

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

Organizers: Maria Chan, Subramanian Sankaranarayanan, and Henry Chan

This workshop will focus on the application of AI/ML techniques in nanoscience and materials research. Besides research highlights, the workshop will also provide an overview and demo of various AI/ML tools and software developed at the CNM. Examples include:

- Ingrained framework for matching simulated and experimental STEM/TEM and STM images.
- FANTASTX framework for determining atomic structures from STEM, PDF, XAS, XRD, STM, and other experimental data types.
- BLAST framework for fitting interatomic potentials for atomistic/coarse-grained molecular dynamics simulations using Ab Initio and experimental data.
- CASTING framework for inverse design of structures and processing-microstructure optimization using molecular dynamics and kinetic Monte Carlo.
- POLYBOT framework for enabling autonomous experiments guided by AI/ML and digital twins.