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Title : Molecular Modeling of the Ionic Liquid [EMIM+][TFMSI-] Inside a Slit Nanoporous Electrode

Abstract Text:

Considering the relevance of ionic liquids as alternative electrolytes in energy-related devices such as electrochemical double-layer capacitors (EDLCs) and dye-sensitized solar cells (DSSCs), it is essential to explore more about their behavior in the vicinity of the charged walls of a nanoporous electrode. Structural properties of an IL confined inside a nanoporous electrode affect macroscopic properties such as the capacitance in an EDLC; and the dynamical properties of the confined IL is one of the factors that determines the macroscopic electrical resistance in electrochemical devices.

Model electrodes represented as slit-like graphitic nanopores and the IL 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide [$EMIM^+$][$TFMSI^-$] are studied using molecular dynamics (MD) simulations. Our goal is to understand the effect of pore size and surface charge density on the structural, dynamical and electric properties of ILs confined inside nanoporous materials. As previous studies have largely concentrated on the structure and electric properties of the confined ILs, we have especially focused on the dynamics of the system, which were studied in detail by measuring mean squared displacements (MSDs), van Hove self correlation functions (VHSCFs) and self intermediate scattering function (SISFs).

Our results indicate that structural properties such as the local density profiles, the local orientation, and the radial distribution functions of the cations and anions vary strongly with pore size and charge density in the pore walls. These variables also affect the dynamical properties of the confined IL. Our results suggest that the dynamics of the ions inside the slit pore are highly heterogeneous and depend strongly on their position with respect to the pore walls, as well as on the surface charge density of the walls. For example, our results show that the layer of cations that is closer to a positively charged wall, as well as the layer of anions closer to a negatively charged wall, exhibit extremely slow dynamics when compared to bulk systems.

Keywords:

Ionic Liquids, Molecular Dynamics and nanopores