

Properties of electrolytes at the nanoscale

Encadrants:

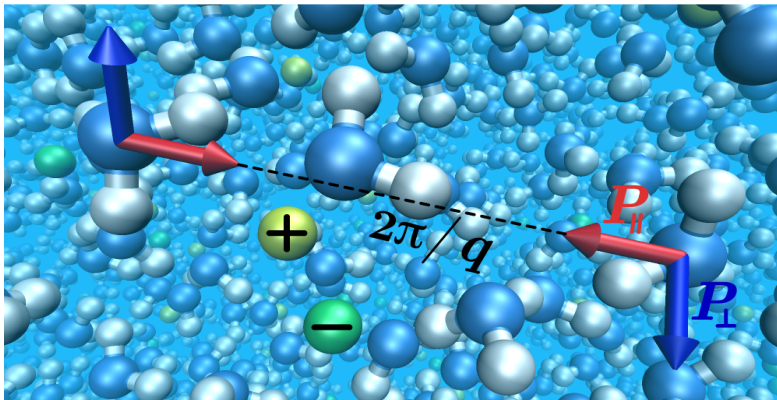
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Possibilité de thèse: Oui

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Sketch of electrolyte at the nanoscale. Water acts as a nonlocal nonlinear dielectric medium to the presence of ions.

Résumé

The properties of confined electrolytes focus a lot of attention. They play a key role in controlling reactivity and transport in confinement. These processes are omnipresent in *in vivo* metabolic pathways and in nanofluidic devices developed to produce non-intermittent green energy. As the properties of the fluid at the nanoscale differ drastically from the macroscopic ones, a theory based on a linear local description of the fluid, such as the Poisson-Boltzmann theory or the method of image charge breaks down at this scale and a new framework is necessary to describe these systems [1,2,3]. In this internship, we will investigate the interplay between the structure of the fluid, the correlations of the ions and the geometry and the physical properties of the confining surface on the dielectric properties of the liquid. Via standard tools of statistical physics and field theory we will derive analytically the properties of this system and will extract the coupling between fluid molecular structure and confinement. Molecular dynamics simulations will be performed to parametrize the field theory model and validate the analytical results.

1. L. Fumagalli, et al. Anomalous low dielectric constant of confined water, *Science*, 360 1339 (2018)
2. G. Monet, et al. The nonlocal dielectric response of water in nanoconfinement, *Phys. Rev. Lett.* 126 216001, (2021)
3. A. Robert et. al. Coupled Interactions at the Ionic Graphene-Water Interface, *Phys. Rev. Lett.* 130 (7), 076201, (2023)

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