Molecular views on nanofluidic transport

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Nanofluidic transport plays a key role in many present-day applications, such as water filtration/desalination, “blue energy” harvesting, etc. However, transport efficiency in state-of-the-art artificial nanofluidic devices is generally not optimal, and far below the performance of biological systems. In order to improve the efficiency of nanofluidic systems and design innovative devices, it is crucial to understand the specificities of nanoscale transport. In particular, surfaces and interfaces play an increasing role when reducing the system size, so that in nanoconfined liquids, the different types of transport (hydrodynamic, ionic, thermal…) and their couplings are controlled by surfaces.

During this talk, I will show that molecular simulations represent a powerful tool to investigate transport in nanoconfined liquids and in liquids at interfaces, accounting naturally for the molecular detail of the systems. To that aim, I will present some recent works where we investigated interfacial hydrodynamics and its consequences on nanofluidic energy conversion using electrokinetic effects.