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The DeNO$_x$ process and NO$_2$ adsorption in MOF74[1] S. ZULUAGA, T. THONHAUSER, Wake Forest University, K. TAN, Y. CHABAL, University of Texas Dallas — Due to the harmful character of NO_2 and its slow decomposition rate, the use of catalytic materials for its removal (DeNO$_x$ process) has attracted a lot of attention. The high porosity and highly reactive uncoordinated metal centers of MOF74 have led us to investigate the use of Mg- and Zn-MOF74 as materials for trapping NO_2 with resistance to poisoning by SO_2. In this combined theoretical and experimental study, we investigate the interaction between the unsaturated metal centers of the MOF and the NO_2 guest molecules. For our theoretical modeling we use ab initio calculations at the DFT level, utilizing vdW-DF to capture the significant van der Waals component of the interaction between NO_2 and the MOF. We present detailed first-principle results concerning the adsorption energies and geometries, as well as vibration frequencies of the NO_2 molecule adsorbed in the MOF. Our experimental efforts (IR and Raman spectroscopy) have shown a blue shift to 1684 cm^{-1} in the vibration stretching mode of the NO_2 upon adsorption and a thermal stability up to 150°C. Our first-principle calculations and experimental results show a remarkable agreement, allowing us to give a complete picture of the adsorption of NO_2 molecules in the MOF74 structure.

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