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Machine learning water cluster from quantum^2 dynamics

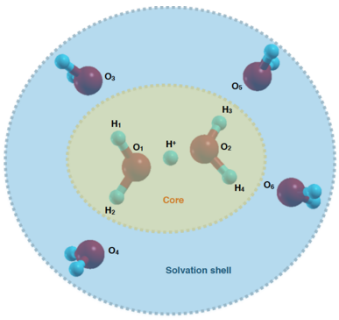
Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie

Campus Pierre et Marie Curie
Tower 23 - 4th floor -23-22
Director: Guillaume Fiquet

Title: *Machine learning water clusters from quantum^2 dynamics.*

Keywords: machine learning, ab initio molecular dynamics, quantum Monte Carlo, water

Scientific description:
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.

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

Techniques/methods in use: python, density functional theory, quantum Monte Carlo, ML libraries
Applicant skills: strong background in statistical physics and/or physical chemistry, propensity for simulations and/or programming.
Industrial partnership: No

Internship supervisor(s):
Michele Casula, Marco Saitta
E-mail: michele.casula@impmc.upmc.fr, Tel: 01 44 27 43 60
Internship location: Institut de Minéralogie, Physique des Matériaux et Cosmochimie (IMPMC)
Possibility for a Doctoral thesis: Yes