Reliability of model-based estimations of the hydrogen adsorption capacities in nanoporous materials: a molecular simulation study

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There has been a recent report regarding the existence of solid-like H_2 adsorption in nanoporous materials. In this work, we employed grand canonical Monte Carlo (GCMC) simulations on a series of metal-organic frameworks with 1-D and 3-D channels to address the pitfalls of model-based approaches in estimating the hydrogen uptake. The excess hydrogen uptakes of several structures with pore sizes ranging from 5 to 37 angstrom were predicted. The pore volume and the density of adsorbed H_2 were obtained by fitting the Tóth equation to the excess H_2 isotherm data from the simulation, and the results were compared with the data obtained from direct simulation. Sensitivity analyses show that the pore volume and the density of adsorbed H_2, obtained from model-based fitting are not accurate enough to estimate the adsorbed H_2 density and the pore volume of the materials, and especially poor for the materials with 1D channels.