



"Soft-Matter Seminar"

Dynamics of water molecules confined in nanoscale space under mechanical perturbation and electrical fields

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Abstract:

Water confined in nanoscale space is of great importance for biological activities as well as the designing of novel molecular devices/machines/sensors. With the development of the experimental and computational facilities, it becomes possible to study the dynamics of water confined in nanoscale space by both experiments and numerical simulations. In this talk, we present our recent progress studied by molecular dynamics simulations. It is found that the water permeation across the channel has an excellent on-off gating behavior when the water molecules form single-file structure inside the channel with an appropriate channel radius. The water conduction across the water channel keeps almost fixed for a considerable deformation and/or a very small distance of the external charge from the channel, and decreases very rapidly when the channel deformation or the charge distance passes a threshold. The nanopore exhibits unidirectional transportation of the water molecules when there is a combination of charges positioned adjacent to a nanopore, inspired from biological water channels, Aquaporins. We also show that the biomolecules with aqueous liquids inside a single-walled nanotube can be controllably manipulated by using an external charge or a group of external charges outside the nanotube, which is expected to serve as lab-in-nanotube for the interactions and chemical reactions of molecules especially biomolecules. Finally, we will report our very recent observation on the signal transduction mediated by water and other polar molecules confined in nanochannels.

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