PVT-Properties and Viscosities of Mixtures of Imidazolium-Based Ionic Liquids and Alcohols from Molecular Simulation

G. Raabe[C,S] and J. Koehler
Institut für Thermodynamik, TU Braunschweig, Braunschweig, Germany
G.Raabe@tu-bs.de

Room temperature ionic liquids have recently attracted increasing interest as replacement solvents for a variety of chemical reactions and separation processes.

The development of designer solvents requires the characterization of the thermophysical properties of not only pure ionic liquids, but also of their mixtures with common liquids, such as alcohols. Molecular simulation is the ideal tool for investigating these complex mixtures, as it provides valuable fundamental insights into their behavior on the molecular level and, with this, yields more detailed information about the systems than available from experiment.

Many molecular simulation studies on ionic liquids have already been reported. Most of the work has been aimed at the development of classical force fields and the investigation of the structural and dynamic properties of pure ionic liquids. Only a few simulations have concerned solutions of salts or gases in ionic liquids, or the behaviors of ionic liquids in mixtures with water, aromatic, or organic compounds.

To our best knowledge, no computer study is available on the thermodynamic properties of ionic liquid mixtures with alcohols and their correlation with microscopic properties. Thus, we will present results on our current study on the pVT-properties and viscosities of imidazolium-based ionic liquids in mixtures with alcohols, as a function of composition. We also give insight into the microscopic structural properties of theses mixtures by investigating the radial distribution functions and self diffusion coefficients of the different species in the mixtures. The simulations are based mainly on the united-atoms force field descriptions of the molecular species involved, but, for the sake of comparison, we will also present some results of all-atom models.