Nanoscale Science and Technology
Room 206 A W - Session NS1-TuM

AI for Material Discovery and Characterization

Moderators: Yongtao Liu, ORNL, **Son Le**, University of Maryland

8:00am **NS1-TuM-1 Advancing Scanning Probe Microscopy as a Tool for Nanoscale Scientific Discovery with AI***, **Rama Vasudevan**, Ganesh Narasimha, Jawad Chowdhury,* Oak Ridge National Laboratory*; Soumendu Bagchi,* Oak Ridge Natinal Laboratory*; Yongtao Liu,* Oak Ridge National Laboratory **INVITED**

Scanning probe microscopy (SPM) methods have been a mainstay of nanotechnology since their inception in the 1980s, helping to image and map functional properties of a wide variety of samples, ranging from ceramics to thin films to nanoparticles to biomolecules. More recently, the advent of machine learning and artificial intelligence (AI) has led to an increasing adoption of AI-based methods within core physical sciences.

In this talk, it will be shown how AI can significantly improve SPM in terms of scientific discovery, by adapting AI algorithms and tailoring them for purposes of microscopy characterization and manipulation. Traditional spectroscopic characterization in SPM is carried out in a point by point manner across a grid of points, which is highly redundant. We propose the use of curiosity-based algorithms that can adaptively sample different locations to improve exploration, and boost the robustness of generated structure-function models. The proposed algorithm is trialed on several microscopy platforms and is shown to be superior to random sampling, and is suitable for circumstances when no scalarizer function is available for optimization.

In contrast to materials characterization, where the task is generally purely one of materials prediction, material manipulation requires knowledge of how to act under different environment states, constuting a sequential decision making problem, which is usually formulated as a reinforcement learning problem. This can be solved via traditional policy-based learning methods such as policy-gradient, Q-learning, etc. Here, we show how RL-policies can be learned to manipulate ferroelectric domain structures in thin films, given a surrogate model for domain wall-SPM tip bias interactions, as well as extensions of this RL approach for atomic scale manipulations with other microscopy platforms. 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.

8:30am **NS1-TuM-3 Understanding and Controlling Atomic Transformations in 2D Materials Through in situ STEM***, **Raymond Unocic**, Caitlyn Obrero,* North Carolina State University*; Kevin Roccapriore,* AtomQ*; Ayana Ghosh,* Oak Ridge National Laboratory*; Maxim Ziatdinov,* Pacific Northwest National Laboratory*; Sergei Kalinin,* University of Tennessee Knoxville*; Matthew Boebinger,* Oak Ridge National Laboratory, USA

The discovery and design of next-generation functional 2D materials demand an atomic-level understanding of how structure and chemistry govern performance. At the nanoscale, where materials are often only a few atomic layers thick, minute structural or chemical changes can trigger profound shifts in electronic, magnetic, optical, and catalytic properties. Unlocking control over these properties requires deep insight into the transformation mechanisms that govern atomic-scale behavior. Scanning transmission electron microscopy (STEM) has emerged as a vital tool due to high spatial resolution imaging, diffraction, and spectroscopy. Recent breakthroughs in *in situ* and *operando* STEM now allow us to go beyond static characterization, opening the door to real-time observation of structural evolution and chemical reactions under dynamic conditions. In this work, we leverage *in situ* STEM to investigate the formation pathways, reaction kinetics, and energy landscapes involved in the synthesis of novel 2D materials. Using controlled heating experiments, we directly visualize the transformation of amorphous precursors into crystalline layered structures, capturing how temperature and electron dose influence nucleation and growth mechanisms at the atomic level. Further, we demonstrate atomic engineering of 2D materials through feedback-controlled electron beam techniques to create targeted defects and nanopores with atomic precision. To deepen our mechanistic understanding, we integrate machine learning tools to analyze transformation dynamics and uncover hidden patterns in atomic-scale behavior. These insights pave the way for predictive control over material design. The presentation will conclude with a forward-looking perspective on how advanced microscopy, paired with machine learning, is redefining the limits of materials discovery - transforming our ability to design and engineer 2D functional materials.

8:45am **NS1-TuM-4 Advancing Autonomous Experimentation with Human-AI Synergy and Cross-Platform Integration***, **Yongtao Liu**,* 1 Bethel Valley Road

Advancements in artificial intelligence are rapidly transforming materials research by enabling autonomous experimentation. In this talk, I will present our recent progress in developing automated and autonomous experimentation frameworks that accelerate discovery across diverse materials systems. Our approach integrates computer vision-enabled high-throughput experimentation, AI-powered decision-making, prior knowledge-guided exploration, and cross-platform co-optimization. By leveraging computer vision, we enable rapid, automated exploration of complex experimental parameter spaces. We further incorporate AI algorithms into experimental loops to perform real-time data analysis and decisions making. A key feature of our framework is the incorporation of expert knowledge and human oversight, enabling context-aware experimentation grounded in physical understanding. Beyond single-platform optimization, we also introduce a cross-platform strategy of autonomous experimentation that enables coordinated operation between synthesis and multimodal characterization tools. This distributed yet collaborative strategy requires no physical integration, offering an approach for autonomous research across diverse research platforms.

9:00am **NS1-TuM-5 Nanovision: An Integrated Platform for Two–Dimensional Material Discovery and Device Assembly***, **Son Le**, Jeffrey Schwartz,* Laboratory for Physical Sciences*; Ruihao Ni, You Zhou,* University of Maryland, College Park*; Karen Grutter, Aubrey Hanbicki, Adam Friedman,* Laboratory for Physical Sciences

Two-dimensional (2D) materials are crucial for enabling next-generation computing, electronics, sensing, and communication technologies. Currently, most breakthroughs in 2D material research rely on atomically thin (few-layer), exfoliated crystals. Frustratingly, identifying candidate crystals typically requires tedious, time-consuming, manual processes performed by trained researchers. This bottleneck severely limits device complexity, fabrication throughput, and overall research efficiency. To address this challenge, we created an integrated hardware and software platform that rapidly and automatically images, identifies, and catalogs exfoliated 2D crystals at full-wafer scales. Our platform enables researchers to visualize and to interact with ultra-high-resolution multimodal images of 2D materials using a web-accessible interface that supports remote operations, promotes data sharing, and enhances researcher productivity. By leveraging artificial intelligence and computer vision strategies, our platform eliminates the need for researchers to engage in tedious visual identification. A working prototype of this platform has helped us to streamline our 2D materials device research while collecting user feedback for continual refinements to our workflow. Moreover, using this platform, we are compiling physical and digital libraries of exfoliated 2D materials with the goal of democratizing access to high-quality materials for researchers. In this presentation, we describe the ongoing development of the hardware, software and control interface used in this impactful materials discovery platform.

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