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Séminaire du Laboratoire de Physique Théorique de la Matière Condensée

Lundi 23 Novembre 2020, 10 :45
LPTMC, On-line zoom seminar(https ://zoom.us/j/94339577111 ID de réunion : 943 3957 7111 Code secret : 117717)
Domaines : cond-mat.mes-hall

Titre : *How a surface affects the dielectric properties of water : A minimal theoretical model supported by molecular dynamics simulation*

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Résumé : *The dielectric permittivity of water in nanometric confinement has been measured in an increasing number of simulations and experiments in the last years [1, 2]. The results confirm that at this scale water is not a homogeneous dielectric medium and that a confinement of up to 100 nanometers leads to an unexplained low permittivity. This property determines the strength of water-mediated electrostatic forces, which in turn affects phenomena such as molecular transport through nanopores, chemical reactions in confinement, and macromolecular assembly.*

Continuum nonlocal electrostatics can be used to model dielectric properties at the nanometric scale of correlated fluids in the bulk (i.e. far from a surface) [3]. In this work, we write an electrostatic energy for water as a functional of its polarization that encodes the correlation lengths of the fluid in the bulk and an interaction energy with the surface as a harmonic potential. By introducing generic higher-order terms in the interaction energy we can explain the differences of the response of interfacial water in the vicinity of isoelectronic surfaces. We validate our approach with Molecular Dynamics simulations of hydrated graphene and hBN surfaces. Moreover, the theoretical model reproduces experimental measures of the dielectric permittivity of water in nanometric slabs.

[1] L. Fumagalli et al., Science 2018, 360, 1339. [2] P. Loche et al., J. Phys. Chem. B 2020, 124, 4365. [3] A. A. Kornyshev, Electrochimica Acta 1981, 26, 1.