

Molecular Simulations Predictions of Thermophysical and Transport Property of Ionic Liquid- Ionic Liquid Mixtures

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In the last decade or so, molecular simulation methodologies have enabled thermophysical and transport property predictions of a large number of ionic liquids and their mixtures. In addition, a number of researchers have predicted phase equilibria of ionic liquids with gases and solvents in order to assess the feasibility of employing ionic liquids as gas separation agents. Such simulations have focused primarily on systems containing only one ionic liquid. Given that ionic liquid-ionic liquid mixtures can greatly expand the range of nonaqueous systems, there is a critical need in determining properties of such mixtures. In this talk, we will describe our initial efforts in addressing this gap in the knowledge. We will report molecular simulation predictions of thermophysical, transport and structural properties of mixtures of ionic liquids based on imidazolium and pyridinium moieties.