Using Molecular Simulation to Understand the Bulk and Interfacial Behavior of Ionic Liquids

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Understanding the bulk and interfacial properties of room temperature ionic liquids (RTILs) is important for several industrial applications of these fluids. In this presentation, we discuss recent progress in the use of Monte Carlo simulation to better understand the phase and interfacial properties of ionic fluids. We first present liquid-vapor saturation properties of the homologous series 1-alkyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ([Cnmim][NTf2]) at temperatures ranging from room temperature to the critical region. We also relate the trends observed in these properties to the microstructure of the saturated liquid and vapor phase. We present results for the homologous series with n ranging from 2 to 12. The calculated properties include saturated liquid and vapor densities, vapor pressures, enthalpies and entropies of vaporization. We also show how the liquid phase microstructure, especially the nano-domains observed for some of these fluids, evolve over the temperature range investigated. In many cases, simulation results are compared to experimental data.We next examine the role of dispersion and electrostatic interactions in the wetting behavior of ionic liquids on non-ionic solid substrates. We study simple models of ionic liquids comprising of spherical cations and anions with variable strengths of electrostatic interactions relative to dispersion interactions. The range of relative ionic strengths that we investigate includes those observed in RTILs and molten alkali halides. Results are presented to show the dependence of contact angle on temperature and substrate strength for fluids with different relative ionic strengths. For all of the fluids studied, we observe a relatively narrow range of substrate-fluid interaction strengths wherein the contact angle is nearly independent of temperature. We discuss now this observation is related to the microstructure of the fluid at the liquid-vapor and solid-liquid interfaces.