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 – semiconduc-
tor transitions with pressure in zigzag nanotubes using the Local density approx-
imation. 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 ap-
proach 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.