Internship offered in M2
2018-2019

Responsible for internship

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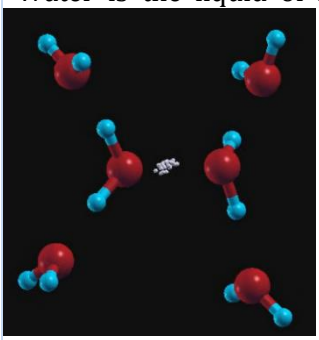
Internship topic: *Quantum^2 dynamics of water through machine learning*



Water is the liquid of life. Fair enough! However, despite its tremendous importance for processes ranging from ion solvation to protein folding, not to speak of chemical reactions and even planetary science, a fully consistent description of water that builds from the fundamental interactions between hydrogen, oxygen and their surrounding electrons is still lacking. It is known that in order to have a reliable description of water, it is necessary to include quantum nuclear effects, whose motion must develop on the top of accurate potential energy surfaces (PES), provided by the solution of the electronic problem at given nuclear coordinates. We have recently developed an innovative method, which couples the accurate determination of the PES by *quantum* Monte Carlo methods with the *quantum* description of nuclei, treated as extended objects and not like point-like particles. The results on protonated water clusters are spectacular, as they indicate major quantum effects in proton transport at room temperature. However, the computational cost of this approach makes it difficult to study fully quantum^2 (*quantum* square!) bulk water.

In this master project, we propose to adapt machine learning techniques to analyse our quantum^2 dynamics of water clusters, and fit new interatomic potentials, with the aim of running the first *quantum^2 dynamics*-based simulation of bulk water. Machine learning methods are more and more used to improve interatomic potentials to spectacular accuracy, *quantum^2 dynamics* is known for its highest reliability. Merging together these two worlds for the first time will allow us to draw an unprecedented picture of water.

M. Dagrada *et al.*, JCTC **10**, 1980 (2014)

F. Mouhat *et al.*, JCTC **13**, 2400 (2017)

F. Mouhat et al., *in preparation* (2018).

We look for a student strongly determined to undertake this ambitious and potentially breakthrough project, within a young and dynamical team. Besides the above-mentioned articles, our team has a consolidated expertise and a strong publication record in the development of advanced approaches, successfully applied to the study of molecular systems, including **7 PNAS, 2 Nature Comm and 8 PRL** in the last few years.

Techniques involved: DFT, QMC

Applicant skills: strong background in statistical physics and/or physical chemistry, propensity for simulations and/or programming

Paid internship: Yes

Can this internship be continued for a PhD? Yes

If yes, type of PhD funding envisaged is: Labex, Ministère, autres