Contribution ID: **320** Type: **Oral Presentation**

Water transport in soft nanoporous materials: Impact of mechanical deformation on collective dynamics, interfacial slippage and permeance

Friday, 4 June 2021 14:00 (15 minutes)

Transport of water in soft porous materials is relevant to a broad range of applications such as ultrafiltration and reverse osmosis processes, where polymeric membranes are employed in filtration/separation, or energy related processes where proton conducting media (Nafion for instance) are used. It also pertains to important fields such as those dealing with wood/cellulosic materials, food processing and is of upmost importance in many biological processes (transport through cellular membranes). While water transport in hard porous materials such as porous silica glasses is well studied, the situation in soft matter is much more puzzling and remains unclear due to the combination of surface heterogeneity, the diffuse boundary location and pore deformations due to mechanical stresses.

In this work we study water in chemically realistic hydrophobic pores at different thermodynamic and mechanical conditions using atomistic molecular dynamics simulations. In detail, we show that the pore swelling can be modeled within a poromechanic framework and analyze the adsorption and confinement effects as well as microscopic diffusion mechanisms and transport effects due to pore size fluctuations. Strikingly, we fund that hydrodynamic continuum models remain valid for planar flow of water even in monolayer confinement in soft pores.

Time Block Preference

Time Block A (09:00-12:00 CET)

References

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