Elucidating Structural Heterogeneity of Materials with Spectroscopy, Machine Learning, and Atomistic Simulations

Anh Pham

Quantum Simulations Group & Computational Chemistry and Materials Science Summer Institute, Lawrence Livermore National Laboratory, Livermore, CA 94550, United States

Email: pham16@llnl.gov

ID: INV15
Invited Talk
Aug. 24, 11.00 - 11.30

Keywords:

Precise determination of atomic structural information in functional materials holds transformative potential and broad implications for emerging technologies. Spectroscopic techniques, such as X-ray absorption near-edge structure (XANES), have been widely used for material characterization; however, extracting chemical information from experimental probes remains a significant challenge, particularly for disordered materials. We present an integrated approach that combines atomic simulations, data-driven techniques and experimental measurements to investigate chemical speciation of amorphous systems, including carbon and carbon nitrides as examples. We discuss the development of machine learning potentials that can efficiently explore the vast configuration space of the systems. By employing statistical methods, this structural database enables the elucidation of the most representative local structures and how they evolve with chemical compositions and density. Density functional theory simulations are used to establish a correlation between the local structure and spectroscopic signatures, which then serves as the basis for interpreting and extracting chemical content from experimental data. Although our framework is specifically demonstrated to XANES, the approach described herein is readily adaptable as applied to other experimental characterization probes and materials classes.