Experimental and theoretical study on hydrogen interaction with unsaturated Metal Organic Frameworks\textsuperscript{1} NOUR NIJEM, JEAN FRANÇOIS VEYAN, University of Texas at Dallas, YONGGANG ZHAO, LINGZHU KONG, JING LI, DAVID C. LANGRETH, Rutgers University, YVES J. CHABAL, University of Texas at Dallas — Infrared absorption spectroscopy (IRAS) is useful to study the interaction of $\text{H}_2$ molecules inside various materials, since the frequency of its internal stretch mode depends on the adsorption site. Unsaturated Metal Organic Frameworks (MOFs) are particularly interesting due to their high $\text{H}_2$ uptakes with relatively large isosteric heats of adsorption ($Q_{st} > 8 \text{ kJ/mol}$). Our study focuses on $\text{H}_2$ in $\text{M}_2(\text{dhtp})$, dhtp=2,5-dihydroxyterephthalate (M= Zn, Ni, Co, Mg) and combines temperature-dependent IRAS measurements and vdW-DF calculations. Results show that the $\text{H}_2$ stretch frequencies are very sensitive to the chemical environment, with no correlation between binding energies and frequency shifts, as previously observed for saturated MOFs.\textsuperscript{2} Moreover, the $\text{H}_2$ stretch vibration closest to the metal site exhibits a strong shift from -30 cm\textsuperscript{-1} to -68 cm\textsuperscript{-1} upon population of neighboring sites (e.g. “oxygen” site).

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