INTERNSHIP PROPOSAL

(One page maximum)

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Internship location: Gulliver, ESPCI

Thesis possibility after internship: YES
Funding: NO

Title Polarization Functional for Water at the Electronic Scale

Summary (half a page maximum)

Understanding the microscopic dielectric properties of water near metal surfaces is key to electrochemistry, catalysis, and nanofluidics. Recent experiments in nanoslits reveal interfacial water structure at subnanometer scales, calling for new theoretical models.

Water-metal interfaces are typically investigated using classical or ab initio molecular dynamics (MD) simulations. Breaking away from these purely numerical approaches, we have developed analytic functionals of the polarization to describe the dielectric properties of water at the nanoscale. These functionals are versatile, analytically tractable, and parametrized to reproduce dielectric properties of bulk water.

The goal of this internship is **to develop and parametrize a Landau–Ginzburg-type functional including electronic correlations.** By introducing coupling with confining metallic surfaces, we use these tools to describe the dielectric properties of confined water and to rationalize its unexpected experimental behavior.

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