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Molecular Transport in Metal Organic Framework Ma- terials P.

CANEPA, Wake Forest University, N. NIJEM, Y.J. CHABAL, University of Texas at Dallas, T. THONHAUSER, Wake Forest University — Metal organic frameworks (MOF) materials are a class of porous materials well suited for hydrogen storage and gas separation. While current work on MOFs focuses mostly on the adsorption properties of small molecules, their diffusion is still poorly understood. To elucidate the diffusion process, we study the diffusion of H_2 , CO_2 , and H_2O in the nano-pores of MOF-74-Mg by combining *ab initio* simulations with infrared (IR) spectroscopy. We present computed adsorption energies and changes in the IR frequencies upon adsorption. We also discuss several diffusion mechanisms and their calculated barriers. We further verify the existence of the debated secondary binding sites for guest molecules and we discuss the role played by H_2O . We find that H_2O is much more likely to adsorb in the MOF than H_2 and CO_2 , leading to a significant reduction of the adsorption capabilities of the MOF towards these target molecules, and hence resulting in limitations for practical applications. Overall, our computational findings are in very good agreement with experiment and they provide a fundamental understanding of the diffusion processes of small molecules in these nano-porous materials, with implication for the usability of MOFs in gas separation and storage applications.

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