Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

First principles study of hydrogen adsorption on carbon nanowires. ALEJANDRO TAPIA, LUIS AGUILERA, Facultad de Ingeniería, Universidad Autónoma de Yucatán, GABRIEL MURRIETA, Facultad de Matematicas, Universidad Autónoma de Yucatán, ROMEO DE COSS, Departamento de Física Aplicada, Cinvestav-Mérida — Recently has been reported a new type of one-dimensional carbon structures. Carbon nanowires formed by a linear carbon-atom chain inside an armchair (5,5) carbon nanotube has been observed using high-resolution transmission electron microscopy. In the present work we have studied the changes in the electronic structure of a carbon nanowires and (5,5) single-walled carbon nanotubes (SWCN) when a hydrogen atom is adsorbed. We used the Density Functional Theory and the calculations where performed by the pseudopotentials LCAO method (SIESTA code) and the Generalized Gradient Approximation (GGA) for the exchange-correlation potential. We have analyzed the changes in the atomic structure, density of states (LDOS), and the local orbital population. We found charge transfer from the nanotube to the linear chain and the hydrogen atom, the electronic character of the chain and nanotube sub-systems in chain@SWCN is the same that in the corresponding isolated systems, chain or SWCN. But the hydrogen adsorption produced changes in the atomic estructure and the electronic properties. This research was supported by PRIORI-UADY under Grant No. FING-05-004 and Consejo Nacional de Ciencia y Tecnología (Conacyt) under Grants No. 43830-F and 49985-J.

Alejandro Tapia
Facultad de Ingeniería, Universidad Autónoma de Yucatán

Date submitted: 05 Dec 2006 Electronic form version 1.4