

## Storage of Molecular Hydrogen in Carbon Based Systems

Sa Li and Puru Jena

*Department of Physics, Virginia Commonwealth University,  
Richmond, VA 23284, USA*

The early promise of nanoscale carbon (activated carbon, single-wall nanotubes and fullerenes, nanofibers, and nanohorns) as hydrogen storage materials has not materialized. It has been demonstrated that any reported capacity of higher than 1 wt% in carbon nanotubes is due to experimental error. Theoretical study also confirms that high hydrogen content in the pure carbon nanotubes cannot be achieved through physical sorption. Although recent theoretical research has shown that doping of transition metal atoms such as Sc and Ti on carbon fullerenes and nanotubes may fundamentally change the nature of hydrogen bonding and lead to materials with hydrogen gravimetric density of up to 8 wt %, later calculations demonstrated that transition metal atoms coated on these surfaces will cluster. This in turn would not only affect the nature of hydrogen bonding but also the amount of stored hydrogen. The clustering of transition metal atoms also has been shown to play an adverse role in transition metal doped polymers.

We will discuss two different carbon based systems where hydrogen can be stored molecularly to meet the requirements of the transportation industry. One such system is Li doped *cis*-polyacetylene while the other is nano-porous carbon. Using density functional theory we show that Li atoms doped in *cis*-polyacetylene, similar to Li doped C<sub>60</sub>, will not coalesce and can bind hydrogen in molecular form with large gravimetric density. However, the binding of hydrogen is weak and cryogenic temperatures are needed for hydrogen sorption. Fortunately, modifying the chemistry of the inner pores of graphite provides certain advantages for hydrogen storage. We show that each Ti atom doped in a graphene pore (porous carbon) can bind up to four H<sub>2</sub> molecules much the same way it does when supported on a C<sub>60</sub> fullerene or carbon nanotube. More importantly, the Ti atoms do not cluster inside the pore and hence can retain their individual hydrogen storing capability.

The calculations also reveal that the nano-porous carbon is magnetic with or without Ti doping, but magnetism disappears when the pores are fully saturated with hydrogen. The observation of magnetic porous carbon may have applications far beyond its ability to store hydrogen.