

Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Ab-initio study of metallic and semi-conducting carbon nanotubes

. SUMIT SAXENA, TREVOR A. TYSON, New Jersey Institute of Technology - Newark — We present first principle calculations to study the metal – semiconductor transitions with pressure in zigzag nanotubes using the Local density approximation. Spin restricted calculations for metallic (9, 0) and semi-conducting (10, 0) carbon nanotubes were performed using the full potential projected augmented wave (PAW) method and using ultra-soft pseudo potentials. Our calculations show qualitative agreement to the reported experimental density of states (DOS) for the semi-conducting (10, 0) nanotubes [1]. The band gap between the valence and the conduction band using the pseudo potential formalism is found to be very close to that predicted using PAW approach. We observe that the DOS obtained using pseudo potentials reproduces the essential features however the full potential approach reproduces most of the features of the experimentally reported results. The details of the calculations and other results will be presented. [1] T. W. Odom, J. L. Huang, P. Kim, C. M. Lieber, J. Phys. Chem. B 104 2794 (2000)

Sumit Saxena
New Jersey Institute of Technology - Newark

Date submitted: 20 Nov 2006

Electronic form version 1.4