

Abstract Submitted
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Neutron Diffraction Studies of Hydrogen Adsorption in a Highly Stable Porous Rare-Earth Metal-Organic Framework JUNHUA LUO, YUSHENG ZHAO, HONGWU XU, LUC L. DAEMEN, Los Alamos National Laboratory — Gas sorption measurements show that a highly stable porous lanthanide metal-organic framework can take up hydrogen of about 2.1 wt. % at 77 K and 10 bar. Difference Fourier analysis of neutron powder diffraction data revealed four distinct D₂ sites that are progressively filled within the nanoporous framework. Interestingly, the strongest adsorption sites identified are associated with the aromatic organic linkers rather than the open metal sites, as occurred in previously reported MOFs. Our results provide for the first time direct structural evidence demonstrating that optimal pore size (around 6 Å, twice the kinetic diameter of hydrogen) strengthens the interactions between H₂ molecules and pore walls and increases the heat of adsorption, which thus allows for enhancing hydrogen adsorption from the interaction between hydrogen molecules with the pore walls rather than with the normally stronger adsorption sites (the open metal sites) within the framework. At high concentration H₂-loadings (5.5 H₂ molecules (3.7 wt. %) per Y(BTC) formula), H₂ molecules form highly symmetric novel nanoclusters with relatively short H₂-H₂ distances compared to solid H₂. These observations are important and hold the key to optimizing this new class of rare metal-organic frameworks (RMOFs) materials for practical hydrogen storage applications.

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