Molecular Simulation Studies on the Structural Properties of Binary Mixtures of Omidazolium-Based Ionic Liquids and Solutes

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Room temperature ionic liquids are a class of organic salts with unusually low melting temperatures that have attracted increasing interest as replacement solvents for a variety of chemical reactions and separation processes. Their development as designer solvents requires not only characterization of the thermophysical properties of the pure ionic liquids but also of their mixtures. In this regard it is also of utmost importance to understand in which way the thermophysical properties are influenced by different parameters. Thus, it is significant to understand how the structure of the ionic liquid changes upon mixing, and in which way the properties of the mixtures are related to their structural characteristics. Molecular simulation is the ideal tool to investigate these relations, as it provides valuable fundamental insights into the behaviour of ionic liquids on the molecular level. Thus, we will present molecular dynamics simulation studies on the structural features of binary mixtures of 1-alkyl-3-methyl-imidazolium based ionic liquids and alcohols, acetonitril and refrigerants as model solutes. Our studies on the local structures of the mixtures by radial and spherical distribution functions provide insight into how microstructural characteristics are related to the solubility of the ionic liquids for different solutes.