UCLA College | Physical Sciences Chemistry & Biochemistry

SPECIAL CHEMISTRY SEMINAR

Prof. Arun Venkatnathan

Department of Chemistry
Indian Institute of Science Education and Research

Wednesday, August 7, 2024

4:00 PM | YH 4222c

Mani L. Bhaumik Collaboratory -

Dongwon Yoo Seminar & Conference Hall

Unraveling Thermal Stability, Structure and Ion Transport in Battery Electrolytes: A Classical Molecular Dynamics Simulation Approach

Soft solid battery electrolytes are promising materials for lithium and sodium ion batteries. In these materials, a lithium or a sodium salt is co-crystallized in low-affinity organic solvents such as DMF or adiponitrile. In this talk, the application of classical Molecular Dynamics (MD) simulations to characterize thermal stability, ion-ion and ion-solvent interactions, ion transport (diffusion, ionic conductivity) in soft solid electrolytes to validate or understand experimental findings will be presented. An application to investigate diglyme based sodium ion liquid electrolyte as an alternative choice to traditionally used carbonate solvents will also be discussed. Another application of MD simulations to examine a pressure/temperature controlled juicing phenomena in a sodium-ion conductor will also be presented.

Please contact letts@chem.ucla.edu for additional information.

This event is made possible by generous donations from our supporters and also through the gifts of the Bhaumik Centennial Collaboratory, Yoo Seminar & Conference Hall, Tsay Study Lab, and Centennial Collaboratory Donor Wall & Space Funds.