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Simultaneous description of strong and weak H_2 adsorption sites coexisting in MOFs MOON-HYUN CHA, KYUNG-SUK KIM, School of Engineering, Brown University, JISOON IHM, Department of Physics and Astronomy, Seoul National University — In designing hydrogen-storage materials, it is a widespread practice to introduce transition-metal atoms into the MOF structures in order to increase the binding energy of H_2. In such systems, it is necessary to understand and describe the H_2 binding behaviors at both strong and weak binding sites. Here, we propose a model that quantitatively characterizes the hydrogen gas adsorption in the presence of different kinds of adsorption sites. Based on equilibrium thermodynamics, this model enables us to figure out the number of H_2 molecules adsorbed to each adsorbing site and the corresponding heat of adsorption. When the present model is applied to real experimental data, different binding sites are identified and the contribution of each term to the storage capacity is obtained. While the virial equation gives the isosteric heat of adsorption averaged over the system, our model gives the heat of adsorption at each adsorbed site. Furthermore, by analyzing the results of fitting, we can estimate the volume occupied by adsorbed H_2 molecules.

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