SCIENCES SORBONNE UNIVERSITÉ

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Master thesis proposal

Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie

Campus Pierre et Marie Curie
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Title: Onset of superionicity in iron-bearing dense water ice

Keywords: superionicity, molecular dynamics, high pressure, ocean planets

Scientific description:

Superionic solids are characterized by a sublattice of highly mobile ions, decoupled from a normal underlying periodic solid structure. The mobility of these ions transforms the otherwise insulating structure into a superionic conductor. These are important materials as solid state ionics, with applications in batteries and various sensors. Surprisingly, such materials can also exist in the deep hot interior of planets. The most ubiquitous such phase is water ice. The presence of a solid layer of superionic ice overlying the core of silicates, oxides, and iron, deep inside planets like Neptune and Uranus has tremendous implications in generating huge and complicated planetary magnetic fields.

The phase diagram of water ice is dominated by molecular crystals at pressures below the megabar. At higher pressures, the structure, based on a bcc lattice of oxygen, becomes ionic. At high temperature, the hydrogen sublattice decouples from the oxygen sublattice, and the high mobility of protons transforms the structure into such a superionic conductor. In planets, reactions at the contact between ice, water, and silicates, lead to various salts, like NaCl, being incorporated in the superionic ice structure. Their presence enhances the onset of superionicity.

In superionic ice, the hydrogen sublattice (white) is highly mobile and decoupled from the oxygen sublattice (red), resulting in a net ionic conductivity

Here we propose to study the incorporation of ferric iron in the superionic phase of water ice. Fe^{3+} is a major weathering product of rocky material in the presence of water. As such, it must be a ubiquitous impurity in superionic ice at planetary conditions.

We will specifically look at the possible mechanism of incorporation of ferric iron in the structure of superionic ice. Then we will investigate the effect of iron on the hydrogen mobility, on the relative stability of various superionic phase of ice, and on the electronic and ionic components of the electrical conductivity of the superionic ice. We will perform large-scale first-principles molecular dynamics calculations. We will run the simulations on the machines of the national supercomputer centres (CCRT and IDRIS).

Techniques/methods in use: *ab initio* molecular dynamics calculations and thermodynamics, statistical analysis

Applicant skills: basic knowledge of unix/linux and python, condensed matter phyics

Industrial partnership: N

Internship supervisor(s) (name, email, phone, webmail):

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Internship location: IPGP

Possibility for a Doctoral thesis: Y (doctoral school)