

## **Nanoengineering of Hybrid Carbon Nanotube-Metal Nanocluster Composite Materials for Hydrogen Storage**

### **Investigators**

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### **Summary of 2006 Research Progress:**

During the two and half years of research, we have developed detailed approaches to implement the framework of nanomaterial design, fabrication and characterization to optimize the catalyzed nanotube for hydrogen storage. Three experimental groups have worked together to develop diameter controlled CNTs and characterize the hydrogen interaction characteristics with CNTs.

(1) The modeling study has refined the results reported in 2005 Progress Report through a systematic study of hydrogen coverage patterns on nanotube surfaces and the kinetic pathways of molecular hydrogen interaction with nanotube surface with and without nitrogen dopants. Modeling study has initiated to explore hydrogen storage materials other than carbon nanotubes, and the hydrogenation of Li-nitride has been examined following a similar modeling method applied to hydrogen interaction with nanotube.

(2) On the controlled fabrication of single wall carbon nanotubes, further progress has been made toward a refined control of fabrication conditions leading to high-yield vertical growth SWNTs. The effects of hydrogen plasma on SWNTs have shown the potential long term reliability issues of using carbon nanotubes as hydrogen storage medium under repeated cycling of storage and discharge conditions. The experiment has shown that the SWNTs can be degraded into hydrocarbons through hydrocracking of C-C bonds with the nanotube leading to a loss of storage capacity. This finding further emphasizes the importance of controlled catalytic processes which can selectively work on H-H bond breaking or reformation during the adsorption or desorption of hydrogen molecules from nanotube surfaces.

(3) The X-ray spectroscopy study of hydrogen-Nanotube interaction has been extended to examine the role of promoters (e.g., K or 3d metals) on the atomic hydrogen binding to carbon nanotubes. The promoters are shown to increase the atomic hydrogen storage capacity from 65% to 90-100%, and these findings strongly indicate that the intrinsic nature of carbon nanotube – H chemical bonding is modified by the promoters. The spectroscopic data also indicate that the nature of CNT-H bonding is changed by the promoters.

(4) The kinetic process of hydrogen molecule adsorption on SWNTs is investigated with Pt and Pd catalysts added on nanotube samples. The systematic study of molecular hydrogen uptake in nanotube-catalyst sample shows a very small weight % storage

capacity of different samples used for the measurement. The morphology of the nanotube sample has been examined and correlated to the update capacity of nanotubes. The addition of Pt or Pd catalysts has shown a promising increase of update capacity of nanotube sample by factor of 2.8 to 4.4, but the weight % storage capacity is still less than 1 wt % for the tested nanotube samples.

In summary, out four research groups have systematically investigated material properties and kinetic processes of hydrogen interaction with carbon nanotubes and have elucidated many underlying mechanisms of nanotube-hydrogen interactions. The future plan is to further refine these experimental works to close the gap between the atomic hydrogen storage capacity and molecular hydrogen storage capacity through engineering of catalysts and promoters as well as improved control of nanotube sample preparations.