Titre de la thèse:
Simulations of nuclear quantum effects in Earth physics

Description du projet (max. 1 page) :

Hydrogen is present in quite a number of materials of utmost importance—the human body among others. However, the hydrogen nucleus—a proton—is, generally speaking, a quantum particle because it is light, but its quantum properties are in general neglected because they are difficult to take into account in simulations. The approximate treatment of nuclear quantum effects (NQE), among which zero-point energy and tunneling, is relatively recent: the Quantum Thermal Bath (QTB), a method which takes into account these effects, has been successfully used for high pressure ice and for aluminium hydroxide, a mineral of geological interest. Proton delocalization, tunnelling and zero-point energy play a crucial and often quite puzzling role in the phase diagram and dynamics at such extreme pressures (tens of GPa). (see, eg http://www.insp.jussieu.fr/L-hydrogene-dans-la-glace-est-il.html)

We shall use the QTB, and possibly other methods if necessary, to study nuclear quantum effects in hydrous minerals, such as silicate hydroxides and aluminum hydroxides, in the conditions of Earth's mantle and their relation with the water cycle inside our planet. Besides those minerals, which attract much attention as they can drive water throughout the Earth's mantle, clathrate hydrates, that is water cages imprisoning other atoms or molecules (such as methane, hydrogen, etc.), present for instance at the bottom of the oceans, constitute a wide class of astonishing and still poorly known systems in which yet to be understood nuclear quantum effects arise.

The thesis will be conducted in a collaborative context: very recent, state-of-the-art experiments, will be essential to validate simulation results and offer a nice opportunity to understand often paradoxical experimental findings that raise challenging questions. Connection with research on alternative simulation methods will also be of great importance.

The thesis project is therefore largely interdisciplinary, between statistical mechanics and geophysics, and implies a continuous exchange with experimentalists in France and abroad. A marked scientific curiosity and communication skills are therefore particularly appreciated. Overall, the work will consist in setting up the models, run the simulations (they will be carried out both on local computational resources and on national computational centres) and interpret the numerical results on theoretical basis. A background in statistical physics as well as some previous experience in scientific computing are required.