

Abstract Submitted  
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**Understanding H<sub>2</sub>-H<sub>2</sub> interactions in Metal Organic Frameworks (MOFs) with unsaturated metal centers<sup>1</sup>** NOUR NIJEM, JEAN F. VEYAN, Univeristy of Texas at Dallas, LINGZHU KONG, YONGGANG ZHAO, JING LI, DAVID LANGRETH, Rutgers University, YVES J. CHABAL, Univeristy of Texas at Dallas — Unsaturated Metal Organic Frameworks (MOFs) are particularly interesting due to their high H<sub>2</sub> uptakes with relatively large isosteric heats of adsorption ( $Q_{st} > 8$  kJ/mol). This work explores H<sub>2</sub>-H<sub>2</sub> interactions between adsorbed H<sub>2</sub> at the different sites in MOF-74 (M<sub>2</sub>(dhtp), dhtp=2,5-dihydroxyterephthalate) and combines IR spectroscopy with vdW-DFT calculations. The adsorption sites in MOF-74 are from highest to lowest binding energies the metal, oxygen, benzene and pore-center sites. The frequency of adsorbed H<sub>2</sub> at the metal site suffers an additional  $\sim 30$  cm<sup>-1</sup> red shift (for Mg and Zn) and  $\sim 84$  cm<sup>-1</sup> (for Co) when the neighboring oxygen site is occupied. The dipole moment of adsorbed H<sub>2</sub> is also affected. These interactions extend to the benzene sites for MOF-74-Co. A decrease in dipole moment of H<sub>2</sub> adsorbed at the metal site is observed with the partial occupation of the benzene sites. However, the complete occupation of the benzene sites induces an additional  $\sim 10$  cm<sup>-1</sup> red shift.

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