



Electrolytes in confinement: a field theory approach

18 month postdoctoral position

Laboratoire Gulliver ESPCI, Paris

Electrolytes in confinement: a field theory approach

The study of nanoconfined electrolytes is exciting both for their ubiquity and for the theoretical challenge they bring. The nanometer scale represents typical confinement size of technological and biological devices, screening length of low concentrated ionic solutions, and range at which water starts to behave as an inhomogeneous medium¹. The structure of interfacial solutions is thus a subtle interplay between short-range charge overscreening generated by the solvent, ion-ion correlations, water- and ion-surface interactions. These effects cannot be captured by macroscopic models such as Poisson-Boltzmann equation.

Can we develop a field theory describing nanoconfined electrolytes? To answer this question, the postdoctorate will extend the Landau-Ginzburg model developed for confined water² to electrolytes under confinement. Particular attention will be paid to the description of the surface-ion³ and water-ion interaction at this scale. Both classical and quantum simulations will be used as inputs to extract essential ingredients of the theory and to parametrize them.

The postdoc will be based in ESPCI, in the center of Paris, under the supervision of H el ene Berthoumieux. The postdoc will be integrated in the lab « Gulliver ». The work will be in collaboration with Alexei Kornyshev, (Imperial College, London) and Marie-Laure Bocquet (ENS, Paris). The postdoc duration is 18 months, start date at latest 1st April 2023, with salary according to experience.

The candidate should have a PhD (or have it completed before the start of the position) in theory in physics or chemical physics. Interest for molecular dynamics/ ab initio simulations is appreciated.

Candidate interested, please send a CV and a short email motivating your interest in the position.

H el ene Berthoumieux: helene.berthoumieux@espci.fr

References: (1) L. Fumagalli et al., Anomalous low dielectric constant of confined water, *Science*, 360, 1339 (2018), (2) G. Monet, et. al, Nonlocal dielectric response of water in nanoconfinement, *Phys. Rev. Lett.* 126 21600 (2021). (3) A. Robert et al., Coupled interactions at the ionic graphene/ water interface, *ArXiv*, arXiv:2204.08779, (2022).