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Experimental and theoretical study on hydrogen interaction with unsaturated Metal Organic Frameworks[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 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 H_2 uptakes with relatively large isosteric heats of adsorption (Q_{st} >8 kJ/mol). Our study focuses on H_2 in M_2(dhtp), dhtp=2,5-dihydroxyterephthalate (M= Zn, Ni, Co, Mg) and combines temperature-dependent IRAS measurements and vdW-DF calculations. Results show that the 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.[2] Moreover, the H_2 stretch vibration closest to the metal site exhibits a strong shift from -30 cm^{-1} to -68 cm^{-1} upon population of neighboring sites (e.g. "oxygen" site).

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[2]N. Nijem *et al.* submitted to J.A.C.S 2009

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