Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

First-principles studies of small-molecule adsorption and mechanical properties of amine-appended metal-organic frameworks JUNG-HOON LEE, JEFFREY B. NEATON, Department of Physics, University of California, Berkeley — Metal-organic frameworks (MOFs) are a class of highly-porous solids, consisting of metal centers (M) connected by organic ligands, that are of interest for gaseous storage and carbon capture. Recently, a new class of amine-appended MOFs, mmen-M_2(dobpdc), have been shown to have exceptional CO2 adsorption properties via a novel phase transition with CO2 concentration. Here, we study this cooperative effect, as well as the mechanical properties of such MOFs with M=Mg, Mn, and Zn, using first-principles density functional theory (DFT) calculations with van der Waals corrections. We find excellent agreement with measured CO_2 heats of adsorption, and demonstrate that amine ligands enhance CO_2 binding energies (by about 30 kJ/mol) and selectivity under humid conditions, in agreement with multi-component adsorption measurements. We further calculate that the polycrystalline Young's modulus of mmen-Mn_2(dobpdc) increases by 70% due to the amine ligands, a dramatic enhancement. All together, our calculations suggest that amine-based ligands can be used to optimize both small gas separation and mechanical properties of MOFs.

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Date submitted: 10 Nov 2016 Electronic form version 1.4