Internships offered in M2
2017-2018

Responsibles for internship

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Internship topic: ***Nuclear quantum effects on protons in hydroxides***

Hydrogen is everywhere ; however, it can be a challenge for theoretical physics and computer simulations because it is light, which means it can exhibit significant quantum properties, as in high-pressure ice and other materials of geophysical interest (see [1,2] and references therein). These effects include zero-point energy and proton tunneling, with sometimes startling results. Including such effects in simulations is by no means easy and has only recently become feasible on a regular basis and community of researchers is presently forming to develop new methods and study new phenomena.

In ice, the proton is connected to two oxygen atoms via a covalent bond for the first and a hydrogen bond for the second. When the O-O distance becomes shorter, the hydrogen can hop by tunneling through the two oxygens and exchange the covalent and hydrogen bonds. Eventually (at very low temperatures or high pressures), it can settle at the mid-point between the two oxygen atoms in a situation in which the distinction between covalent and hydrogen bonds does not apply anymore. The replacement of hydrogen by heavier deuterium often has drastic effects in that respect [2]. When the composition of the material is more complex than in pure ice, other contributions can either impede or modify such behavior.

Hydroxides are a diverse family of materials which offers a wealth of structures, some of which are likely to show quantum effects connected with proton delocalization. The scope of the internship is to explore the proton behavior in selected hydroxides by simulations that are able to take into account nuclear quantum effects, and to quantify their relevance. The simulations will be mainly done within the recently developed « *quantum thermal bath* » (QTB) method [3], which attempts to reproduce the quantum indetermination by the application of a suitable stochastic force on the nuclei. The system will be represented either by suitable interatomic potentials or via the Density Functional Theory (DFT), using a parallelized version of the Quantum Espresso code. The internship will involve setting up the simulations, running them on our computer cluster, and finally producing significant physical interpretations with the usual critical physicist's eye. A taste for computer simulations and applied quantum mechanics is clearly a must.

[1] Y. Bronstein, P. Depondt, F. Finocchi, A.M. Saitta, « Quantum-driven phase transition in ice described via an efficient Langevin approach ». Phys. Rev. B 89, 214101 (2014) ; Y. Bronstein, Ph. Depondt, F. Finocchi, « Thermal and nuclear quantum effects in the hydrogen bond dynamical symmetrization phase transition of δ-AlOOH », Eur. J. Mineralogy, 29, 1 (2017);
[2] http://www.insp.jussieu.fr/L-hydrogene-dans-la-glace-est-il.html
[3] H. Dammak et al., Phys. Rev. Lett. 103, 190601 (2009)

Techniques involved: Quantum calculations on model systems, ab initio (DFT) molecular dynamics simulations.
Paid internship: Yes
Can this internship be continued for a PhD? yes
If yes, type of PhD funding envisaged is: École doctorale