Sequestration and Diffusion of Small Non-Polar Molecules in MOF Materials

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Distressing scenarios of fossil fuel shortages and increasing green-house effects have intensified scientific efforts to find innovative materials capable of efficient/effective hydrogen storage and gas separation. Metal organic frameworks (MOF) are a broad class of novel porous materials that exhibit the necessary prerequisites for feasible hydrogen storage and gas separation. For example, MOFs have large surface areas, high porosity, high thermal stability, high structural flexibility, and easily tunable chemical and physical properties [1, 2, 3]. A great deal of experimental effort has been made in synthesizing MOFs and tailoring their chemical properties, but insight into the physisorption phenomena that govern MOF macroscopic properties is best obtained through a combination of experiment and theory. We will present promising results from such a combined study, focusing on theoretical DFT simulations of the adsorption and diffusion of small, non-polar molecules such as H_2, CO_2, and N_2 throughout the MOF scaffold. Standard exchange-correlation functionals are not capable of describing weak van der Waals interactions responsible for binding these molecules inside MOFs; however, we will show that the truly non-local functional vdW-DF [4, 5] gives results—for a variety of properties of MOFs—in remarkable agreement with our experiments.

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