INTERNSHIP PROPOSAL

(One page maximum)

Laboratory name: Gulliver, ESPCI & LPENS (ENS)
CNRS identification code: 7083
Internship director'surname: Hélène Berthoumieux
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Internship location: Gulliver, ESPCI

Thesis possibility after internship: YES
Funding: NO

Title: Machine-Learning Force Fields and Simulation Methods for the Dielectric Properties of Water

Summary (half a page maximum)
The dielectric behavior of water governs key processes in electrochemistry, nanofluidics, and materials science. While *ab initio* molecular dynamics (AIMD) captures its electronic structure accurately, it remains computationally demanding. Recently, **machine-learning force fields (ML-FFs)** trained on AIMD data have emerged as powerful tools to reproduce quantum accuracy at a fraction of the cost. However, their ability to describe long-range polarization and dielectric properties remains to be fully assessed and improved.

This internship aims to test and refine ML-FFs for liquid water. The student will perform molecular dynamics simulations using existing machine-learning potentials and compute dielectric observables including polarization correlations, charge structure factors, and frequency-dependent permittivity. These results will be compared with reference *ab initio* and classical simulations in order to assess the strengths and limitations of current ML approaches.

This internship is part of a broader project investigating the properties of the water/metal interface, including the capacitance and friction of water flowing over metal.

References:
J. Carrasco *et al. A* molecular perspective of water at metal interface, Nature Materials, 11 (2012), N. Kavokine et al.,Fluctuation-induced quantum friction in nanoscale water flows, Nature, 602, 7895 (2022) A. Robert, H. Berthoumieux, ML. Bocquet, Coupled Interactions at the Ionic Graphene-Water Interface, Phys. Rev. Lett. 130, 076201 (2023). J. Hedley, K.Bhatt, H. Berthoumieux, A. Kornyshev, What does an ion feel at the electrochemical interface? Revisiting electrosorption through nonlocal electrostatics, J. Chem. Phys. 162, 114703 (2025), D. Labavic, F. Brunig, R Netz, ML. Bocquet, H. Berthoumieux, Nonlocal dielectric properties of water: the role of electronic delocalisation, arXiv2505.11101 (2025).

Please, indicate which speciality(ies) seem(s) to be more adapted to the subject:

Condensed Matter Physics: YES/NO Soft Matter and Biological Physics: YES/NO
Quantum Physics: YES/NO Theoretical Physics: YES/NO