

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Theoretical study of Hydrogen Storage in Nanotubes and Nanoscrolls. GEORGE FROUDAKIS, University of Crete — A combination of *ab-initio* and Molecular Dynamics methods is used for investigating the nature of atomic and molecular hydrogen interaction with C, SiC and BN Nanotubes and Nanoscrolls. The curvature of the tube wall together with the direction of the hydrogen approach is considered and evaluated. In addition the improvement of the storage capacity is tested under various conditions of doping, pressure and temperature.

George Froudakis
University of Crete

Date submitted: 25 Nov 2005

Electronic form version 1.4