On the phase behavior of water-like fluids with square-well attractions and site-site association in slit-like pores. Density functional approach.

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We study the adsorption and phase behavior of water-like fluid models with square-well inter-particle attraction and site-site association in slit-like pores by using a density functional theory. The models for water taken from [1] reproduce the bulk equation of state well [2]. The mean field theory and the first-order mean spherical approximation have been applied to account for the attractive interactions. The chemical association effects are taken into account by using the first-order thermodynamic perturbation theory. The influence of the slit-like pore width, the gas-solid interaction energy, and of the square-well width on the phase behavior have been explored [3]. A comparison with computer simulation data has been performed. Some results and perspectives concerning the adsorption of water-like models in a slit-like pore with walls modified by pre-adsorbed tethered chain molecules are presented. The presence of molecular brushes on the pore walls has important consequences for the behavior of water in pores [4].

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