

Abstract Submitted
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Understanding CO₂/N₂ Selectivity and Binding in MOFs Using Dispersion-Corrected DFT¹ JOSHUA HOWE, KYUHO LEE, UC Berkeley Department of Chemical and Biomolecular Engineering; Molecular Foundry, LBNL, BEREND SMIT, UC Berkeley Department of Chemical and Biomolecular Engineering, JEFFREY NEATON, Molecular Foundry, LBNL — Metal-organic frameworks (MOFs) are a class of highly ordered, highly customizable nanoporous materials that are attractive for use in energy-relevant gas separations. MOF-253 (AlOH)(bpydc) can be post-synthetically modified by introduction of metal cations and charge-stabilizing anions [1]. Post-synthetically modified MOF-253 samples have been shown to exhibit enhanced CO₂/N₂ selectivity over the unmodified framework [1]. Here we focus on the following series of post-synthetic modifications: CoCl₂, CuCl₂, FeCl₂, NiCl₂, PdCl₂. We use the vdW-DF, vdW-DF2, and DFT-D2 dispersion-corrected density functional theory (DFT) methods to study CO₂ and N₂ binding trends in this series of modified frameworks. Particular focus is paid to examining the predictive power of our calculations on both the modified framework and modified bipyridine clusters as a proxy for the full framework. Additionally, we examine the suitability of an approximate Henry coefficient model to predict measured gas selectivity trends [1].

[1] E. Bloch, et. al, J. Am. Chem. Soc., 132, 14382-14384, 2010.

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