

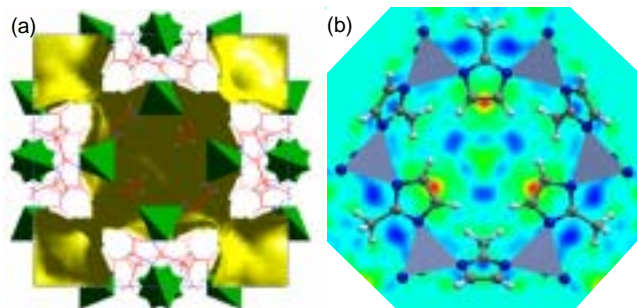
Engineered Nano-Materials for High Capacity Hydrogen Storage

T. Yildirim^{1,2}

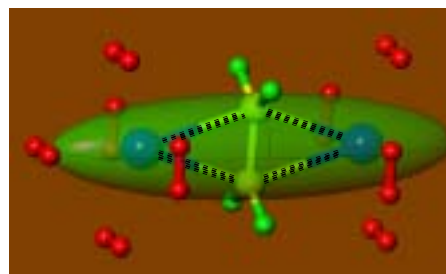
¹National Institute of Standards and Technology, NCNR, Gaithersburg, MD 20899

²Department of Materials Science and Eng., University of Pennsylvania,
Philadelphia, PA 19104

Developing safe, cost-effective, and practical means of storing hydrogen is crucial for the advancement of hydrogen and fuel-cell technologies. The current state-of-the-art is at an impasse in providing any materials that meet a storage capacity of 6wt% or more required for practical applications. The main obstacles in hydrogen storage are slow kinetics, poor reversibility and high dehydrogenation temperatures for the chemical hydrides, and very low desorption temperatures/energies for the physisorption materials such as activated carbon. In this talk, we first discuss several neutron experiments for hydrogen absorption properties of several novel high-surface nano-porous materials such as metal-organic-frameworks (MOFs) and zealic imidazolate frameworks (ZIFs). Even though these new materials have large surface area to absorb up to 10 wt% hydrogen molecules at low temperature, the interaction is weak and therefore at room temperature there is no absorption. In the second part of the talk, we will propose a new “nano-guest host concept” to increase the H₂ binding energy in these light-weight high-surface area materials such as MOFs and ZIFs. From accurate quantum mechanical calculations, we show that light transition metals (TM) such as a Ti-atom affixed to several nanostructures such as nanotubes/C₆₀ and small organic molecules (C₂H₄) strongly bind up to five hydrogen molecules. The first H₂ adsorption is dissociative with ~0.25 eV energy barrier while other adsorptions are molecular with significantly elongated H-H bonds. The metal-hydrogen interaction is found to be very unique, lying between chemi and physisorption, with a binding energy of 0.4 eV compatible with room temperature desorption and absorption. Simulations at high temperature indicate that such hybrid systems of transition metals affixed to nanostructures are quite stable and exhibit associative desorption upon heating, a requirement for reversible storage. These results not only advance our fundamental understanding of dissociative adsorption of hydrogen on transition metals in nano-structures but also suggest new routes to better storage and catalyst materials.



(a) ZIF8 host lattice from neutron powder diffraction along with the available free space (pore structure) for H₂ occupation (b) A real-space Fourier-difference scattering-length density superimposed with 6-ring pore aperture of the ZIF8 structure, indicating the location of the first absorption sites (red-yellow regions). *J. Am. Chem. Soc.*; **2007**; *129*(17) pp 5314 - 5315



Results of modeling studies indicate that attaching titanium atoms (blue) to the ends of an ethylene molecule (yellow-green) will result in a capsule-shaped complex that absorbs 10 hydrogen molecules (red), (14wt% capacity). *Phys. Rev. Lett.* 97, 226102 (2006)