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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.

[1]J. Y. Lee et al. Adv. Func. Mater., **17**, 1255 (2007)
[2]M. Dion et al. Phys. Rev. Lett., **92**, 246401 (2004)
[3]T. Thonhauser et al. Phys. Rev. B, **76**, 125112 (2007)

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