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

Author Index

Bold page numbers indicate presenter