Abstract Submitted
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Analyzing the frequency shift of physi-adsorbed CO2 in metal organic framework materials[1] YANPENG YAO, Rutgers, The state university of New Jersey, NOUR NIJEM, University of Texas at Dallas, JING LI, Rutgers, The state university of New Jersey, YVES CHABAL, University of Texas at Dallas, DAVID LANGRETH, Rutgers, The state university of New Jersey, TIMO THONHAUSER, Wake Forest University — Combining first-principles density functional theory simulations with IR and Raman experiments, we determine the frequency shift of vibrational modes of CO_2 when physi-adsorbed in the iso-structural metal organic framework materials Mg-MOF74 and Zn-MOF74. Surprisingly, we find that the resulting change in shift is rather different for these two systems and we elucidate possible reasons. We explicitly consider three factors responsible for the frequency shift through physi-absorption, namely (i) the change in the molecule length, (ii) the asymmetric distortion of the CO_2 molecule, and (iii) the direct influence of the metal center. The influence of each factor is evaluated separately through different geometry considerations, providing a fundamental understanding of the frequency shifts observed experimentally.

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