

# Sunday Afternoon, November 5, 2023

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

### Room B113 - Session NSP-SuA

## Nanoscience and Technology Division Plenary Session (ALL-INVITED SESSION)

**Moderators:** Georg Fantner, EPFL, Adina Luican-Mayer, University of Ottawa, Canada

### 2:00pm NSP-SuA-1 Bits to Atoms and Atoms to Bits: Atomic Fabrication in Electron Microscopy, *Sergei Kalinin*, University of Tennessee Knoxville INVITED

The last note left by Richard Feynman stated “*What I cannot create, I do not understand.*” Building solid state quantum computers, creating nanorobots, and designing new classes of biological molecules and catalysts alike requires the capability to manipulate and assemble matter atom by atom, probe the resulting structures, and connecting them to macroscopic world. Until now, the only viable approach for atomic fabrication was the Scanning Tunneling Microscopy, often integrated with the bespoke surface science techniques. Over the last decade, it has been shown that electron beams in Scanning Transmission Electron Microscopy can be used not only to probe structure and electronic properties of materials on atomic level, but also to modify materials on the atomic level. Harnessing electron beam changes for direct atomic fabrication however requires synergy between machine learning methods and microscope control. In this presentation, I will illustrate the progression of automated electron microscopy from real-time data analysis to physics discovery to atomic manipulations. Here, the applications of classical deep learning methods in streaming image analysis are strongly affected by the out of distribution drift effects, and the approaches to minimize though are discussed. The robust approach for real-time analysis of the scanning transmission electron microscopy (STEM) data streams, based on the ensemble learning and iterative training (ELIT) of deep convolutional neural networks, is implemented on an operational microscope, enabling the exploration of the dynamics of specific atomic configurations under electron beam irradiation via an automated experiment in STEM. Combined with beam control, this approach allows studying beam effects on selected atomic groups and chemical bonds in a fully automated mode. We demonstrate atomically precise engineering of single vacancy lines in transition metal dichalcogenides and the creation and identification of topological defects graphene. The ELIT-based approach opens the pathway toward the direct on-the-fly analysis of the STEM data and engendering real-time feedback schemes for probing electron beam chemistry, atomic manipulation, and atom by atom assembly. We further illustrate how deep kernel learning (DKL) methods allow to realize both the exploration of complex systems towards the discovery of structure-property relationship, and enable automated experiment targeting physics (rather than simple spatial feature) discovery. The latter is illustrated via experimental discovery of the edge plasmons in STEM/EELS. Jointly, these developments open the pathway for creation and characterization of designed defect configurations and artificial molecules in 2D materials.

### 3:00pm NSP-SuA-4 NSTD Early Career Competition Finalist Talks: N. Hosseini, Y. Liu, S. Challa,

### 3:40pm NSP-SuA-6 NSTD Graduate Competition Finalist Talks: N. Asmari, L. Kuo,

### 4:20pm NSP-SuA-8 Co-Localizing Atomic Force Microscopy with Other Microscopies and Spectroscopies: Elucidating Material Composition, Structure, and Properties at the Nanoscale, *B. Bailey, O. Maryon, J. Tenorio*, Boise State University; *D. Cintron Figueroa*, Pennsylvania State University; *J. Benzing*, National Institute for Science and Technology (NIST); *F. DelRio*, Sandia National Laboratories; *J. Robinson*, Pennsylvania State University; *M. Hurley, S. Hues, E. Graugnard, Paul Davis*, Boise State University

A wide variety of scanning probe microscopy (SPM) modes based on atomic force microscopy (AFM) have been developed to probe the nanoscale electrical, electrochemical, magnetic, mechanical, and thermal properties of surfaces. As a result, AFM and associated SPM modes enjoy widespread use in the surface characterization of materials. However, AFM typically does not directly report on chemical composition or optical properties. This talk will show how this limitation can be overcome through sub-micron

precision co-localization of AFM and associated advanced SPM modes with other analytical techniques such as scanning electron microscopy (SEM), Raman microscopy, and/or fluorescence-based super-resolution optical microscopy. In particular, co-localization of Kelvin probe force microscopy (KPFM) with SEM, energy dispersive spectroscopy (EDS), and electron backscatter diffraction (EBSD) has enabled correlation of surface Volta potentials with the composition and/or orientation of microstructural phases present in metal alloys. Additionally, the recently developed technique of photothermal AFM-IR, which simultaneously couples AFM and infrared spectroscopy to enable chemical identification at the nanoscale, has been applied to the study of few-layer atomic layer deposited and etched (ALD/ALE) transition metal dichalcogenides (TMDCs).

### 4:40pm NSP-SuA-9 Electron Paramagnetic Resonance of Individual Rare-Earth Atoms, *Gregory Czup, C. Lutz*, IBM Almaden Research Center; *H. Brune*, EPFL, Switzerland

Lanthanide series atoms are promising candidates for realizing single molecule magnets which remain magnetically stable at elevated temperatures. They are also being explored for their use as qubits both in the solid state and within molecules due to the long phase coherence time of the magnetic  $f$ -electrons and especially their nuclear spins. Recently, Electron Spin Resonance combined with the Scanning Tunneling Microscope (ESR-STM) has been developed into a powerful tool to address individual atomic spins on surfaces. However, driving and sensing spin resonance in lanthanide atoms with ESR-STM has remained a challenge due to  $f$ -electron shielding by the nonmagnetic valence electrons, which inhibits magnetoresistive sensing required for the technique. On the other hand, rare earths with an open valence shell have been shown to facilitate stronger interactions with tunneling electrons through intraatomic exchange coupling between the  $f$  electrons and valence shell. Here we demonstrate the detection of spin resonance in two different open-shell rare earth elements adsorbed on a thin insulating film using the STM. In one case, our measurements reveal an unexpectedly rich spectral structure which arises from the combination of a large electronic manifold of states and nuclear hyperfine interactions which can all be accessed at GHz energy scales. In the other case, a relatively large  $g$  factor presents opportunities for magnetic sensing at the atomic scale. Our results demonstrate the ability to drive and sense spin resonance of individual rare earth atoms with atomic resolution while providing a route to studying uncommon open valence shell lanthanide species.

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