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First-Principles Prediction of Small Molecule Adsorption in MOF-74 Variants JOSHUA HOWE, KYUHO LEE, Dept. of Chemical and Biomolecular Engineering, University of California, Berkeley; The Molecular Foundry, LBNL, LI-CHIANG LIN, Dept. of Chemical and Biomolecular Engineering, University of California, Berkeley, BEREND SMIT, Dept. of Chemical and Biomolecular Engineering, University of California, Berkeley; Materials Sciences Division, LBNL, JEFFREY NEATON, The Molecular Foundry, LBNL; Dept. of Physics, University of California, Berkeley — Using density functional theory (DFT), we predict binding energies of flue gas molecules (CO, CO_2, H_2O, H_2S, N_2, NH_3, SO_2, and H_2) and small hydrocarbons (CH_4, C_2H_2, C_2H_4, C_2H_6, C_3H_6, and C_3H_8) in a variety of "MOF-74" variants. Using a harmonic approximation to compute quantum zero-point and thermal corrections, we compute binding enthalpies for comparison with experimental heats of adsorption. Our study is performed using vdW-DF2, a fully nonlocal dispersion-corrected density functional along with Hubbard U corrections on $3d$-orbital electrons as appropriate. We study MOF-74 variants, "M-MOF-74", where "M" is chosen to be any divalent third-row metal cation (M= Mg, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn). Additionally, we study "M-MOF-74" systems with "meta-dobdc" as the linker (as compared to the traditional "para-dobdc"). We compare with experiment when available and find reasonable agreement. We identify trends, and compare with experiment where available, finding excellent agreement. This work supported by DOE through the EFRC on Gas Separations for Clean Energy Technologies; computational resources provided by NERSC.

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