A theoretical and experimental study of hydrogen storage in metal organic framework materials. VALENTINO R. COOPER, JEONG YONG LEE, JING LI, YVES CHABAL, DAVID C. LANGRETH, Rutgers University — Metal-organic framework (MOF) materials, assembled by linking metal ions or clusters through molecular bridges, have been shown to be good candidates for H$_2$ storage. We have been successful in fabricating and characterizing MOFs with increased H$_2$ uptake$^1$, though still too low for commercial applications. Here we present a coordinated theoretical-experimental effort to understand the mechanism of H$_2$ adsorption in true MOF materials. Using the completely ab initio van der Waals density functional (vdW-DF)$^{2,3}$ we simulate the interactions of H$_2$ within Zn$_2$(bdc)$_2$(ted). We demonstrate that modeling the entire MOF structure can result in different H$_2$ adsorption geometries, binding energies and vibrational frequencies than observed in calculations on fragments of the MOF. Combining these results with experimental IR vibrational frequency studies may provide insights into modifying MOF structure and composition for enhanced H$_2$ uptake.