Pacific Northwest
NATIONAL LABORATORY

PHYSICAL SCIENCES DIVISION PRESENTS:

Shehan Parmar, Georgia Institute of Technology

Understanding Ionic Liquids via Polarizable Molecular Dynamics Simulations

Ionic liquids (ILs) are prime candidates for a broad range of applications, including battery electrolytes, spacecraft propulsion propellants, and water purification media. Unlike molecular solvents, ILs have large liquid cohesive energies due to strong Coulombic interactions between cation/anion pairs, giving rise to their unique thermophysical and transport properties. Over the past two decades, the success of classical molecular dynamics simulations has spawned the development of numerous force fields aimed at linking quantum mechanics to macroscopic behavior. In this seminar, we will first highlight the importance of developing ab-initio-based polarizable force fields. I will then present two simulation case-studies involving (1) a candidate battery electrolyte, N1888/TFSI (methyltrioctylammonium/bistriflimide), and (2) a propellant mixture, HAN/HEHN (2-hydroxyethylhydrazinium and hydroxylammonium nitrate), for which we investigate various thermophysical, bulk-phase, or interfacial structural properties.

Through collaborations with experimental groups, we seek to characterize these ionic liquids to understand nanoscale behavior and ultimately enhance technology applications. Drawing from our group's research and others', we show how polarizability--the electronic density's response to local electric fields--fundamentally modulates IL electrostatic and dynamic properties.

Tuesday, October 10
11:00 PM to 12:00 PM PST
ESC Titanium (1003)
Microsoft Teams

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