Influence of pore geometry on the structural and dynamic properties of confined ionic liquids

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Ionic liquids (ILs) confined in nm-sized pores are of interest for their potential use in applications such as electrochemical double layer capacitors. In these devices, interactions exist between the nanoporous electrodes and the ionic liquids and the behavior of the confined ionic liquids is not fully understood. This project focuses on the influence of the carbon geometry on the confined ILs. We investigate the behavior of the ionic liquid, 1-*n*-butyl,3-methylimidazolium hexafluorophosphate, [bmim][PF6] confined inside three carbon models: (1) a slit-like graphitic pore model, (2) a multi-walled carbon nanotube, and (3) a model CMK-3 material, which consist of amorphous carbon rods arranged in a hexagonal array. Molecular dynamics simulations were performed using the non-polarizable potential for [bmim][PF6] developed by Bhargava and Balasubramanian [[[1]](#endnote-1)] to understand the influence of pore size and geometry on the structural and dynamic properties of the confined IL. We observe that the IL exhibits similar layering effects near the carbon surfaces of the three pore models. It has also been found that the dynamics of the ions depend strongly on their location with respect to the carbon surface, with slower dynamics generally observed near the pore surfaces. To identify the behavior of the ILs in these simulations we performed analysis on the density profiles, orientation of the ions, and the dynamics at specific locations within the carbon pore models.

1. [] B. L. Bhargava and S. Balasubramanian, *J. Chem. Phys.* **127**, 114510 (2007) [↑](#endnote-ref-1)