Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

First-Principles Study of Carbon Nanoframeworks Tailored for Hydrogen Storage[1] EUNJA KIM, PHILIPPE WECK, BALAKRISHNAN NADUVALATH, University of Nevada, Las Vegas, HANSONG CHENG, Air Products and Chemicals, Inc., BORIS YAKOBSON, Rice University — Based on first-principles calculations, we propose a novel class of 3-D materials consisting of small diameter single-walled carbon nanotubes (SWCNTs) functionalized by organic ligands as potential hydrogen storage media. Specifically, we have carried out density functional theory calculations to determine the stable structures and properties of nanoframeworks consisting of (5,0) and (3,3) SWCNTs constrained by phenyl spacers. Valence and conduction properties, as well as normal modes, of pristine nanotubes are found to change significantly upon functionalization, in a way that can serve as experimental diagnostics of the successful synthesis of the proposed framework structures. Ab initio molecular dynamics simulations indicate that such systems are thermodynamically stable for on-board hydrogen storage. In order to increase the hydrogen uptake in the interstitial cavity of such nanoframeworks, we are currently investigating the possibility of Li deposition on these nanostructures.

[1]This work was supported by DOE under Cooperative Agreement No. DE-FG36-05GO85028.

Eunja Kim
Dept. of Physics and Astronomy, Univ. of Nevada, Las Vegas

Date submitted: 04 Dec 2007 Electronic form version 1.4