Using Monte Carlo simulation to understand the bulk and interfacial behaviors of ionic fluids

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Ionic fluids consist of a collection of dissociated ions. Notable examples are room temperature ionic liquids (RTILs) and molten alkali halides. This class has recently gained considerable attention, mainly due to the potential applications of RTILs in nanotechnology, energy storage and chemical processing. At the same time, studies on theoretical models continue to provide insight into the behavior of electrolyte solutions and colloids. This field has greatly benefitted from different types of molecular simulation due to the ability for one to use this tool to relate the macroscopic properties of a system to the underlying microscopic interactions. One type of simulation, called Monte Carlo, employs statistical thermodynamics to generate different configurations of molecules in order to calculate the thermophysical properties of a given system. In this presentation, we first describe how MC simulations are used to compute bulk and interfacial properties of interest. For the bulk behaviors, we present the vapor and liquid phase properties of different RTILs having a wide variety of structures and inter-ionic interactions. We examine thermodynamic properties, such as the saturated densities, vapor pressure, and enthalpy of vaporization, as well as metrics that describe the structure molecules adopt in the liquid and vapor phases. Regarding interfacial phenomena, we consider how different ionic fluids wet a particular solid surface. Here, we use a simple model for ionic fluids to systematically understand the influence of electrostatic interactions on wetting properties. Results are presented to show how the strength of the interaction between the fluid and solid as well as the system temperature affect the properties and microscopic structure of the fluid near the surface.