Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Hydrogen adsorption and storage in porous single-wall carbon nanotubes[1] WALTER ORELLANA, Universidad Andres Bello — Efforts to increase the hydrogen capacity in carbon nanotubes (CNTs) point to find energetically favorable access to its inner space. Following this way, we investigate the incorporation of H_2 molecules inside CNTs through pores in their walls by density functional theory calculations and molecular dynamic simulations. The pores are constructed by multivacancies defects (nV) with n missing atoms. CNTs of 1.1 and 1.4 nm in diameter were considered. We find that 16V has the limit size where the defect reconstruction is unlikely, preserving the unsaturated border. Under hydrogenation, the border is passivated by H_2 dissociative reactions, leaving an inert pore of about 6 Å in diameter (16V-H).We verify that the incorporation and release of H_2 molecules through this pore occur barrierless and its stability in contact with a gas of 32 and 64 H_2 molecules for exohedral and endohedral adsorption is preserved at high temperatures up to 600 K. Our results show that at room temperature, the endohedral adsorption energy is high enough for a reversible adsorption-desorption process, suggesting that porous CNTs, as produced for instance by electron irradiation under a H_2 atmosphere, could be an effective H_2 storage medium, allowing the access to the CNT inner space.

[1]Research supported by FONDECYT Grant 1090489 and PBCT ACT24/2006 (Chile).

Walter Orellana
Universidad Andres Bello

Date submitted: 07 Dec 2009 Electronic form version 1.4