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Understanding the kinetics of adsorption in narrow channel metal organic frameworks WEI ZHOU¹, JASON SIMMONS, TANER YILDIRIM², NIST Center for Neutron Research — Advancements in the controlled synthesis of metal organic frameworks (MOFs) have lead to impressive increases in hydrogen storage capacities and enhanced binding energies that may offer higher temperature operation. Given that the optimum pore size for hydrogen adsorption is on the order of 7 Angstroms, diffusion of hydrogen into these materials can play an important role in their ultimate implementation. In this presentation we use a combination of experimental and computational techniques, including gas sorption and neutron scattering measurements and detailed first-principles calculations, to better understand the kinetic limitations to adsorption in narrow channel MOF. In particular we show that the adsorption is diffusion limited with a significant activation barrier of ~ 70 meV, and that this barrier is phonon-mediated. This work demonstrates the importance of considering kinetic effects in addition to pore volume and heats of adsorption when optimizing MOF materials for hydrogen storage.

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