

CNM Short Course: Using AI/ML for Modeling and Characterization of Nanoscale Materials

Wednesday, May 3, Morning

- 9:00 – 9:15 Subramanian Sankaranarayanan (Argonne National Laboratory)
Overview of CNM Theory and Modeling Group
- 9:15 – 9:30 Michael Sternberg (Argonne National Laboratory)
Carbon High Performance Computing Cluster
- 9:30 – 10:30 Aditya Koneru, Suvo Banik, (University of Illinois-Chicago), and Subramanian Sankaranarayanan (Argonne National Laboratory)
BLAST Framework for Fitting Interatomic Potentials for Atomistic/Course-grained Molecular Dynamics Simulations Using Ab Initio and Experimental Data
- 10:30 – 11:30 Aditya Koneru, Suvo Banik, (University of Illinois-Chicago), and Subramanian Sankaranarayanan (Argonne National Laboratory)
CASTING Framework for Inverse Design of Structures and Processing-microstructure Optimization
- 11:30 – 12:00 Break and Q&A

Wednesday, May 3, Afternoon

- 12:00 – 1:00 Henry Chan (Argonne National Laboratory)
POLYBOT Framework for Enabling Autonomous Experiments Guided by AI/ML and Digital Twins
- 1:00 – 1:30 Joshua Paul (Northwestern University)
Ingrained Framework for Matching Simulated and Experimental STEM/TEM and STM Images
- 1:30 – 2:30 Chaitanya Kolluru, Davis Unruh, and Maria Chan (Argonne National Laboratory)
FANTASTX Framework for Determining Atomic Structures from STEM, PDF, XAS, XRD, STM, and Other Experimental Data Types
- 2:30 – 3:00 Katerina Vriza (Argonne National Laboratory)
EXSCLAIM/Plot2Spectra for Extraction of Microscopy and Spectroscopy Data from Literature
- 3:00 – 4:00 Q&A