkumar Prabhakaran, Oliva M. Primera-Pedrozo, Xue-Bin Wang, Niranjan Govind, Zbynek Novotny, Grant E. Johnson,* Pacific Northwest National Laboratory

Polyoxometalates (POMs) represent a class of molecular materials with significant potential for next-generation electronics, but their application requires precise control of their electronic properties on surfaces and in addressable arrays. This study investigates the electronic structures and self-assemblies of Lindqvist hexavanadate polyoxometalates (V_6POMs) on highly oriented pyrolytic graphite (HOPG). Using ion soft landing (ISL), we deposited intact, mass-selected V_6POMs functionalized with azide, succinate, and hydroxyl groups. X-ray photoelectron spectroscopy (XPS) confirms the retention of the V^{5+} oxidation state upon deposition. High-resolution scanning tunneling microscopy/spectroscopy (STM/S), supported by density functional theory (DFT) calculations, reveals a key finding: while isolated V_6POMs are semiconducting, their lateral aggregation, driven by hydrogen bonding between organic linkers, substantially reduces the molecular transport gaps. This demonstrates that the electronic properties of surface-supported V_6POMs may be tuned by controlling both the choice of organic functional group and the degree of aggregation. These results establish a clear pathway toward developing chemically programmable, multi-state resistive switching elements for future memristive devices and energy-efficient microelectronics.

9:15am **NS-TuM-6 Scalable HfN Based AlScN Ferroelectric Diode Memories for High-Temperature Operation up to 500 °C*, Chao-Chuan Chen,*** University of Pennsylvania*; Tzu-Yu Peng,* National Taiwan University, Taiwan*; Yunfei He, Zekun Hu, Kefei Bao, Roy Olsson,* University of Pennsylvania*; Yu-Jung Lu,* Academia Sinica, Taiwan*; Deep Jariwala,* University of Pennsylvania

Ferroelectric AlScN has attracted significant attention for next-generation non-volatile memory applications owing to its large remanent polarization, high thermal stability, and CMOS compatibility. However, the intrinsically high coercive field of AlScN results in large operating voltage, while aggressive thickness scaling is often limited by increased leakage current, premature breakdown, and unstable ferroelectric switching behavior. To address these issues, HfN has emerged as a promising bottom electrode material because its small lattice mismatch with AlScN enables coherent interface formation and reduced leakage current, potentially facilitating ultrathin and thermally robust ferroelectric devices.

In this work, HfN-based AlScN ferroelectric diode memories with different AlScN thicknesses (20 and 45 nm) and different oxide interlayers (Al_2O_3 and HfO_2) were investigated to evaluate the effects of thickness scaling and interface engineering on high-temperature ferroelectric operation. The influence of oxide interlayers on switching characteristics, leakage current, and self-rectifying behavior was also compared. Electrical characterizations, including DC, AC switching, and PUND measurements, were performed over a wide temperature range from room temperature to 500 °C to evaluate thermal stability and ferroelectric switching behavior under elevated-temperature operation.

Stable ferroelectric switching behavior was successfully maintained up to 500 °C under both AC and DC measurements. Both 20 nm and 45 nm AlScN devices demonstrated stable ferroelectric operation over a wide temperature range. A gradual reduction in coercive field with increasing temperature was observed, indicating thermally assisted polarization switching and reduced switching voltage. In the 45 nm devices, the remanent polarization reached |2Pr| values of ~150 μC/cm^2 and further increased at higher temperatures, suggesting enhanced polarization switching behavior. Although leakage current increased at elevated temperature, the devices retained clear ferroelectric switching characteristics and finite self-rectifying behavior with on/off ratio of ~10. In addition, the effects of AlScN thickness and oxide interlayers on switching stability and leakage behavior were systematically compared. These results highlight the thermal robustness and scalability of HfN-based AlScN ferroelectric diodes for high-temperature non-volatile memory applications.

9:30am **NS-TuM-7 Imaging Atomic Dynamics in Real-Time: Current Capabilities and Future Horizons at SLAC MeV-UED***, Alexander Reid,* SLAC National Accelerator Laboratory **INVITED**

High-brightness radio-frequency photocathode technology enables the generation of ultrashort electron bunches for a variety of frontier application. In the megaelectronvolt (MeV) energy range, these bunches serve as a powerful probe of atomic dynamics at the timescale of lattice vibrations, chemical reactions and phase rearrangement. MeV electrons combine ultrashort durations (<100 fs), with high momentum resolution, tens-of-nanometer scattering depths, and low energy deposition. The MeV ultrafast electron diffraction facility at SLAC National Accelerator Laboratory leverages these properties to allow sensitive measurement of atomic motions in solid, liquid and gas phase systems. This presentation details the current MeV-UED instrument at SLAC, its scientific achievements and the ongoing developments. A special focus will be emerging opportunities in in-situ, in-operando and multi-modal measurements capabilities.

11:00am **NS-TuM-13 Cavity Electrodynamics of Van der Waals Heterostructures***, James McIver,* Columbia University **INVITED**

Van der Waals (vdW) heterostructures host many-body quantum phenomena that can be tuned *in situ* using electrostatic gates. These gates are often microstructured graphite flakes that naturally form plasmonic cavities, confining light in discrete standing waves of current density due to their finite size. Their resonances typically lie in the GHz - THz range, corresponding to the same μeV - meV energy scale characteristic of many quantum effects in the materials they electrically control. This raises the possibility that built-in cavity modes could be relevant for shaping the low-energy physics of vdW heterostructures. However, capturing this light-matter interaction remains elusive as devices are significantly smaller than the diffraction limit at these wavelengths, hindering far-field spectroscopic tools. Here, we report on the sub-wavelength cavity electrodynamics of graphene embedded in a vdW heterostructure plasmonic microcavity. Using on-chip THz spectroscopy, we observed spectral weight transfer and an avoided crossing between the graphite cavity and graphene plasmon modes as the graphene carrier density was tuned, revealing their ultrastrong coupling. Our findings show that intrinsic cavity modes of metallic gates can sense and manipulate the low-energy electrodynamics of vdW heterostructures. This opens a pathway for deeper understanding of emergent phases in these materials and new functionality through cavity control.

11:30am **NS-TuM-15 Dynamical Control of Tip-Induced Light-Matter Interactions at the Surface of Quantum Materials***, Kyoung-Duck Park,* Pohang University of Science and Technology (POSTECH), Republic of Korea **INVITED**

Structure, function, dynamics, and interactions are fundamental concepts for understanding physical systems in nature. Among them, light-matter interactions have been a central subject of modern optics and condensed matter physics. However, conventional optical approaches have largely been limited to the classical regime at the microscale because of the diffraction limit. Recent advances in plasmonic nanocavities and tip-enhanced nano-spectroscopy have opened new opportunities to induce and probe light-matter interactions at the nanoscale. Nevertheless, these two approaches have mostly developed independently: plasmonic nanocavities can strongly enhance optical fields but lack spatially resolved spectroscopic access, while tip-enhanced nano-spectroscopy provides nanoscale optical information but has rarely been used as an active platform to dynamically control light-matter interactions. In this talk, I will introduce the concept of tip-enhanced cavity-spectroscopy (TECS) as a unique approach to induce, probe, and dynamically control tip-induced light-matter interactions at the surface of quantum materials. By using a plasmonic tip as a movable and tunable nanocavity, TECS enables nanoscale access to strong and ultrastrong light-matter interactions, including regimes where quantum tunneling and cavity-induced modification become important. This platform allows the optical, mechanical, polarization, and electrical degrees of freedom of the tip-sample junction to be actively controlled in real time. I will further discuss several emerging directions enabled by this concept. First, we exploit the extremely high local pressure generated by a nanoscale tip, reaching the GPa scale, to directly modify lattice structures and electronic properties at material surfaces. Second, we demonstrate dynamic control of near-field polarization by incorporating adaptive optics into near-field spectroscopy. Third, we develop conductive TECS, in which electrical current is directly introduced through the cavity junction to control local electronic and optical responses. These advances establish tip-induced light-matter interactions as an active and dynamically controllable platform for nanoscale spectroscopy, imaging, and quantum-material manipulation.

12:00pm **NS-TuM-17 Magneto – THz Correlated Electronic Behavior at the Nanoscale Through Scanning Near-Field Optical Microscopy***, Samuel Haeuser,* Iowa State University*; Richard H.J. Kim,* Ames National Laboratory*; Randall K. Chan,* Iowa State University*; Joong-Mok Park, Thomas Koschny,* Ames National Laboratory*; Jigang Wang,* Iowa State University

Probing real space magnetic responses at terahertz (THz) scales is challenging but highly desired, as the local responses are less affected by the topologically trivial inhomogeneity that is ubiquitous in spatially averaged measurements. We explore a variety of material sets that contain strong electronic correlation behaviors at the nanoscale. Inherent properties of materials directly provide us with a playground of electrons but generally require special circumstances to manifest coherently. For example, $ZrTe_5$ hosts topologically protected helical edge states localized to atomically sharp boundaries, where magnetic fields can tune preferred electrical channels. $Pr_{(1-x)}Ca_xMnO_3$ hosts the colossal magnetoresistance transition from an insulator to a metal that has long been described to originate as nanoscopic phase transition on the order of the crystal lattice itself, also tuned by the combination temperature and magnetic field. Both systems are not guaranteed to remain under high energy excitations that may break such states. Thus, to probe the nanoscale electron correlated phenomena we apply a custom-built cryogenic magneto-THz/infrared scattering-type scanning near-field optical microscopy (cm-sSNOM) platform. We resolve the nanoscale, THz spectroscopic evolution of the magnetic field-driven colossal magnetoresistance transition [1] and magnetic brightening of helical edge states in quantum spin Hall transport [2].

[1] S. Haeuser, et al., "Terahertz-nanoscale visualization of the microscopic spin-charge architecture of colossal magnetoresistive switching" arXiv:2603.07941

[2]S. Haeuser, et al., "Magnetic Brightening and Nanoscale Imaging of Spin-Polarized Helical Edge Modes," **Nature Nanotechnology**, in press (2026) arXiv:2605.04883

Nanoscale Science and Technology
Room 320 - Session NS-TuA

Multimodal Techniques in Surface and Interface Engineering at the Nanoscale II

Moderators: Dr. Son Le, University of Maryland, **Dr. Taisuke Ohta**, Sandia National Laboratories

2:15pm **NS-TuA-1 Multimodal Investigation and Interface Engineering of Near-Surface Diamond Quantum Defects***, Nazar Delegan,* Argonne National Laboratory **INVITED**

Solid-state spin defects, such as the nitrogen-vacancy (NV) center in diamond, are premier candidates for quantum sensing and information processing due to their long spin coherence times and robust room-temperature operation. However, when brought within nanometers of the surface to maximize coupling to external targets, their quantum properties degrade due to interface defects, uncontrolled surface terminations, and parasitic "dark" electron spins. Overcoming these challenges requires a multimodal approach that pairs sub-nanometer characterization with precise chemical control of the interface.

In this talk, we address this problem by leveraging atomic layer etching (ALE) and atomic layer deposition (ALD) as a dual framework for highly sensitive surface diagnostics and precise interface engineering. We show that sub-angstrom ALD nucleation profiles serve as an analytical probe capable of distinguishing between common diamond (001) surface terminations. Expanding on this capability, we deploy ALD-grown ultrathin titanium oxide (TiO_2) films to passivate the diamond interface, drastically reducing the background density of deleterious dark surface spins.

This controlled processing allows for the realization of pristine diamond surfaces. Enabled by this approach, we present direct atomic-scale imaging, spectroscopic characterization, and charge-state manipulation of individual near-surface NV centers using scanning tunneling microscopy (STM). By utilizing a conductive graphene capping layer to circumvent diamond's bulk insulating nature, we identify clear spectroscopic signatures of NV- defects. Critically, we demonstrate local control over the defect's electronic environment, dynamically tuning the charge state from NV^- to NV^0 via tip-induced gating. Together, these complementary nanoscale imaging and conformal engineering paradigms offer a robust toolkit for mitigating surface noise and optimizing diamond-based quantum architectures.

2:45pm **NS-TuA-3 Multi-Technique Nanoscale Probe Studies of Intercalated Phases of Pb, Gd and Dy Under Graphene on SiC***, Shen Chen, Salma Khatun, Umamahesh Thupakula,* Ames National Laboratory*; Zhe Fei,* Iowa State University*; Marek Kolmer,* Ames National Laboratory*; Michael C. Tringides,* Iowa State University

Metal intercalation beneath epitaxial graphene on SiC (Gr/SiC) can host different subsurface phases, which is a way to control the band structure, subsurface superstructure, metal nucleation and charge transfer. Realizing and controlling these subsurface phases requires identifying the galleries occupied by the intercalants and the types of intercalated phases formed. Here, we use complementary techniques, including STM/STS, SPA-LEED, and ARPES to address the previous questions. Among Pb-intercalated phases, $(10\times10)_{gr}$ is of particular interest because the large supercell generates replica Dirac cones at the corners of mini-Brillouin zones. However, establishing reproducible growth conditions for the $(10\times10)_{gr}$ phase remains challenging. By monitoring deposition and annealing cycles, we quantitatively show that during growth the $(10\times10)_{gr}$ and Pb(10) intensities are correlated, suggesting that Pb(111) islands preferentially nucleate on $(10\times10)_{gr}$ domains[1]. For Gd intercalation, multiple phases with different gallery occupancies form, depending on growth conditions of coverage and annealing temperature, all of which have been comprehensively studied with the previously listed techniques. Multiprobe STM transport confirm the decoupling of the top graphene by the large displacement field generated by intercalated Gd[2]. Recent experiments show the formation of pre-designed Gd intercalated phases by kinetically controlling the Gd subsurface occupation[3]. Dy [4] intercalation shares similar intercalated phases and growth as Gd and both metals are ideal metals to control graphene magnetism. These experiments show that metal intercalation is a very promising approach for further engineering graphene's exceptional electronic properties. They establish a framework to identify metal intercalated phases in Gr/SiC heterostructures and to generate 2-d quantum materials with tunable electronic properties.

[1] S. Chen, M. Kolmer, L. Wang, Y. Han, M. Blank, J.W. Evans, M.C. Tringides, *Phys. Rev. B*. **112**, 045418 (2025).

[2] M. Kolmer, W. Ko, J. Hall, S. Chen, J. Zhang, H. Zhao, L. Ke, C.-Z. Wang, A.-P. Li, M.C. Tringides, *J. Phys. Chem. Lett.* **13**, 11571 (2022).

[3] S. Khatun, S. Chen, J. Hall, M. Fralaide, U. Thupakula, M. Hupalo, Y. Han, Z. Fei, M.C. Tringides, M. Kolmer, *Carbon*. 121670 (2026).

[4] S. Chen, Y. Han, M. Kolmer, J. Hall, M. Hupalo, J.W. Evans, M.C. Tringides, *Phys. Rev. B*. **107**, 045408 (2023).

3:00pm **NS-TuA-4 Multidimensional Characterizations of Pyrrolidine Dissociations on Cu(100) Surface with the Single-Bond Resolution***, Liya Bi, Hao Zhou, Zihao Wang, Shaowei Li,* University of California San Diego

Here, we report the development of a multidimensional characterization platform for identifying surface adsorbents with the single-bond resolution. This platform is based on low-temperature scanning tunneling microscopy, encompassing the bond-resolved STM (BR-STM), STM-inelastic electron tunneling spectroscopy (STM-IETS) and infrared-integrated STM (IRiSTM). We demonstrated both its chemical sensitivity and spatial resolution through fully characterizing the dissociation products from a pyrrolidine (C_4H_9N) to a dehydrogenated pyrrole (C_4H_4N) on Cu(100) surfaces. We unambiguously assigned a series of products after step-by-step dehydrogenation to dehydrogenated pyrrolidine (C_4H_8N), 1-pyrroline (C_4H_7N), dehydrogenated 2-pyrroline (C_4H_6N), 3H-pyrrole (C_4H_5N) and dehydrogenated 1H-pyrrole (C_4H_4N), which was supported by bond-resolved topographic imaging and/or IETS mapping and/or single-molecule IR spectroscopy. Our experimental scheme is expected to aid in chemical identification in on-surface synthesis or catalysis with both structurally and vibrationally sensitive probes.

3:15pm **NS-TuA-5 Linking Sers Spectral Variability to Reliable Detection of Low-Affinity Analytes via Plasmonic Substrate Physics and Machine Learning***, Amit Kumar, Fengbo MA,* University of Georgia*; Susu M. Zughaier,* Qatar University, Qatar*; Xianyan Chen, Yiping Zhao,* University of Georgia

Surface-enhanced Raman spectroscopy (SERS) provides ultrasensitive molecular detection through localized plasmonic field enhancement; however, reliable sensing of low-affinity analytes remains limited by spectral variability arising from heterogeneous electromagnetic enhancement and adsorption-orientation-dependent Raman tensor projections. In this work, we establish a physics-informed and machine-learning-assisted framework linking SERS spectral variability with sensing reliability on oblique-angle-deposited silver nanorod (AgNR) substrates. A comprehensive SERS dataset was constructed using 1,2-bis(4-pyridyl) ethylene (BPE) under six controlled experimental conditions, including defect mapping, batch-to-batch variation, nanorod-length variation (200-1000 nm), concentration-dependent drop-casting (10^{-3}-10^{-12} M), static immersion (10^{-3}-10^{-10} M), and real-time adsorption (10^{-5} M). Hierarchical cluster analysis (HCA) partitioned the spectra into seven reproducible spectral clusters spanning high- and low-SNR regimes, while principal component analysis (PCA) revealed that cluster separation originates from systematic redistribution of Raman modes rather than stochastic noise. The results show that geometry-dependent plasmonic enhancement redistributes Raman peak intensities through electromagnetic weighting, while tensor-based orientation analysis demonstrates orientation-selective enhancement governed by Raman polarizability anisotropy. Building on this spectral variability framework, HCA and PCA were further applied to concentration-dependent bacterial biomarker datasets to identify distinct spectral evolution regimes associated with adsorption affinity and concentration variation. Strongly adsorbing biomarkers, including 2,3-DHBA, 2,5-DHBA, and pyocyanin, produced stable high-intensity spectra, whereas weakly adsorbing biomarkers, including lipoteichoic acid (LTA), enterobactin, and β-carotene, exhibited weak enhancement and non-monotonic spectral evolution that limited conventional calibration-based quantification. Using HCA/PCA-derived spectral patterns, convolutional neural network (CNN) classification and regression models were implemented directly on the SERS spectra. The CNN classification model achieved 99.99% classification accuracy, while regression models yielded concentration prediction performance exceeding R^2 >0.97 with MAE <0.27 despite substantial spectral variability. These results establish SERS spectral variability as a physically interpretable phenomenon governed by coupled plasmonic and molecular-orientation effects and demonstrate a scalable framework for robust nanoscale sensing in complex chemical and biological environments.

Nanoscale Science and Technology
Room Ballroom A - Session NS-ThP

Nanoscale Science and Technology Poster Session

NS-ThP-1 Improving Mechanical Integrity in Wearable Solid-Carbon Microneedle Sensors, ***Nicolas Manning***, Commonwealth University of Pennsylvania - Lock Haven

Nanostructured carbon used as solid contact enables stable, calibration-free all-solid-state ion-selective electrodes (SC-ISEs) in miniaturized formats. It is typically coated on top of a metallic electrode, such as a microneedle, followed by an ion-selective membrane (ISM) coating. When this microneedle is inserted into artificial skin, the coatings do not always stay intact. Here we investigate an alternate approach by preparing self-supporting mesoporous carbon-based microneedles, which can be infiltrated and covered with the ISM. We hypothesize that this helps to maintain the ISM coating during insertion of the microneedle into skin. Silicone molds were prepared from steel microneedle arrays and then infiltrated with a resol containing colloidal silica as sacrificial template for the mesopores. After polymerization and carbonization, the resulting microneedle arrays were etched to remove the silica, introducing mesopores. Structural features were verified by scanning-electron microscopy. Future work will incorporate reference membranes and assess ion selectivity under physiological conditions, advancing SC-ISE microneedles for real-time on-skin or in vivo ion monitoring.

NS-ThP-2 Single-Molecule Spectro-Microscopic Visualization of Surface-Supported Configurational Flexibility and Intramolecular Transformations, ***Soumyajit Rajak***, *Nan Jiang,* University of Illinois, Chicago

Understanding physicochemical transformations at surfaces with molecular-scale precision is essential for advancing nanoscale materials characterization and the rational design of functional interfaces for catalysis, molecular electronics, and optoelectronic devices. A major challenge in surface characterization is the direct identification of intermediates, adsorption geometries, and reaction products with simultaneous chemical specificity and sub-molecular spatial resolution, capabilities that are difficult to achieve with conventional ensemble-averaged techniques. Although scanning tunneling microscopy (STM) provides atomic-scale structural information, it often lacks definitive chemical sensitivity, particularly for nonplanar and conformationally flexible molecular systems. A single-molecule tip-enhanced Raman spectroscopy (TERS) methodology integrated with ultra-high vacuum (UHV) STM has been utilized to achieve correlative nanoscale structural and chemical characterization of thermally induced surface transformations and surface-dependent molecular arrangements. Coupling light with an atomically sharp plasmonic probe creates highly localized surface plasmons (LSPs), which allow the overcoming of the diffraction limit and confined enhancement of the Raman signals. As a model metal-organic interface, we investigate tetraphenyl tetrabenzoporphyrin adsorbed on Cu(100) and Cu(111), representative systems relevant to heterogeneous catalysis and organic electronic materials. Porphyrin derivatives are especially attractive for nanoscale studies because of their tunable electronic structure, metal-coordination functionality, and conformational flexibility arising from σ-bonded meso-substituents.Our measurements demonstrate that TERS provides chemically specific vibrational fingerprints of individual adsorbed molecules while simultaneously resolving symmetry variations and local conformational changes induced by molecule–substrate interactions at the sub-nanometer scale. Spatially resolved vibrational mapping enables discrimination between coexisting adsorption geometries and thermochemically transformed species that exhibit distinct chemical identities. The results further reveal how substrate interactions stabilize nonplanar conformations and alter molecular symmetry, establishing direct structure-property relationships at the single-molecule level.

NS-ThP-3 Intrinsic Stability of Rhodium Nanoclusters on HOPG: An Atomic-Scale Investigation of Heat Treatment and CO Adsorption, ***Charbel Tawny***, *Maxwell Gillum, Gallage KPA Ariyaratne, Mausumi Mahapatra,* Loyola University Chicago

Understanding structure-reactivity relationships in heterogeneous catalysis requires well-defined model systems that enable atomic-scale characterization. In this work, Rhodium (Rh) nanoclusters were deposited on Highly Oriented Pyrolytic Graphite (HOPG), an inert support, to investigate their nucleation, growth and changes in morphology under ultra-high vacuum (UHV) conditions. By systematically varying Rh coverage (0.09 ML to 0.6 ML), Scanning Tunneling Microscopy (STM) was used to resolve cluster size, morphology, and spatial distribution. Our experiments reveal the formation of highly dispersed Rh nanoclusters with a notably narrow size distribution; for instance, a 0.09 ML deposition produced particles with an average width of 1.74 ± 0.5 nm and height of 0.85 ± 0.1 nm. Crucially, these nanostructures exhibit exceptional thermal stability, maintaining their size and distribution even after annealing to elevated temperatures up to 850 K. Subsequent CO exposure at both 300 K and 500 K allowed for the visualization of surface interactions. While CO induced streaking was observed in STM images due to adsorbate mobility, the Rh clusters remained structurally stable without significant redispersion or morphological changes. This study establishes the robustness of Rh nanoclusters in response to various stimuli that would be present in an industrial reaction, such as high temperatures and gas exposure, further deepening our knowledge of surface catalysis.

NS-ThP-4 Characterization and Analysis of Rhodium Oxide Nanoparticles on HOPG Surface, ***Gallage KPA Ariyaratne***, *Maxwell Gillum,* Loyola University Chicago*; Charbel Tawny,* loyola University Chicago*; Mausumi Mahapatra,* Loyola University Chicago

This study investigates the characterization and analysis of rhodium oxide (RhO_x) nanoparticles formed on highly oriented pyrolytic graphite (HOPG), with the aim of understanding how oxygen influences nanoparticle stabilization and behavior on a weakly interacting support. HOPG serves as an ideal model surface for probing intrinsic nanoparticle properties in the absence of strong substrate interactions. Rh nanoparticles are vapor-deposited onto freshly cleaved HOPG under ultra-high vacuum conditions and subsequently oxidized at controlled temperatures (300–850 K) to generate RhO_x nanostructures. Scanning Tunneling Microscopy (STM) is employed to examine nanoparticle morphology, size distribution, and structural evolution as a function of temperature and Rh coverage. Oxidation at room temperature results in the formation of RhO_x nanoparticles with an apparent reduction in particle density and surface coverage relative to metallic Rh. At elevated temperatures, larger RhO_x nanoparticles are observed, with average widths of 9.14 nm. High temperatures like 850 K, result in the formation of triangular channels on HOPG surface, originating from step edges. These features are not due to direct structural failure of HOPG but rather arise from oxygen mediated anisotropic etching of the graphite surface. Oxygen can dissociate on RhO_x which then migrate onto the HOPG surface where the atomic oxygen react with uncoordinated carbon atoms at defect sites and step edges which lead to the removal of carbon atoms as CO/CO_2 and leads to anisotropic etching on surface. Post oxidation exposure to carbon monoxide (CO) is performed to evaluate redox reversibility and stability under reducing conditions, with the evolution of gaseous species such as CO_2, O_2, and CO observed, while the crack and particle size remains unchanged. In parallel, Density Functional Theory (DFT) calculations using (PBE-GGA) model RhO_x adsorption on graphite, identifying favorable configurations, and electronic properties with nanoparticle stability, reactivity, and catalytic performance on carbon supports.

NS-ThP-5 Spatiotemporal Defect Engineering of Charge Transport in TiO2 by Time-Resolved Atomic Force Microscopy, *Nuray Basaran, Mohammad Safikhani-Mahmoudi,* École de technologie supérieure, University of Quebec, Canada*;* ***Bugrahan Guner***, Yale University*; Omur Dagdeviren,* École de technologie supérieure, University of Quebec, Canada

The performance of photocatalysts, sensors, and oxide-based devices is governed by how charge carriers migrate, recombine, and interact with defects at surfaces and interfaces. Titanium dioxide (TiO_2), a model photocatalyst, provides a versatile platform for exploring these dynamics. Recent advances in*time-resolved atomic force microscopy (TR-AFM)* now allow direct nanoscale mapping of carrier motion under realistic conditions, uncovering defect-controlled pathways that were previously inaccessible.

We establish findings from our recent studies to build a coherent picture of light-induced defect dynamics in TiO_2. In "thin" TiO_2films, it was shown that ultraviolet irradiation generates photoinduced surface oxygen vacancies (PI-SOVs) that shorten carrier migration time constants but raise activation barriers, indicating a trade-off between faster trapping and reduced mobility. Extending this framework,*we*revealed that PI-SOVs impact both fast and slow timescales, with spatially heterogeneous distributions leading to locally distinct transport regimes.*Moreover, we explored* surface chemistry by introducing methanol as a prototypical hole scavenger: methanol adsorption further reduced time constants and modified activation energies, demonstrating how molecular adsorbates tune vacancy-carrier interactions.

By bridging molecular adsorption, defect generation, and irradiation penetration, this body of work highlights spatiotemporal defect engineering as a promising strategy for controlling charge transport in oxides. TR-AFM emerges as a uniquely powerful platform for resolving these processes at the nanoscale, offering pathways to rationally design oxide-based systems with tunable photocatalytic efficiency, sensor responsiveness, and energy-conversion robustness.

NS-ThP-6 Ce-Doped TiO_2 Nanoparticles from Commercial P25 and Flame Spray Pyrolysis Synthesis Routes for Enhanced Visible-Light Photocatalysis, *Selda Topcu Sendogdular,* Stony Brook University, Turkey*;* ***Ilker Keseroglu****, Pelagia-Iren Gouma,* The Ohio State University

Ce-doped TiO_2 nanoparticles were synthesized by modifying commercial Degussa P25 and flame-made TiO_2 produced by flame spray pyrolysis (FSP), followed by thermal treatment at 500 °C. The effects of Ce doping on the structural, morphological, optical, and photocatalytic properties of TiO_2 were investigated for undoped and Ce-doped samples containing 5 and 40 wt% Ce.

X-ray diffraction (XRD) analysis showed that both P25 and FSP TiO_2 consisted primarily of anatase and rutile phases, while Ce doping suppressed the anatase-to-rutile transformation and promoted CeO_2 phase formation at higher Ce loading. Ce doping reduced the anatase crystallite size and altered the phase composition, with brookite contributions observed in CE5-P25 and CE5-TiO_2 samples. SEM and TEM analyses revealed morphological differences between P25 and FSP TiO_2 particles, where P25 exhibited irregular elongated and polygonal particles, while FSP-derived TiO_2 showed predominantly spherical particles. Ce doping decreased particle size to approximately 14–34 nm, whereas high Ce loading (40 wt%) resulted in particle agglomeration and cube-like Ce-rich structures. SAED and HRTEM analyses confirmed the coexistence of anatase and rutile phases and verified lattice fringes corresponding to anatase (101) and rutile (110) planes.

UV–Vis spectroscopy demonstrated enhanced visible-light absorption and a red shift in the absorption edge with increasing Ce content. The bandgap decreased from approximately 3.06 eV for pure TiO_2 to 2.48 eV for Ce-doped samples, indicating improved visible-light response. Photocatalytic performance was evaluated through methylene blue degradation under visible-light irradiation using a Xe lamp with AM 1.5G and a 400 nm cut-on filter. Among all samples, CE5-TiO_2 exhibited the highest photocatalytic activity, achieving approximately 90% methylene blue degradation under visible light.

The enhanced photocatalytic performance is attributed to reduced crystallite size, suppression of rutile phase growth, modified phase composition, and improved visible-light absorption induced by Ce doping. These results demonstrate that Ce modification effectively enhances the photocatalytic activity of both commercial P25 and flame-made TiO_2 for environmental remediation applications.

NS-ThP-7 Roll-to-Plate Nanoimprint Lithography for Fabrication of Biomimetic Structures, ***Daniela Topasna****, Juan Gonzalez, Sebastian Ziegler,* Virginia Military Institute

Nanoimprint Lithography (NIL) fabrication technique consists of transferring a pattern from a template by pressing it onto a resin coated substrate, yielding structures with nanometer resolution. The resin can be cured thermally or by exposure to UV radiation. This is a simple, low-cost and high-throughput technique, which has been used as an alternative to photolithography in semiconductor industry, optics and photonics, and biomedical field. NIL roll-to-plate method was used in this project to replicate microstructures of Cicada wings which are of interest due to their antibacterial properties. We report the results on the fabrication of these biomimetic structures and on their characterization by scanning electron microscopy.

NS-ThP-8 Nanoscale Surface and Interface Engineering of Asymmetric Electrode Screen Length for Advanced Nanoscale Ferroelectric Devices, ***Philip (Sanghyun) Lee***, University of Kentucky*; Kent Price,* Morehead State University*; M. David Henry,* Sandia National Laboratories, USA

The continued scaling of ferroelectric tunnel junctions (FTJs) has placed unprecedented importance on understanding and controlling nanoscale surface and interface interactions within ultrathin HfO_2–based ferroelectrics. At thicknesses below 6 nm, the electronic structure, bonding environment, and screening behavior at metal/ferroelectric interfaces dominate the tunneling landscape, often more strongly than the bulk ferroelectric properties themselves. Conventional symmetric Metal-$Hf_{0.5}Zr_{0.5}O_2$-Metal (MFM) stacks such as TiN/HZO/TiN exhibit negligible tunneling electroresistance (TER) because their interfaces screen polarization charges in an identical manner, suppressing any barrier asymmetry. While inserting dielectric interlayers can restore asymmetry, these additional interfaces introduce variability, trap formation, and integration challenges.

This contribution presents a materials–driven strategy that leverages intrinsic nanoscale surface and interface asymmetry between dissimilar metal electrodes to enhance FTJ performance without modifying the ferroelectric layer. We focus on five CMOS compatible metals such as TiN, W, Ru, TaN, and Mo about possessing distinct electronic screening behavior, interfacial bonding characteristics, and surface chemistries with HZO. These differences affect how polarization-bound charges are compensated at the interface, reshaping the tunneling barrier.

To assess these nanoscale interfacial effects, multiple devices including Ta/HZO/TaN were developed and their nanoscale interfacial structures and chemistry were compared in agreement with theoretical research for MFM devices. This study incorporates realistic ferroelectric switching, nonlocal tunneling transport, and metal–specific screening behavior, enabling direct correlation between nanoscale interface physics and device–level performance. Surface and interface characteristics with multiple HZO thicknesses were quantified to confirm how interfacial screening, depolarization stability, and surface-induced barrier shaping collectively determine TER, read current, and write voltage.

Our results show that electrode pairs with different interfacial screening length create strong asymmetry in the tunneling barrier, enabling enhanced TER without the need for additional interlayers. Energy band analysis reveals how nanoscale surface interactions such as metal-oxygen bonding, interfacial dipole formation, and screening charge distribution directly affect the tunneling mechanism in opposite polarization states. Finally, we mapped optimal metal combinations that support low–voltage switching and stable ferroelectric behavior <6nm HZO for interface–engineered MFM devices.

NS-ThP-9 Time-Delayed Measurements of Heterogeneous Dynamic Data, ***Petro Maksymovych***, Clemson University*; Sabine Neumayer,* Oak Ridge National Laboratory, USA

In neuromorphic and memory devices, accessible multistability is enabled by the dynamics of the constitutive materials rather than by their equilibrium structures alone. Hysteresis loops, oscillatory responses, and other time-dependent signatures reflect the multiplicity of accessible material states. Yet deciphering the underlying dynamics remains persistently elusive — in no small part because the dynamic information itself is treated qualitatively rather than as a quantitative observable.

I will present a systematic approach based on time-delayed embedding and dynamic mode decomposition that treats dynamic data as a structured object, extracting its nonlinearity, topology, and a predictive numerical model of the underlying process. Applied to resistive switching in memory oxide materials [1,2], nonlinearity alone can discriminate between specific microscopic mechanisms. In ferroelectrics, the same framework separates genuine switching from spurious hysteresis and detects the signatures of a multiwell potential [3,4]. Effective denoising strategies extend the approach to noisy nanoscale and device measurements without loss of physical interpretability.

Time-delayed methodologies provide a transparent and interpretable connection between hysteresis loops and physical mechanisms, complementing machine learning methods and enabling parameter-free comparison between modeling and experiments of driven dynamics. R

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NS-ThP-10 Chirality Retention in Aqueous Propylene Oxide Hydration: Chirality of the Transition State*, **Nisha Shukla,*** Carnegie Mellon University, USA*; Marcus Yu,* University of Columbia*; Andrew Gellman,* Carnegie Mellon University, USA

The hydration kinetics of enantiomerically pure propylene oxide (PO) to chiralpropylene glycol (PG) in aqueous solution have been studied using FTIRwhile simultaneously monitoring the net chirality of the reaction mixture. The hydration reactionappears to be first-order in the PO concentration with a rate constant of 0.05 hr. Moreimportantly, the reaction is enantioselective; the product PG retains the chirality of the 2C carbonin PO with ~2:1 selectivity. The fact that there is some inversion of the chirality suggests thatthe dominant transition state is one in which the 2C-O bond in PO is cleaved, resulting in a closeto planar transition state capable of inversion during hydration. If the transition state involved1C-O cleavage it would retain the rigid chiral center of the PO reactant, preventing significantinversion.

NS-ThP-11 Understanding the Structural Orientation of Iron Tetraphenylporphyrin (Fe-TPP) on HOPG through Scanning Tunneling Microscopy for Electrocatalytic CO_2 Reduction*, **Hritvik Bhosale,*** *Mausumi Mahapatra,* Loyola University Chicago

Homogeneous molecular catalysts provide precise control over the steric and electronic properties of active sites, enabling tunable catalytic activity and selectivity. However, these systems often suffer from limited stability, poor recyclability and reduced long-term durability under homogeneous operating conditions. Consequently, strategies that combine the tunability of molecular catalysts with the robustness of heterogeneous platforms have attracted considerable attention. Despite advances in catalyst heterogenization, developing structurally well-defined systems that bridge homogeneous and heterogeneous catalysis remains a challenge.

Porphyrin-based systems have emerged as attractive molecular platforms owing to their structural versatility, electronic tunability and catalytic relevance. Among them, iron porphyrins are particularly promising for electrocatalytic CO_2 reduction through successive electron-transfer processes that have demonstrated efficient, CO-selective and durable catalytic performance.

Understanding molecule-surface interactions at the nanoscale is essential for rational catalyst heterogenization. Scanning tunneling microscopy (STM), with submolecular and atomic-scale spatial resolution, provides a powerful platform for directly visualizing molecular arrangements, conformations, electronic structures and intermolecular interactions at surfaces. STM has proven especially effective for investigating the adsorption behavior and self-assembly of porphyrin systems on conductive substrates.

The present study investigates the adsorption behavior of iron tetraphenylporphyrin (FeTPP) on highly oriented pyrolytic graphite (HOPG) using STM as the primary investigative technique. By correlating molecular structure with surface organization, intermolecular interactions, and local electronic properties, this work aims to provide fundamental insights into molecule-surface interactions relevant to catalyst heterogenization and to establish structure–property relationships for the development of heterogenized iron porphyrin systems for efficient electrocatalytic CO_2 reduction.

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NS-ThP-12 Nano-Projectile SIMS: Guiding EUV Resists Fabrication Process with Nanoscale Compositional Insights*, **Christelle Guillermier,*** Biennetechnology*; Michael J Eller,* University of Mississippi*; Stanislav V Verkhoturov, Richard Rickman,* Biennetechnology*; Serge Della Negra,* Universite Paris Saclay, France*; Emile A Schweikert,* Texas A&M and Biennetechnology

The semiconductor industry is rapidly adopting extreme ultraviolet (EUV) lithography to pattern features below 10 nm. However, there remains a critical need for methods capable of probing nanoscale compositional uniformity throughout the multi-step fabrication process. Secondary Ion Mass Spectrometry (SIMS) has long been a key analytical technique in semiconductor process control due to its high sensitivity and high-resolution depth profiling capabilities, but its lateral resolution is limited to ~50 nm, restricting its application to critical dimension analysis. In this work, we present results from the newly commercialized Nano projectile Secondary Ion Mass Spectrometry (NP-SIMS) instrument, the Orion MkII, which overcomes this limitation by examining surfaces with individual nano-projectiles. Each projectile samples an area of ~10–15 nm in diameter and ~10 nm in depth, enabling nanoscale inspection with lateral resolution that matches the requirements of advanced EUV photoresist characterization. We demonstrate the capabilities of NP SIMS for identifying material inhomogeneities that can lead to defects during resist fabrication and compromise pattern quality. More specifically, NP-SIMS enables examination of characteristic molecular species for homogeneity and co-localization with other resist components. The integration of a multi-anode detector further allows identification and characterization of sites containing multiple instances of the same analyte. Finally, NP-SIMS provides detailed chemical analysis of defect sites, which can significantly affect the resist performance. Altogether, NP-SIMS delivers essential insights to guide the optimization of EUV resist chemistry and processing conditions.

NS-ThP-13 Probing the Electron Screening Process in 2d Semiconductor WS_2*, Alex Boehm, Christopher Smyth,* Sandia National Laboratories*; Kory Burns,* University of Virginia, USA*; Andrew Kim,* Sandia National Laboratories, USA*; Jordan Hachtel,* Oak Ridge National Laboratory, USA*; Don Bethke, Tzu-Ming Lu, Catalin Spataru,* Sandia National Laboratories, USA*; Hayden Barry,* University of Virginia, USA*; Jose Fonseca, Jeremy Robinson,* Naval Research Laboratory, USA*; **Taisuke Ohta,*** Sandia National Laboratories, USA

The confinement of charge carriers within an anisotropic two-dimensional (2D) geometry leads to reduced, variable dielectric screening, which gives rise to strongly bound excitons, correlated electron phases, and band gap renormalization. We employ electronic structure probes (photoelectron and electron energy loss spectroscopies) to assess the impact of the supporting substrate and the sulfur vacancy defects on the screening characteristics of the 2D semiconductor WS_2. Exploiting the contrasting external dielectric screening environments achieved in gold-supported and free-standing (i.e. suspended) configurations, we show how the electronic states of one-layer WS_2 align at a built-in junction across the effective and ineffective screening environments. Photoelectron spectroscopy points to the close alignment of the charge neutrality levels of WS_2 between each screening environment. We further reveal through ion irradiation that the introduction of a modest defect density (n_V) of 1×10^{13} cm^{-2} reduces the electronic band gap from 2.4 eV to 2.2 eV in poorly-screened suspended WS_2 because of the exciton binding energy reduction. The band gap renormalization accompanies the diminishing photoelectron core-hole relaxation and the expansion of the screened radius beyond the inter-defect distance around 4 nm when n_V reaches ~8×10^{12} cm^{-2}. Collectively, these findings provide key insights into the interrelationships of the polarizability of WS_2 with its electronic behavior and photoemission process.

We thank P. Mantos for measurement support. A.B., C.M.S., D.B., T.L., C.D.S., and T.O. acknowledge support from the Laboratory Directed Research and Development program at Sandia National Laboratories. A.R.K. acknowledges support from the U.S. Department of Energy, Office of Science, Division of Materials Sciences and Engineering (grant BES 20-017574). J.J.F. and J.T.R. were supported through Base Programs and the Nanoscience Institute at the Naval Research Laboratory via the Office of Naval Research. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly-owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. This abstract describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the abstract do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

NS-ThP-14 Local Electronic and Transport Properties of Epitaxial Graphene on Sic(0001) Studied by Scanning Tunneling Microscopy and Spectroscopy*, **Marek Kolmer,*** *Umamahesh Thupakula, Shen Chen, Yong Han,* Ames National Laboratory*; Michael C. Tringides,* Iowa State University

Despite long-standing efforts to understand the interface between epitaxial graphene and the Si-terminated silicon carbide (0001) substrate, the exact atomic-scale structure, its complex bonding configurations, and the resulting electronic properties of the first epitaxial graphene carbon layer (C_{buffer}) remain open problems. We will present how to control the local

structure of the epitaxial graphene-SiC interface with a low-temperature scanning tunneling microscope (STM) [1]. We will show that the covalent bonds between C_{buffer} and the SiC substrate may be reversibly broken and restored using the polarity of the electric field from the STM tip, generating protrusions at the interface of slightly higher amplitude. This buried interface manipulation enabled us to pattern epitaxial graphene with lateral precision, reaching the scale of a single 1.8 nm unit cell of the graphene-SiC interface $(6\times6)_{SiC}$ moiré lattice. However, the STM manipulation experiments also provide direct evidence of silicon vacancies at the topmost reconstructed SiC(0001) layers [2]. Bias-voltage- and epitaxial graphene thickness-dependent characterization of the collective C_{buffer}-SiC interface showed that 'Si' vacancy sites exhibit stable, non-switching behavior under STM electric fields. Moreover, vacancies introduce localized electronic states below the Fermi level. Our experimental results directly elucidate the atomic-scale interface and the influence of atomic and bonding configurations on the local density of states for graphene of different thicknesses on SiC(0001). Finally, we will present the consequences of the local epitaxial graphene structure on electronic transport properties.

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NS-ThP-15 The Nature of Photodoping in van der Waals Heterostructures, ***Son Le***, Laboratory for Physical Sciences*; Thuc Mai, Maria Munoz, Riccardo Torsi, Angela Hight Walker, Curt Richter,* NIST*; Aubrey Hanbicki,* Laboratory of Physical Sciences*; Adam Friedman,* Laboratory for Physical Sciences

A unique photoinduced modulation doping is achieved via integration of common 2D materials and inexpensive light sources. Under applied electric field and incident light, the doping level of 2D materials heterostructures consisting of multiple dielectric layers can be precisely controlled and tuned *in situ*. This photodoping also offers local control of charge with submicron spatial resolution with lifetimes on the order of months to years. For 2D materials systems there is no current agreement on the exact mechanism underlying this effect, with studies pointing to charge generation and trapping in various layers/interfaces. In this work, we present photoinduced doping of van der Waals heterostructures with various compositions in order to pin-point the exact spatial location of the photoactive defects that responsible for the doping phenomena. Regardless of the mechanistic details, this photodoping effect yields high-quality reconfigurable devices in a variety of 2D material systems including graphene, TMDs, and 2D superconductors.

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NS-ThP-16 Ternary Gold Nanoparticle-Corona-Neurotransmitter Plasmonic Complexes for Probing Resonant Electronic Coupling, ***Tefera Entele Tesema***, *Kahmeria Smith,* Prairie View A&M University

Plasmonic gold nanoparticles generate localized electromagnetic fields under resonant excitation, making them powerful platforms for probing nanoscale metal–molecule interactions. Although the molecular corona is often treated as a passive stabilizing layer, its composition can regulate interfacial charge distribution, optical damping, adsorption geometry, and plasmon-mediated coupling. Here, we develop a ternary plasmonic complex consisting of a gold nanoparticle core, a plant-derived molecular corona, and neurotransmitter molecules as a model system for resonant electronic coupling at bioactive noble-metal interfaces, using surface-enhanced Raman scattering (SERS) as the primary readout.Purple sweet potato (Ipomoea batatas, PSP)-derived extract functions as a reducing/stabilizing medium and forms a molecular corona containing anthocyanins, phenolic acids, and related polyphenols. This corona is treated as an electronically active, chromophoric interface whose absorption can influence resonance conditions. Dopamine is used as an initial catecholamine model to probe how bioactive adsorbates perturb the corona-mediated optical and vibrational response.Preliminary UV–visible spectroscopy shows that extraction protocol, pH, and solvent environment influence the optical identity of the PSP extract and nanoparticle formation. Unpeeled PSP extracted in 0.05 M acetate buffer at pH 4.75 produces a wine-colored, colloidally stable AuNP suspension that remains visually stable for five days. In contrast, TFA extraction at pH ~3 preserves anthocyanin absorption near 522 nm but is associated with black precipitate during AuNP formation, consistent with uncontrolled nucleation or aggregation. These observations indicate that mildly acidic acetate conditions provide a more suitable window for controlled AuNP–corona assembly. Anthocyanin interconversion among flavylium, hemiketal, quinonoidal, and related forms provides a handle for tuning corona absorption relative to the AuNP plasmon and SERS excitation.The phenolic and catechol-like functionalities in the PSP corona overlap chemically with catecholamine neurotransmitters and may compete for or reorganize interfacial binding sites on gold. SERS will monitor these interactions through vibrational fingerprints that report adsorption geometry, orientation, and binding competition. Coupling corona electronic transitions, nanoparticle plasmon resonance, and laser excitation is expected to amplify neurotransmitter-sensitive interfacial signatures. This work provides a tractable model for signal transduction at biotic–abiotic interfaces and may inform plasmonic chemical sensing and bioactive nanoparticle design.

NS-ThP-17 Exciton-Polaritons in Metal-Organic Chalcogenolates: From UV to Visible, ***Deep Jariwala***, University of Pennsylvania

Exciton-polaritons (EPs), hybrid light–matter quasiparticles formed by strong coupling between excitons and confined photons, offer a route to engineer semiconductor optical response without chemical modification. Here, I present strong and ultrastrong coupling in metal-organic chalcogenolates (MOCs), layered van der Waals hybrid semiconductors that act as natural multi-quantum-well structures with strong excitons, large oscillator strengths, and high refractive indices. These properties make MOCs promising self-hybridized polaritonic materials from the ultraviolet (UV) to visible range.

I will first discuss silver phenylselenolate (AgSePh, mithrene), which has a direct optical bandgap of ~2.65 eV, exciton binding energy of ~400 meV, and refractive index of ~2.5. Mueller matrix ellipsometry reveals giant in-plane birefringence (~1.01) and three anisotropic exciton resonances, enabling polarization-dependent linear dichroism up to ~77% when coupled to an optical self-cavity. Thickness-controlled mithrene flakes on reflective substrates support self-hybridized EPs in the ultrastrong coupling regime, with normalized coupling g/Ex = 0.13–0.14 and Rabi splitting >650 meV, the largest reported for a non-organic semiconductor in the visible range.

I will then present self-hybridized EP photodetectors in mithrene, where thickness-tunable multimode polariton states enable sub-bandgap photodetection extending >130 nm (~0.55 eV) below the optical bandgap. Trap-assisted two-photon absorption sustains strong coupling under sub-bandgap excitation, addressing a key limitation for polaritonic light harvesting. The polariton dispersion yields ultrafast group velocities (~65 μm ps−1), extending effective exciton diffusion from hundreds of nanometers to several micrometers and producing a 2.38-fold enhancement in photo-to-dark current ratio.

Finally, I will extend these concepts to the UV using silver phenylthiolate (AgSPh, thiorene), a wider-bandgap MOC with a sharp excitonic resonance at 3.46 eV (~60 meV linewidth) and refractive index of ~2.1. In open and closed cavities, thiorene shows clear anticrossing with Rabi splittings of 488 and 512 meV, respectively, among the largest reported in the UV and 6–10× larger than conventional ZnO and GaN platforms. Together, these results establish MOCs as a versatile platform for polariton-enhanced optoelectronics.

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