

Materials Science and Technology Division

Materials Theory Seminar

“From fundamental understanding to predicting new nanomaterials for high capacity hydrogen storage and fuel cell technologies”

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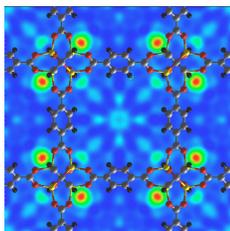
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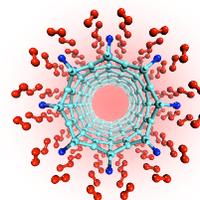
Abstract:

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 metal-organic frameworks (MOF). Recently we have proposed a novel concept to overcome these obstacles. From accurate quantum mechanical calculations, we show that light transition metals (TM) such as a Ti-atom affixed to several nanostructures such as nanotubes/ C_{60} and small organic molecules (C_2H_4) strongly bind up to five hydrogen molecules. The first H_2 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 nanostructures but also suggest new routes to better storage and catalyst materials. Finally, time permitted, we will discuss the possibility of dimerization, polymerization, and incorporation of the predicted TM-nanostructures in nanoporous materials such as MOF to improve the life-cycle and kinetics of the predicted storage materials.

Host: David Singh



Neutron scattering image of MOF, showing the absorption sites for H_2 (red-green circles.)



Ti (blue) decorated (8,0) carbon nanotube (light blue) binds many H_2 (red) molecules.