MOLECULAR HYDROGEN ADSORPTION IN METAL-ORGANIC FRAMEWORKS

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There is presently much interest in studying hydrogen storage materials for fuel cell applications. A promising class of physisorbents for this purpose is metal-organic frameworks, which consist of metal ions bridged by rigid organic molecules that assemble as highly porous molecular "scaffolds". We will report on a novel application of diffuse reflectance IR spectroscopy to probe the ro-vibrational modes of molecular hydrogen adsorbed within these materials. Experiments with H_2, HD, and D_2 illustrate the importance of quantum mechanical considerations and the necessity for rotational translational coupling models. Data reveal the propensity of exposed metals sites to produce some of the largest recorded interaction energies with adsorbed hydrogen. This leads to large frequency redshifts in the H_2 vibrational mode (65 - 130 cm^{-1}) along with a dramatic increase in the overtone intensity. The magnitude of the effect is shown to follow the Irving-Williams sequence in which the frequency shift for H_2 bound to $Ni^{2+} > Co^{2+} > Zn^{2+}$.