

Ionic and water transport in nanofluidics for blue energy conversion from *ab initio* methods

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Abstract

A vast amount of energy, so-called blue energy, may be harnessed from the mixing of salty and fresh water at river estuaries. Yet, blue energy remains an unexplored source, due to the limited efficiency of conventional membranes. Although the electronic structure of materials has been suggested to be highly relevant for osmotic energy conversion, a number of questions concerning its role on nanoscale water and ionic transport are so far unanswered. In this talk I will answer some of these questions by means of *ab initio* molecular dynamics, for which the extensive use of HPC facilities (Piz-Daint) has been essential. In particular, I will first show that subtle changes in both the molecular structure and dynamics of water at the interface with graphene, hBN and MoS₂ are responsible for pronounced changes in water slippage, amounting to up to one order of magnitude change between the different two-dimensional materials. Additionally, I will present a framework to compute the transport properties of

ions at liquid/solid interfaces simply by computing the water and ions' density profile and discuss the application of this strategy to the the problem of electro-osmosis and diffusio-osmosis at the water/graphene and water/hBN interfaces. I will conclude highlighting the relevance of specific electronic structure effects to both water and ion transport in connection with osmotic power generation.