

Ionic liquids confined in nanopores

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Ionic liquids are mixtures of cations and anions which stay in the liquid state at room conditions, a feature making them potentially ideal electrolytes for energy storage and conversion technologies. In these applications (*e.g.*, supercapacitors) ionic liquids are often found 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[1][2] and sometimes in mutual contradiction, failing so far to provide a generally accepted answer.

I have tackled this issue systematically by massive Molecular Dynamics simulation of a simple model ionic liquid confined in slit nanopores[3]. In this talk I will discuss how, by appropriately tuning size and temperature of the latter, I have revealed unexplored phase modifications. For instance, following an increase of the confinement, I have observed the formation of ionic liquid-crystal structures, which unexpectedly transform into plain stable liquid states and subsequently freeze in new crystal phases, with a remarkable reentrant behavior.

I will also show how these changes reflect on the relative organization of the ions (charges) and on their dynamical state. Building on the simulation results, I will try to provide a consistent general picture of these systems, by involving in the discussion disparate theoretical and experimental inspiring work.

REFERENCES

- [1] J. Comtet et al., Nature Materials, 16 (2017) 634
- [2] R. Futamura et al., Nature Materials, 16 (2017) 1225
- [3] S. Mossa, Physical Review X, 8 (2018) 031062