# Properties of polar fluids at the nanoscale

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Summary
The properties of confined fluids focus a lot of attention. They play a key role in controlling reactivity and transport in confinement. These processes are omnipresent 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 homogeneous 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 geometry and the physical properties of the confining surface on the dielectric properties of the liquid.

To do so, we will describe the fluid molecules with an increasing complexity (starting from punctual dipoles to explicit extended charge distributions). The confinement will first be described as purely geometric and in second step physical properties of the surface (metallic/dielectric) can be included. 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.
Simulations will be performed to parameterize the field-theory model and validate the analytical results.

1. A. Schlaich, E. W. Knapp, and R. R. Netz, Phys. Rev. Lett. 117 048001 (2016).
2. L. Fumagalli, A. Esfandiar, R. Fabregas, S. Hu, P. Ares, A. Janardanan, Q. Yang, B. Radha, T, Tanigushi, K. Watanabe, G. Gomila, Anomalous low dielectric constant of confined water, Science, 360 1339 (2018)
3. G. Monet, F. Bresme, A. Kornyshev, H. Berthoumieux, The nonlocal dielectricresponse of water in nanoconfinement, Phys. Rev. Lett. 126 216001, (2021)