

### Internship proposal 2009-2010

**Laboratory :** Institut de Minéralogie et de Physique des Milieux Condensés (IMPMC)

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### *Superionicity of salty ice*

**Scientific project:** Within the many peculiarities of water, the richness of its solid phase diagram is one of the most surprising. More generally, water in nature and in the universe only exists as an aqueous solution, more or less concentrated, containing a certain amount of dissolved salts, which has enormous consequences in biology/medicine, physics/chemistry, Earth and planetary sciences, and makes its description even more complicated. Until recently, a common belief was that a saline solution at solidification separates spontaneously in pure ice and salt. This hypothesis is at the basis of all models describing the low temperature behaviour of water-containing systems.

Recently, we demonstrated (*The preparation and structure of salty ice VII under pressure*, **Nature Materials** **8**, 405 (2009)) that an aqueous solution of LiCl may form a salty crystalline ice, that is a form of ice whose crystalline sites are randomly occupied by water molecules or chlorine anions, while the Li<sup>+</sup> cations occupy interstitial sites. Not only this discovery was extraordinary, it also allows to access an unexplored domain. The presence of small-size lithium suggests that this system may exhibit superionicity, an electric conductivity of certain solids where the charge is carried by some ionic species free to diffuse within the crystal lattice.

We propose to study this phenomenon by ab initio simulations of its dynamical properties and of lithium diffusivity. The candidate will learn the basics and use of freeware ab initio codes, will set up the system, and study its behaviour in the pressure/temperature region of stability of salty ice VII. The vibrational and dynamical properties, and the possible existence of superionicity, will be compared to the experimental results obtained at the same time by the experimentalists of our team.

**Techniques in use :** Ab initio and Classical Molecular Dynamics Simulations

**Applicant skills :** Basic computer and programming skills, strong motivation

**Granted internship :** yes ( 398.32 €/month)

**C'nano IdF laboratory (France only) :** yes

**Possibility for a thesis :** yes (type of grant : Ministère)