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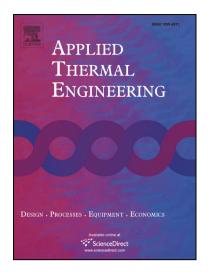
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## ACCEPTED MANUSCRIPT

Theoretical and Experimental Investigations of Isosteric Heats for Water Adsorption on

Silica Gel Surfaces

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**Abstract** 

The knowledge of the isosteric heats  $(\varrho_{st}^{o})$  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 isosteric heats for water adsorption on SiO2 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<sub>2</sub> 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: Isosteric heat of adsorption, Pore width, adsorption interaction, LJ Potentials

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