Nanoscale Science and Technology
Room 320 - Session NS-MoA

Frontiers in Nanoscale Electron, Ion, and Scanning Probes II

Moderators: Alex Belianinov, Sandia National Laboratory, **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 Venturing Off-the-Rails: Localized Reconstruction of the Partial Density of States of Complex Oxide Heterostructures***, Hayden Barry, **Kory Burns***[2], 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.

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

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

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

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

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

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

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

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

New materials exhibiting robust polarization reversal and CMOS-compatible processing (e.g. alloys based on AlN, ZnO, and HfO_2) provide new opportunities for integrated ferroelectrics. To understand the mechanisms that control and induce switchable states in these materials, including the influence of microstructure and electrode interfaces, we employ a variety of transmission electron microscopy (TEM) and spectroscopy techniques to

[1] **Medard W. Welch Award Winner**
[2] **JVST Highlighted Talk**

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 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**[1],* Sandia National Laboratories, USA

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

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

[1] **JVST Highlighted Poster**

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**[1], Connor Vernachio2, Chris Howard,* University of Tennessee Knoxville*; Panchapakesan Ganesh,* Oak Ridge National Laboratory*; Wonhee Ko,* University of Tennessee Knoxville*; An-Ping Li,* Oak Ridge National 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.

[1] **JVST Highlighted Talk**

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