

Abstract Submitted
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Gas Adsorption and Selectivity in Zeolitic Imidazolate Frameworks from First Principles Calculations KEITH RAY, UC Berkeley Department of Physics, DAVID OLMSTED, UC Berkeley Department of Materials Science and Engineering, NING HE, University of Kansas Department of Chemistry, YAO HOUNDONOUGBO, Eastern Washington University Department of Chemistry and Biochemistry, BRIAN LAIRD, University of Kansas Department of Chemistry, MARK ASTA, UC Berkeley Department of Materials Science and Engineering — Zeolitic Imidazolate Framework (ZIFs) are excellent candidate materials for carbon capture and gas separation. Here we employ the van der Waals density functional (vdW-DF) [1] in an analysis of the binding energetics for CO₂, CH₄ and N₂ molecules in a set of ZIFs featuring different chemical functionalizations. We investigate multiple low-energy binding sites, which differ in their positions relative to functional groups on the imidazole linkers. In all cases an accurate treatment of van der Waals forces appears essential to provide reasonable binding energy magnitudes. We report results obtained from different parameterizations of the vdW-DF, providing comparisons between calculations and experimental values of the heat of adsorption [2]. This research is supported by the Energy Frontier Research Center “Molecularly Engineered Energy Materials,” funded by the US Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0001342. [1] M. Dion, H. Rydberg, E. Schroder, D. C. Langreth, B. I. Lundqvist, Phys. Rev. Lett. 92, 246401 (2004) [2] W. Morris, B. Leung, H. Furukawa, O. K. Yaghi, N. He, H. Hayashi, Y. Houndonougbo, M. Asta, B. B. Laird, O. M. Yaghi, J. AM. CHEM. SOC. 2010, 132, 11006-11008

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