UNIVERSITY OF DELAWARE

MATERIALS SCIENCE and ENGINEERING SEMINAR

Dr. Ayana Ghosh

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Oak Ridge National Laboratory, TN

Physics-guided AI for complex materials

Traditional methods such as density functional theory, molecular dynamics have long been foundational in exploring electronic, thermodynamic, and transport properties in functional and quantum materials. The integration of AI/machine learning/deep learning (ML/DL) has transformed this process, enabling faster, broader exploration of materials space, moving us closer to autonomous labs where the domain of theory interacts with experiments in real time. However, to truly advance our scientific understanding, it is crucial to embed reasoning into these approaches. This will allow us to move beyond surface-level correlations while learning about the underlying interactions, governing physical principles that together determine complex materials behavior. This presentation will focus on our recent efforts to derive comprehensive understanding on an array of physical phenomena such as cation ordering, polarization switching, mode coupling, energy landscape in perovskites, emergent electronic behaviors in two-dimensional heterostructures driven by interlayer coupling, lattice construction, and twist angle-dependent periodicity. Our multifaceted theoretical approach integrates first-principles computations, theoretical proxy design, scientific hypotheses formulation/testing, ML, causal reasoning. These efforts advance a novel paradigm of integrated, self-learning AI models designed to unravel complex phenomena through real-time theory-experiment feedback, driving materials innovation.

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MSEG SEMINAR
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BIOGRAPHY

Dr. Ayana Ghosh is a R&D Staff Scientist at the Computational Sciences & Engineering Division at Oak Ridge National Laboratory (ORNL). Her research harnesses state-of-the-art first-principles computations, integrated with scientific machine learning methods and experimental insights to learn about a diverse range of materials systems, including inorganic perovskites, two-dimensional materials, and their organic counterparts. She received her Ph.D. in Materials Science and Engineering from the University of Connecticut in 2020, her B.S. in Physics and Mathematics from the University of Michigan in 2015. Prior to her current role, she completed her postdoctoral training at ORNL. *She has contributed to numerous peer-reviewed publications, with articles featured in journals such as Chemistry of Materials, ACS Nano, Nature Physics, npj Computational Materials and Nature Machine Intelligence.* Her most recent accolades include the 2025 MRS Early Career Distinguished Presenter, 2024 Director's Award for Individual Accomplishment in Science and Technology, 2024 Early Career Research Accomplishment at ORNL, and the 2024 Early Discovery Award from the American Ceramics Society, among other honors.