

Abstract Submitted
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Enhanced H₂ adsorption in metal-organic frameworks with open metal sites: Binding mechanism and strong dependence on metal ions¹

WEI ZHOU, HUI WU, NIST and Univ. of Maryland, TANER YILDIRIM, NIST and University of Pennsylvania — Metal-organic frameworks (MOFs) with open metal sites exhibit much stronger H₂ binding strength than classical MOFs, due to the direct interaction between H₂ and the coordinately unsaturated metal ions. [1] Here we will present a systematic study of the H₂ adsorption on a series of isostructural MOFs, M₂(dhtp) with open metals M = Mg, Mn, Co, Ni, Zn. The experimental, initial isosteric heats of adsorption for H₂ (Q_{st}) of these MOFs range from 8.5 to 12.9 KJ/mol, with increasing Q_{st} in the following order: Zn, Mn, Mg, Co, and Ni.[2] The H₂ binding energies derived from first-principles calculation follow the same trend as the experimental observation on Q_{st} , confirming the electrostatic Coulomb attraction between the H₂ and the open metals being the major interaction. We also found a strong correlation between the metal ion radius, the M-H₂ distance and the H₂ binding strength, which provides a viable, empirical method to predict the relative H₂ binding strength of different open metals. [1] J. Phys. Chem. C, 112, 8132 (2008). [2] J. Am. Chem. Soc., 130, 15268 (2008).

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