Abstract Submitted
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Rotational Dynamics in Ionic Liquids CHRIS RUMBLE, MARK MARONCELLI, PSU — Our group has been investigating rotational dynamics of small molecule solutes in ionic liquids (ILs, a class of salts which are molten below 100 °C) using experimental methods and molecular dynamics (MD) simulations. The strong self-association between IL molecules due to Coulombic attractions results in slow dynamics and structural heterogeneity, which reveal themselves in rotations through large angle jump motion, distributed dynamics, and deviations from predictions made using hydrodynamic theory. To explore the effects of solute size and charge distribution on rotations in ILs, we have performed fluorescence anisotropy and NMR T1 relaxation experiments on a series of charged and uncharged solutes of differing sizes in an IL and 1-propanol, as a comparison to a simple glass forming liquid. In conjunction, MD simulations of each solute were performed using our group's coarse-grained IL model to model the dynamics we observe in experiment. The poster will include a discussion of our experimental and simulation results with comparison to hydrodynamic predictions and comments on the similarity of rotational dynamics in ILs and other systems such as glasses and polymer melts.

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