8. Water in TiO_2 Nanopores: a study on structure, dynamics, phase behavior and optical properties of confined water

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Molecular dynamics simulations of water confined in TiO_2-rutile pores of diameters 1.3, 2.8 and 5.1 nm, were carried out at various water contents. Water density and diffusion coefficients were obtained as a function of the distance from the surface. The proximity to the interface affects density and diffusivity within a distance of around 10 Å from the walls, beyond which all properties tend to converge. Different filling mechanisms were observed as a function of the pore size. Capillary condensation takes place in equilibrium for the 2.8 and 5.1 nm pore. In the former case, the surface density increases uniformly with filling until condensation, whereas in the larger nanotube, a cluster of water molecules develops on a localized spot on the surface for fillings just below transition. In the smaller pore, no phase transition is detected. For all the systems studied, the first monolayer of water is strongly immobilized on the interface, thus reducing the accessible or effective diameter of the pore by around 0.6 nm. Finally, our results show how confinement affects the dynamic properties of water inside the pores. The mobility observed for the water molecules is strongly dependent on their proximity to the surface as well as the rotational dynamics, having in turn a significant impact on the dielectric and optical responses of the confined water.