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Molecular views on surface-driven flows: the case of thermo-osmosis

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Surface-driven flows (also called osmotic flows) are generated at interfaces by various thermodynamic gradients (e.g. electric potential gradient: electro-osmosis, solute concentration gradient: diffusio-osmosis, temperature gradient: thermos-osmosis). They represent powerful tools to manipulate liquids in micro and nanofluidic systems, and play a key role in living systems, in sustainable energies, or in water treatment and desalination processes. Osmotic flows arise from the coupling between hydrodynamics and liquid-wall interactions in the nanometric vicinity of the interface, and yet standard descriptions are usually based on continuum models and liquid-wall interactions only.
During this talk I will illustrate with recent work on thermo-osmosis how molecular dynamics simulations can be used to investigate the mechanisms underlying surface-driven flows. In this work, our main objective was to understand the effect of the wetting properties of the liquid on the solid surfaces. We have shown the critical role of interfacial hydrodynamics, which can reverse the direction of the flow, and strongly amplify it. In particular, we have predicted giant thermos-osmotic flows at the water-graphene interface. These theoretical results open many perspectives for the efficient generation of flows using waste heat, which could be applied for instance to sea water desalination.

References

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