

Mechanical Engineering Dissertation Defense

Integrated Design of Ionic Liquid Systems: Linking Microstructural Architecture to Functional Performance in Thermal Fluids and Electrochemical Sensors

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Abstract

Liquid systems are commonly used in the management and control of thermal, electrochemical, and chemical processes. Among promising liquid systems, ionic liquids (ILs) and ILs coupled with a non-ionic co solvent have emerged as a novel chemical framework from which a broad range of chemical properties and functionalities can be engineered. This is made possible through distinct features and evolutions within the microstructural regime where a network of competing ion-ion, ion-dipole, dipole-dipole interactions results in functional improvements to bulk system behavior.

This work focuses on engineering task specific IL/solvent systems by tailoring molecular architectures to balance key properties, targeting significant improvements in phase stability, low viscosity, and favorable transport properties at low temperatures. This is carried out through an integrated design approach to develop two application specific IL/solvent systems for use in: advanced heat transfer fluids, capable of maintaining low viscosity over an extended low temperature regime, and an electrolyte for use in molecular electronic transducer (MET) sensors, optimizing ion transport, stability, and redox mediation for improved electrochemical performance for seismic sensing.

A suite of experimental studies is carried out to elucidate the response of heat capacity, phase behavior, viscosity, and conductivity across a target set of ion pairs and their use and as an additive in conventional non-ionic solvent systems. Specifically, by targeting key structural variation across cation classes and task-specific anion pairings, key functional indicators are mapped against application specific use cases to guide molecular design of ionic liquid systems. This provides a framework to describe how strategic ion/solvent pairing and compositional tuning can favorably influence emergent system properties while also allowing for novel and tailored system level performance improvements.

Experimental results demonstrate significant improvements in low temperature performance and identify key features including a synergistic shift in viscosity as well as a compositional threshold where divergent behaviors emerge in phase behavior and ionic conductivity. This is coupled with computational simulation, including molecular dynamics (MD), conformer searching, and ab initio geometry optimization, elucidating chemistry-structure-property relationships by linking microstructural architecture to the experimentally observed behaviors.

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