167f Molecular Dynamics Study of Pyridinium- and Triazolium-Based Ionic Liquids

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Recently, ionic liquids have found a great interest in the research community due to their promising applications that rely on their extremely low volatility. Molecular simulations can provide valuable insight into the link between the chemical composition and structure of these liquids and their resulting properties. Such understanding is critical for the development of ionic liquids given that there are literally billions of potential ionic liquid compounds that could be made.

In this paper, we present the results of extensive molecular dynamics simulations of ionic liquids based on the pyridinium and triazolium cations. Classical forcefields for both types of ionic liquids are developed and used to simulate both the crystalline and liquid phases. Computed liquid phase volumetric properties agree well with experiment, as do the crystal structures of the salts. Self-diffusivities of the liquid pyridinium-based materials were obtained through pulsed field gradient NMR measurements. Computed self-diffusivities were lower than experiment, possibly due to the neglect of polarization effects. It was also found that the liquids exhibit strong dynamic heterogeneity at room temperature, even through this is above the solidification temperature. This finding suggests that to properly compute the dynamics of these systems, extraordinarily long simulations are required.