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Transport properties of interfacial water

Nanofluidic systems (i.e. natural and artificial systems where fluids are confined at the nanoscale) offer alternative and sustainable solutions to problems relating to energy harvesting and water treatment. New behaviors arise in nanoconfined liquids due to the predominant role of surfaces. Indeed, surfaces can limit the performance of nanofluidic devices, through e.g. liquid-solid friction, but they also provide new opportunities to manipulate liquids, through e.g. the so-called osmotic flows, generated at surfaces by non-hydrodynamic forcing (e.g. electric potential gradient: electro-osmosis, solute concentration gradient: diffusio-osmosis, temperature gradient: thermos-osmosis). Here, I will illustrate with recent work how atomistic simulations can help relate the interfacial transport properties of water and aqueous solutions to their equilibrium structure and dynamics.

First, I will show how classical and ab initio molecular dynamics simulations can reveal the molecular mechanisms of liquid-solid friction, controlling the hydrodynamic boundary condition. In particular, I will show that the commonly accepted relation between wetting and friction can fail in the case of water on graphene and boron nitride, and that the electronic structure of the interface plays a critical role on friction in these systems [1,2]. I will also explain why adding a very small amount of alcohol in water can dramatically decrease interfacial friction [3]. I will then discuss how osmotic flows depend on both interfacial structure and dynamics [4], taking as examples electro-osmotic flows in foam films [5,6], diffusio-osmotic flows of water-alcohol mixtures [7], and thermo-osmotic flows on graphitic walls [8,9].

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