

The fate on an ionic liquid confined at the nanoscale

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Ionic liquids are mixtures of cations and anions which stay liquid at room conditions, a feature making them potentially ideal materials for energy storage and conversion technologies. Here they are often employed in contact with solid interfaces, or even constrained in pores whose size can be less than a nanometer. In such extreme environments the properties of matter are drastically modified compared to the bulk counterparts. In this context one can address a primary issue: Does the phase nature of an ionic liquid change when it is confined in pores of nanometric size? The simplicity of this question is misleading. Experiments which probe ionic liquids at the nanoscale, in fact, are extremely difficult and sometimes in mutual contradiction, failing so far to provide a generally accepted answer.

I have tackled this issue systematically by extensive Molecular Dynamics simulation of a model ionic liquid confined in a slit pore[1]. In this talk I will discuss how, by appropriately tuning size and temperature of the latter, I revealed unexplored phase modifications. For instance, following an increase of the confinement, I observed the formation of ionic liquid-crystal structures, which unexpectedly transform into plain stable liquid states and subsequently freeze in new crystal phases. I will also show how these changes reflect on the relative organization of the ions and on their dynamical state. I will finally build on the MD results to provide a consistent general picture of these systems, by also involving in the discussion disparate very recent inspiring work.

[1] Stefano Mossa, Re-entrant phase transitions and dynamics of a nanoconfined ionic liquid, pre-print arXiv:1803.08888

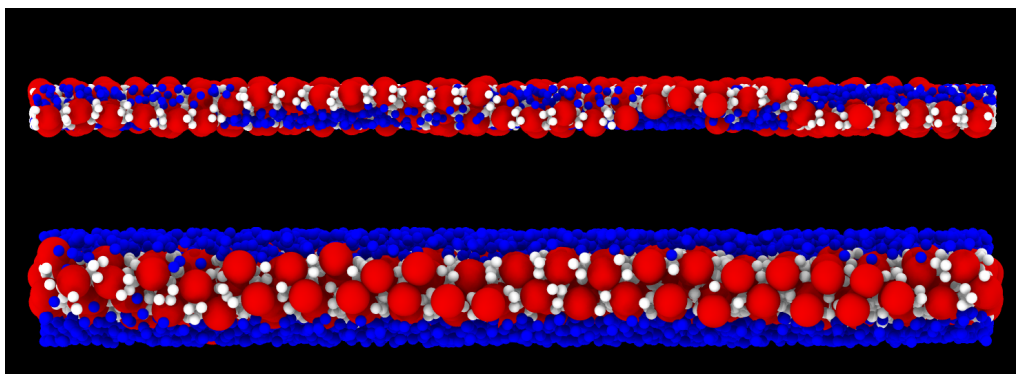


Figure 1: Side views of the considered ionic liquid system adsorbed in the pore in different conditions of confinement. Red beads identify the anions ($[PF_6]$), while white and blue correspond to polar and apolar parts of the cation ($[C_{10} mim]$), respectively.