Abstract Submitted
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van der Waals Density Functional Studies of Gas Binding and Transport in Zeolitic Imidazolate Frameworks[1] KEITH RAY, Department of Physics, University of California, Berkeley, DAVID OLMSTED, Department of Materials Science and Engineering, University of California, Berkeley, NING HE, Department of Chemistry, University of Kansas, YAO HOUNDONOUGBO, Department of Chemistry and biochemistry, Eastern Washington University, BRIAN LAIRD, Department of Chemistry, University of Kansas, MARK ASTA, Department of Materials Science and Engineering, University of California, Berkeley — Gas adsorption selectivity and transport barriers in a series of Zeolitic Imidazolate Frameworks (ZIFs) are calculated with the van der Waals density functional [1]. In these microporous materials, promising for natural gas upgrading applications, CO2 molecules are found to preferentially adsorb [2] when compared with CH4 depending on the ZIF chemical functionalization. The role of the interaction between the CO2 quadrupole and the host framework, as well as the significant dispersion contribution to both CO2 and CH4 binding are discussed. Diffusion barriers are calculated with the nudged elastic band method (NEB) and results are found to depend on the inclusion of the van der Waals energy.

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