Structure and Dynamics of Imidazolium-based Ionic Liquids

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Room-temperature ionic liquids (RTILs) are receiving increased attention due to their unique properties, including nonvolatility and solvating capability, leading to a wide range of potential uses in catalysis, separation technology, photovoltaics and fuel cells. High freezing temperatures are generally achieved by combining large, asymmetrically substituted organic cations with either small or large anions. We have studied the structures of liquid and solid 1-ethyl, 1-butyl and 1-hexyl-3-methylimidazolium bromide with high-energy x-ray diffraction measurements and atomistic molecular dynamics numerical simulations. Excellent agreement between experiment and simulation is obtained, including the region of the low-Q peak that characterizes the nanoscale heterogeneity in these liquids. We have also carried out quasi-elastic neutron scattering (QENS) measurements to determine the translational and reorientational dynamics. Both experiment and simulation demonstrate that, in the length and time scales probed by QENS (fractions of a nm and a few ps), the dynamics are dominated by activated translational diffusion in the liquid phase and reorientations of the ethyl groups in both solid and liquid.