Nanofluidic water transport for blue energy conversion

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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. Recent experiments have reported on exceedingly high power generated from ionic transport across two-dimensional materials and nanotube membranes. Additionally, water flow under confinement has received increased attention in the recent years, also driven by the interest to develop efficient osmotic power generators. Although the electronic structure of materials has been suggested to be highly relevant for osmotic energy conversion, its role on nanoscale water flow and ionic transport is not known. In this talk I will present results on water flow and ion adsorption at the interface between water and graphene, hBN and MoS_2 sheets by means of *ab initio* molecular dynamics. In particular, I will show that subtle changes in both the structure and dynamics of interfacial water are responsible for pronounced changes in water slip, amounting to up to one order of magnitude change between the different two-dimensional materials. I will also compare the adsorption properties of a prototypical electrolyte to explore the role of the electronic structure of materials in the adsorption of ions at liquid/solid interfaces. Extensive

use of HPC facilities (Piz-Daint) has been and will continue to be essential due to the substantial cost of *ab initio* simulations of liquid/solid interfaces. The CP2K code, which is being used to perform these simulations, is especially suited to perform *ab initio* molecular dynamics of complex liquid/solid interfaces on large HPC facilities. Overall, this work bridges the gap between experiments and first principles simulations of liquid and ionic transport across nanomembranes and answers a few of the fundamental questions related to the molecular and electronic properties of materials for osmotic power generation.