Abstract Submitted
for the DFD07 Meeting of
The American Physical Society

Hydrogen Transport And Storage Inside Carbon Nanotubes In Presence Of Encapsulated Metal Ions. SOUMIK BANERJEE, ISHWAR PURI, Virginia Tech — We investigate the hydrogen storage potential of carbon nanotubes (CNTS) through fundamental molecular dynamics (MD) simulations. We suggest possible changes in the structure and conditions of CNTS that could enhance their storage capacity. Our parametric investigation involves the variation of crucial parameters that influence hydrogen storage in carbon nanostructures, i.e., (1) pressure; (2) temperature; and (3) metal particle encapsulation. Our MD simulation results suggest that increased pressure and low temperature improve hydrogen storage inside carbon nanotubes, which is intuitive. We also obtain a more novel result, i.e., that the presence of encapsulated metal ions inside CNTS is a vital factor that considerably modifies their adsorption characteristics, enhancing storage. In addition, we determine that an open-ended nanotube stores more hydrogen than a closed nanotube.

Soumik Banerjee
Virginia Tech

Date submitted: 14 Aug 2007 Electronic form version 1.4