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Theoretical and Experimental Investigations of Isothermic Heats for Water Adsorption on Silica Gel Surfaces

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Abstract

The knowledge of the isothermic heats (Q_{st}^o) is essential to design porous adsorbents for calculating the performances of adsorption-assisted cooling, separation and gas storage systems. This paper presents a thermodynamic framework to calculate the interaction potentials and isothermic heats for water adsorption on SiO_2 structures. Here both Lennard Jones (LJ) and electrostatic potentials are considered. It is found that (i) Q_{st}^o varies from 1.37 eV (~131 kJ/mol) to 0.54 eV (~52 kJ/mol) for the adsorption of one water molecule on various pore sizes of SiO_2 structure, and (ii) Q_{st}^o depends on the pore size (H). Q_{st}^o is found to be very high in the super-micro-pore regions. The density functional theory (DFT) is applied to calculate Q_{st}^o for the adsorption of water on silica. Here water-water interactions are not considered. Later Q_{st}^o for five types of silica gels are obtained from experimentally-measured isotherms data at low pressures (up to 0.15 kPa) and wide range of temperatures. The simulation result agrees well with the experimental data.

Keywords: Isothermic heat of adsorption, Pore width, adsorption interaction, LJ Potentials

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