STRUCTURE AND DYNAMICS OF IONIC LIQUIDS CONFINED IN SLIT PORES

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The structure and dynamical behaviour of a room temperature ionic liquid (RTIL) under confinement between two pore walls resembling a graphite slit-like pore were studied by molecular dynamics simulations. The walls were modelled as flat surfaces interacting with the fluid molecules through a continuous potential that depends on the perpendicular distance from the wall [1,2]. We computed molecular and charge density profiles as well as solvation forces and self-diffusion coefficients across the pore axis, for several pore widths. The effect of the inter-wall distance on the density inhomogeneity was studied. The anisotropy in the translational dynamics and the molecular orientation of the confined fluid were analyzed as a function of the distance from the walls. The diffusional dynamics of the confined fluid was compared to bulk properties [3].
These studies are relevant for the understanding of the different microscopic effects leading to the macroscopic behaviour of RTILs in confined media in order to optimize their use for specific applications such as alternative electrolytes for dye-sensitized solar cells [4], electrochemical sensors employing carbon composite materials, and activated carbon or carbon nanotube based supercapacitors.

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