Master 2: ***International Centre for Fundamental Physics***

INTERNSHIP PROPOSAL

Laboratory name: IMPMC
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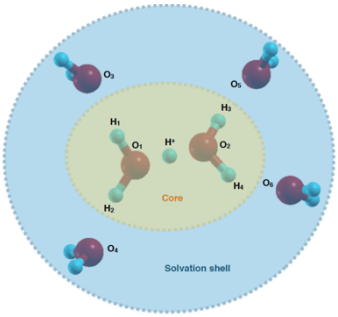
Internship location: IMPMC

Thesis possibility after internship: YES
Funding: YES If YES, which type of funding: IMPMC

Machine learning water clusters from quantum^2 dynamics

A fully consistent description of water that builds from the fundamental interactions between hydrogen, oxygen and their surrounding electrons is still lacking. To have a reliable description of water, it is necessary to include nuclear quantum 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 (QMC) methods with the quantum description of nuclei. The results on protonated water clusters are spectacular, as they indicate major quantum effects in proton transport persisting till 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 machine learning water from quantum^2 (*quantum dynamics + quantum Monte Carlo*) -based simulations. Merging together these two worlds for the first time will allow us to draw an unprecedented picture of water.

We are seeking for a highly motivated student with strong background in statistical physics and/or physical chemistry, propensity for simulations and/or programming. He will work in a stimulating environment, in a young and dynamical team with high publication score.

M. Dagrada et al., JCTC 10, 1980 (2014)
F. Mouhat et al., JCTC 13, 2400 (2017)
F. Mouhat et al., in preparation (2020)

Condensed Matter Physics: YES Macroscopic Physics and complexity: YES
Quantum Physics: YES Theoretical Physics: YES