Dottorato di Ricerca in Fisica dell'Università degli Studi di Messina
21 Novembre 2011, ore 15.00, Sala Seminari IPCF-CNR,
V.le F. Stagno d'Alcontres 37, S. Agata, Messina

Seminar title:
Salty ice under pressure

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Abstract

Water, wherever it exists in nature, contains unavoidably significant amounts of dissolved ionic species. Nonetheless, surprisingly little experimental attention has been paid on the high pressure behaviour of "salt water" compared to pure water. In a recent study combining neutron diffraction and molecular dynamics simulations we showed the existence [3] of a polyamorphic transition in LiCl:6D_2O between a high-density (*HDA*) and a very-high-density amorphous (*VHDA*) form. In spite of the high amount of salt, LiCl:6D_2O vitrifies at ambient pressure in a structurally compact form very similar to the relaxed high-density amorphous phase of pure water (*e-HDA*) [1]. We show that the transition to *salty-VHDA* takes place abruptly at 120 K and 2 GPa under annealing at high pressure, is reversible. We suggest that the transition is linked to a local structural reorganization of water molecules around the Li ions. The possible connection of this transition with the analogous observed [1] in pure water and the generality of the occurrence of a polyamorphism phenomenon in solutions in which one component, water, can have two critical points [2] will be discussed.

Under further annealing at high pressure (~4GPa), the *salty-VHDA* amorphous crystallizes, for a temperature of ~270 K, in a new and unexpectedly simple salt hydrate [4], which can be regarded as an "alloyed" high-pressure ice phase. Such "salty" ice VII has significantly different structural properties compared to pure ice VII, such as a 8% larger unit cell volume, 5 times larger displacement factors, frozen rotational disorder, absence of transition to an ordered ice VIII structure, and most likely ionic conductivity. Our study strongly suggests that there is 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.

[1] R. J. Nelmes *et al*., Nature Phys. **2** 414, (2006).
[2] P. G. Debenedetti and H. E. Stanley, Phys. Today **40** (2003).
[3] L. E. Bove, S. Klotz, J. Philippe, and A. M. Saitta, Phys. Rev. Lett. **106**, 125701 (2011).
[4] S. Klotz, L. E. Bove, T. Strassle, T. C. Hansen, and A. M. Saitta, Nature Materials **8**, 405 (2009