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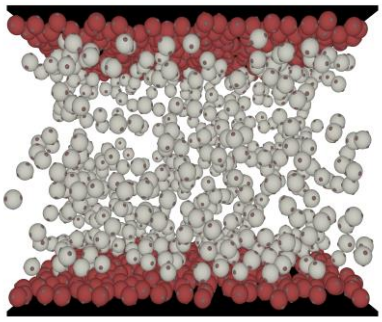
On the phase behavior of model fluids with square-well attraction in slit-like pores: Density functional approach and molecular simulation.



The phase behavior of a model fluid with square well inter-particle attraction in slit-like pores has been studied by using a density functional theory and molecular simulation. The mean field theory, the first-order mean spherical approximation and the statistical associating fluid theory have been applied to account for the attractive interactions.

The influence of the pore width, the gas-solid interaction energy and of the square well width on the phase behavior have been explored in detail. Dependent on the values of parameters of the model, we observed capillary condensation and capillary evaporation, in some cases layering phase transition has been obtained as well. Also, a crossover between condensation and evaporation can be observed for a single specific model dependent on the temperature of adsorption. The theory and the results obtained in the present work are valuable for future theoretical exploration of water-like and other models under confinement that intrinsically involve square well as a reference ingredient.