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Structure, lattice dynamics, and hydrogen adsorption properties of zeolitic imidazolate framework-8 W. ZHOU, NCNR, NIST and MSE Dept., U. Penn., H. WU, NCNR, NIST and MSE Dept., U. Maryland, T. YILDIRIM, NCNR, NIST and MSE Dept., U. Penn. — Zeolitic imidazolate frameworks (ZIFs) are a new family of nanoporous metal-organic framework compounds that possess interesting zeolite-type structures with very high chemical stability [1,2]. We performed high-pressure isotherm measurements at various temperatures to characterize the H_2 adsorption properties of ZIF8, which consists of ZnN_4 clusters linked by 2-methylimidazole [$H_2C_3N_2$-(CH_3)]. We find that the adsorption capacity is 1.2 wt% at 77 K and 1 atm, while the maximal adsorption is 4.5 wt% at 30 K and 3 atm. The initial heat of adsorption is $\sim$5 kJ/mol. Using neutron powder diffraction, we investigated the structure of ZIF8 and its associated hydrogen adsorption sites. These sites were directly determined using difference Fourier analysis and agree well with first-principles predictions. Furthermore, we studied the structural stability and lattice dynamics of ZIF8, combining inelastic neutron scattering and first-principles calculations. Several interesting phonon modes were identified. [1] X. C. Huang et al., Angew. Chem. Int. Ed. 45, 1557 (2006). [2] K. S. Park et al., Proc. Natl. Acad. Sci. U.S.A. 103, 10186 (2006).

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