

Abstract Submitted  
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**Design of a metal-organic framework with enhanced back bonding for the separation of N<sub>2</sub> and CH<sub>4</sub>** KYUHO LEE, Molecular Foundry, Berkeley Lab, WILLIAM ISLEY, ALLISON DZUBAK, PRAGYA VERMA, SAMUEL STONEBURNER, Department of Chemistry, University of Minnesota, LI-CHIANG LIN, JOSHUA HOWE, Department of Chemical and Biomolecular Engineering, UC Berkeley, ERIC BLOCH, DOUGLAS REED, Department of Chemistry, UC Berkeley, MATTHEW HUDSON, CRAIG BROWN, Center for Neutron Research, NIST, JEFFREY LONG, Department of Chemistry, UC Berkeley, JEFFREY B. NEATON, Department of Physics, UC Berkeley, BEREND SMIT, Department of Chemical and Biomolecular Engineering, UC Berkeley, CHRISTOPHER J. CRAMER, DONALD G. TRUHLAR, LAURA GAGLIARDI, Department of Chemistry, University of Minnesota — Removing dinitrogen, an omnipresent but noncombustible contaminant, from natural gas or other methane-rich gases is an extraordinarily difficult separation based on physical properties alone, as both gases lack a permanent dipole and have similar polarizabilities, boiling points, and kinetic diameters. In this work, by using dispersion-corrected density functionals and wavefunction approaches, we predict a new metal-organic framework (MOF) of potential utility for the highly selective and efficient separation of dinitrogen from methane, a particularly challenging separation of critical value for utilizing natural gas. Selective back bonding interactions from the vanadium(II) cation centers in V-MOF-74 to the unoccupied  $\pi^*$  orbitals of N<sub>2</sub> can be used to separate N<sub>2</sub>/CH<sub>4</sub> mixtures. We compare our calculations with the experimentally characterized Fe-MOF-74.

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