Title: Application of Ionic Liquids: Thermodynamics and Properties



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Proposal

In general, researchers have found that the potential application of ionic liquids (ILs) in processes of reactions, gas separations, liquids separations, cleaning operations, electrolytes/fuel cells, heat-transfer fluids, biomass utilization, analytical chemistry, petrochemical industrials.

Design of IL solvents requires fundamental knowledge of how the nature of the cation, anion, and substituents affects chemical and physical properties. This fundamental knowledge can be developed in two ways: via targeted experimentation and through molecular thermodynamics and simulations. Because ILs are relatively new, experimental measurements of fundamental properties, like phase behavior, solubilities, heat capacities, viscosities, thermal conductivity, and electrical conductivity are extremely scarce. However, they are clearly needed. At the other end of the molecular modeling spectrum are statistical cheminformatics-based modeling methods, such as quantitative structure-property relationship (QSPR) modeling. Another important issue is how to efficiently remove ILs from aqueous streams that they may have entered in the process operation.

Achieving the full potential of these exciting new classes of solvents will require that chemical engineers bring to bear the full assortment of our unique mathematical and technical skills on the many problems involved in the design and development of ionic liquids for practical applications.

We invite authors to submit original research as well as review articles to this special issue. Potential topics include, but are not limited to:

- 1. Study of thermodynamics and properties of ionic liquids.
- 2. Modeling and simulation of application of ionic liquids to potential processes.
- 3. Unique mathematical and technical skills in design and development of ionic liquids.