

Structure and Dynamics of Ionic Liquids from Atomistic Simulations

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Ionic liquids (ILs) are pure salts that are liquid near ambient temperatures. They have several unique properties such as a tunable structure, a low vapor pressure, good solvation ability, high thermal stability and slow dynamics at room temperature. These properties make ILs attractive for many applications such as mass spectrometry, chemical separation, pharmaceuticals, solar thermal energy, and carbon capture. Understanding the fundamental structure-dynamics relationship of ILs is the key to optimizing their use in various applications.

Experimentally, structural differences in anions have been observed to lead to different dynamics in ILs. In some situations, ILs with smaller cations and anions yielded a higher conductivity than those with large ions, due to higher diffusivities of the ions. For some ILs, however, the trends are reversed. It has been observed that the temperature dependence of the diffusion coefficient, conductivity and viscosity of several ILs can be quantified by means of the Vogel-Fulcher-Tammann (VFT) equation. IL structure has been measured using x-ray and neutron scattering, and it has been found that there are several length scales of order, unlike conventional liquids.

In this talk, I will report the results of extensive molecular simulation studies carried out to better understand how the structure and dynamics of ILs are related to their chemical constitution and molecular architecture. We compare our calculations against experimental data and show how relatively simple ion exchange dynamics can be used to predict bulk transport properties.