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CO2 Binding in Zeolitic Imidazolate Frameworks from First Principles Calculations KEITH RAY, DAVID OLMSTED, NING HE, YAO HOUNDONOUGBO, BRIAN LAIRD, MARK ASTA — Zeolitic Imidazolate Frameworks (ZIFs) are excellent candidate carbon capture materials owing to their high surface area, selectivity, and stability. In this work we use electronic-structure based methods to investigate the binding of CO2 in a set of ZIFs that share the same topology but feature different functionalized linkers [1]. Since a large portion of the CO2 binding comes from van der Waals (vdW) forces, we explore several different schemes for incorporating these contributions into ab-initio density-functional-theory (DFT) including vdW-DFT [2]. The results are combined with those of classical simulation studies to allow comparisons between calculations and experimentally measured values of the heat of adsorption and adsorption isotherms [1]. 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] W. Morris, B. Leung, H. Furukawa, O. K. Yaghi, N. He, H. Hayashi, Y. Houndonougbo, M. Asta, B. B. Laird, and O. M. Yaghi, J. AM. CHEM. SOC. 132, 11006-11008 (2010)
[2] M. Dion, H. Rydberg, E. Schroder, D. C. Langreth, and B. I. Lundqvist, Phys. Rev. Let. 92, 246401 (2004)

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