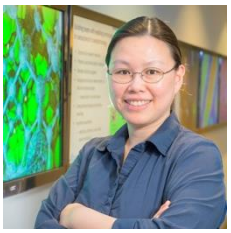
Department of Chemistry & Biochemistry Seminar

Friday, February 19th, 2021

1:30pm – 2:45pm

Zoom ID: 960 452 0800

Password: Materials



An Automated Framework to Integrate Materials Modeling and Characterization

Speaker: ***Dr. Maria Chan***, **Argonne National Laboratory**

Abstract: Advances in both operando materials characterization and atomistic modeling of materials have made possible in-depth, real time probing and quantitative predictions of materials properties and transformation, respectively. Yet, inversion of characterization data is often an under-determined problem, and the structural space for atomistic models under constrained. Therefore, an iterative model for materials inquiry combining both types of tools have become essentially standard. We will discuss examples of combined inquiries in the study of energy storage and photovoltaic materials. In addition, a framework for direct, intimate integration of modeling and characterization, utilizing machine learning techniques, will be introduced, with applications in the studies of nanocatalysts and grain boundaries in polycrystalline materials.

Biography: Maria Chan holds a BSc in Physics and Applied Mathematics from the University of California, Los Angeles, and a PhD in Physics from the Massachusetts Institute of Technology. Since 2012, Chan has been a staff scientist at the Center of Nanoscale Materials, part of Argonne National Laboratory near Chicago. She is also a member of the University of Chicago Consortium for Advanced Science and Engineering, and a senior fellow at the Northwestern-Argonne Institute of Science and Engineering. Chan's research is on the computational prediction of materials properties, using first principles, atomistic, and machine learning methods, particularly in applications towards materials relevant to energy technologies, such as energy storage, photovoltaics, catalysis, and thermal management