Abstract Submitted
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Trends in CO_2-MOF Binding from First Principles: Implications for Gas Separations[1] JOSHUA HOWE, Department of Chemical and Biomolecular Engineering, UC Berkeley; The Molecular Foundry, LBNL, BEREND SMIT, Department of Chemical and Biomolecular Engineering, UC Berkeley, 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 Al(OH)(bpydc) can be post-synthetically modified by introduction of metal cations and charge-stabilizing anions [1]. These post-synthetically modified MOF-253 samples have been shown to exhibit enhanced CO_2-N_2 selectivity over the unmodified framework [1]. Here we use van der Waals-corrected density functional theory (DFT) to study CO_2 binding energy trends in this series of modified frameworks. Particular focus is paid to examining the predictive power of our calculations on modified bipyridine fragments as a proxy for the full framework, as well as the suitability of binding energy trends to predict measured gas selectivity trends [1]. We focus on the following series of 10 post-synthetic modifications: $CoCl_2$, $CuCl_2$, $FeCl_2$, $NiCl_2$, $PdCl_2$, $Co(BF_4)_2$, $Cu(BF_4)_2$, $Fe(BF_4)_2$, $Ni(BF_4)_2$, $Pd(BF_4)_2$.

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

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