

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Ligand-Assisted Enhancement of CO₂ Capture in Tunable MOFs: Balancing Electrostatic and van der Waals Interactions¹ ROBERTA POLONI, Molecular Foundry, LBNL and UC Berkeley, BEREND SMIT, UC Berkeley, JEFFREY B. NEATON, Molecular Foundry, LBNL — Metal-organic frameworks (MOFs) are promising nanoporous materials for CO₂ separation technologies. Here, we use first-principles van der Waals (vdW)-corrected calculations to identify and understand how CO₂ binds to a novel “BTT-type” MOF [1] featuring open metal centers. Our study indicates that CO₂ binds to the open metal cation sites, but with an adsorption energy that can be enhanced by more than a factor of two depending on the choice of the bridging ligand. Judicious choices for metal cations and bridging ligands are shown to lead to a maximum binding energy of 0.67 eV for MgBTT. In all cases, the binding can be attributed to a combination of electrostatics and dispersion, both critically sensitive to the local environment, and contributing nearly equally to the overall binding strength. The possibility to independently tailor these energetics in a manner optimal for CO₂ capture is discussed in the context of recent experiments.

¹We acknowledge DOE-BES for support, and NERSC for computational resources

Roberta Poloni
Molecular Foundry, LBNL and UC Berkeley

Date submitted: 22 Dec 2011

Electronic form version 1.4