

Atomistic study of water confined in silica

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In this work, we have used a combined of atomistic simulation methods to explore the effects of confinement of water molecules between silica surfaces. Firstly, the mechanical properties of water severe confined ($\sim 3\text{\AA}$) between two silica alpha-quartz was determined based on first principles calculations within the density functional theory (DFT). Simulated annealing methods were employed due to the complex potential energy surface, and the difficulties to avoid local minima. Our results suggest that much of the stiffness of the material (46%) remains, even after the insertion of a water monolayer in the silica. Secondly, in order to access typical time scales for confined systems, classical molecular dynamics was used to determine the dynamical properties of water confined in silica cylindrical pores, with diameters varying from 10 to 40 \AA . In this case we have varied the passivation of the silica surface, from 13% to 100% of SiOH, and the other terminations being SiOH₂ and SiOH₃, the distribution of the different terminations was obtained with a Monte Carlo simulation. The simulations indicates a lowering of the diffusion coefficients as the diameter decreases, due to the structuration of hydrogen bonds of water molecules; we have also obtained the density profiles of the confined water and the interfacial tension.