15 September 2025 SSM 104

MATERIALS AND BIOMATERIALS SCIENCE AND ENGINEERING

Modeling Materials Interfaces for Energy Applications

ABSTRACT: Understanding physicochemical processes at materials interfaces is critical in a wide range of emerging technologies, from energy storage and conversion to chemical separation. In this talk, I will review our recent activities in the simulation of materials interfaces using first-principles approaches accelerated by machine learning (ML). I will discuss how first-principles simulations have been combined with ML potentials to elucidate reactivity and degradation mechanism of electrocatalysts at the interface with aqueous electrolytes in hydrogen production systems. In addition, I will discuss how ML is integrated with multi-modal characterization techniques, including X-ray absorption and vibrational spectroscopy, to probe evolving chemistry at oxide interfaces. Finally, I will discuss how large-scale MD simulations and ML potentials are leveraged to investigate the impact of confinement on mass transport, reactivity, and electronic properties of hydrophobic and hydrophilic interfaces in energy-water systems. Opportunities for facilitating UC-LLNL collaboration, including student internships, will also be discussed.

BIOGRAPHY: Anh Pham is the Group Leader of the Quantum Simulations Group in the Materials Science Division at LLNL. His research interests lie in the integration of multiscale simulation, high performance computing, and data science for predicting properties of functional materials under non-equilibrium conditions. Primary topics of interest include energy conversion and storage, degradation and corrosion science, and chemical separation. At LLNL, he currently serves as a coordinator for AI/ML activities across the Physical and Life Sciences Directorate. He also is the thrust lead for degradation science and sustainable materials at the Laboratory for Energy Applications for the Future (LEAF) Center. Since 2017, Dr. Pham has served as Director/co-Director of the Summer Institute on Computational Materials Science and Chemistry (CCMS), a two-month summer school and mentorship program for graduate students at LLNL.

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Refreshments: 1:45pm, **Seminar**: 2-3pm