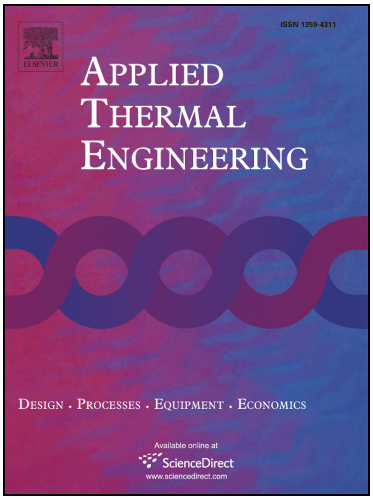

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PII: S1359-4311(18)31648-X
DOI: https://doi.org/10.1016/j.applthermaleng.2018.05.096
Reference: ATE 12235

To appear in: *Applied Thermal Engineering*

Received Date: 14 March 2018
Revised Date: 23 May 2018
Accepted Date: 24 May 2018

Please cite this article as: W. Fan, A. Chakraborty, K. Choong Leong, Theoretical and Experimental Investigations of Isosteric Heats for Water Adsorption on Silica Gel Surfaces, *Applied Thermal Engineering* (2018), doi: https://doi.org/10.1016/j.applthermaleng.2018.05.096

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 $\left(Q_{st}^{o}\right)$ 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 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: Isosteric heat of adsorption, Pore width, adsorption interaction, LJ Potentials