

269a An Application of Mean-Field Perturbation Theory for the Adsorption of Water Molecules in Nanoslit-Pores

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In the present research study, we present the development of a model for characterizing and predicting the adsorption of water molecules between two parallel plates based on mean-field perturbation theory. The electrostatic forces between fluid-fluid molecules in the slit shaped pore are modeled by considering permanent dipole-dipole interactions and permanent dipole-induced dipole moment interactions. The intermolecular potential for the electrostatic interactions was obtained by considering statistical averages over all possible orientations of the molecules. The proposed model is then used to study the sorption of water molecules in the slit shaped pore and an explicit equation for the Helmholtz free energy of the pore phase fluid is derived. Adsorption isotherms for different pore sizes are simulated and the relative contributions of fluid-wall and fluid-fluid interactions to the Helmholtz free energy are calculated as an illustration and compared with the results of existing models in the literature.