

PhD thesis title: Exploring the Phase Diagram of Electrolyte solutions in extreme

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Abstract

It is widely accepted that ice, no matter what phase, is unable to incorporate large amount of salt into its structure. This conclusion is based on the observation that upon freezing of salt water, ice expels the salt almost entirely into brine, a fact that can be exploited to desalinate seawater. We have shown, by neutron diffraction measurements under high pressure and molecular dynamic simulations, that this behaviour is not an intrinsic physico-chemical property of ice phases [*S. Klotz, L.E. Bove et al., Nature Materials 2009, L.E. Bove, S. Klotz et al., PRL 2011*].

We find that, in spite of the high amount of salt, dense LiCl-water solutions vitrify at ambient pressure in an amorphous and structurally compact form very similar to the relaxed high-density amorphous phase of pure water (e-HDA). Under high pressure annealing the system crystallizes into the ice VII structure incorporating homogeneously the salt into the ice lattice. Such an `alloyed` ice VII has significantly different structural properties compared to pure ice VII, such as 8% larger unit cell volume, absence of transition to the ordered ice VIII structure, plasticity, and most likely ionic conductivity. Our study strongly suggests that there could be a whole new class of salt hydrates based on various kinds of solutes and high-pressure ice forms. If these exist in nature in significant quantity, their physical properties would be highly relevant for the understanding of icy bodies in the solar system. To probe this fascinating hypothesis we will explore the phase diagram of electrolyte solutions of geological interest under extreme conditions of pressure and temperature, by neutron and x-ray diffraction measurements and MD simulations.

Requested skills : English spoken, good experimental skills, background in condensed matter physics and/or chemical-physics

For a detailed project, please contact livia.bove@impmc.jussieu.fr