ME Seminar

AI/ML-Driven Multiscale Modeling for Materials and Devices

Dr. Sukriti Manna, Research Assistant Professor, Mechanical and Industrial Engineering, University of Illinois Chicago

ABSTRACT

Accurate prediction of nanoscale structure, dynamics, and properties remains computationally demanding, limiting the pace of materials discovery. To address this challenge, I leverage AI/ML-driven multiscale modelling to develop computationally efficient and predictive frameworks for material behaviour. In this talk, I will introduce the Quantum Cluster Database (QCD), the largest high-accuracy quantum dataset of nanoclusters, which enables the training of machine-learning interatomic potentials that achieve near–density functional theory (DFT) accuracy at dramatically reduced computational cost. Building on this foundation, I will discuss our Monte Carlo Tree Search reinforcement-learning framework for autonomously developing physics-based interatomic potentials across the periodic table. Next, I will show how this reinforcement-learning strategy enables efficient structural sampling in complex energy landscapes, revealing key mechanisms underlying emergent electronic functionality such as resistive switching and neuromorphic behaviour. Building on these results, I will then outline my proposed research on multiphysics thermal management in microelectronics, integrating atomistic insights with continuum-scale phase-field modelling to predict heat transport, phase change, and interfacial effects in microchannel cooling systems. Together, these advances establish a predictive, AI-augmented ecosystem for designing next-generation materials and microelectronic devices.

ABOUT THE SPEAKER

Dr. Sukriti Manna is a Research Assistant Professor in the Department of Mechanical and Industrial Engineering at the University of Illinois Chicago (UIC), with a joint appointment at Argonne National Laboratory (ANL). He earned a B.E. in Metallurgical & Materials Engineering from Jadavpur University, an M.E. in Materials Engineering from the Indian Institute of Science, and a Ph.D. in Mechanical Engineering from the Colorado School of Mines. He subsequently held postdoctoral positions at Johns Hopkins University and Argonne National Laboratory. Dr. Manna's research integrates density functional theory, molecular dynamics, phase-field modeling, and artificial intelligence/machine learning to investigate multiscale structure–property relationships in functional materials. His work spans piezoelectrics, neuromorphic oxides, metal alloys, quantum clusters, nano-colloids, high-entropy alloys, and advanced microelectronic cooling systems. He has co-authored approximately 50 publications in high-impact journals, including Science, Science Advances, Nature Communications, and leading ACS journals and is a co-inventor on a United States Patents. His research has attracted support from the National Science Foundation (NSF), U.S. Department of Energy (DOE), and he collaborates extensively with experimental groups across the U.S. and internationally to accelerate materials discovery through computational–experimental integration.

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