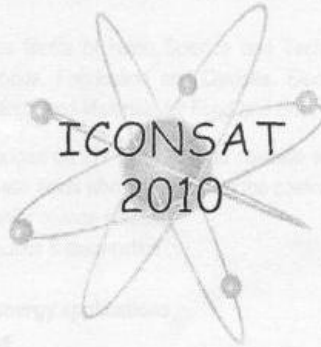


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### **Ab Initio Calculations of Electronic Structure and Optical Spectra of (13-0) Carbon Nanotube**

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Graphite structures, such as carbon nanoscrolls, fullerenes, carbon nanotubes, conjugated oligomers and polymers, represent hot research topics in current chemistry, physics and materials science. SWNTs present novel electronic, optical, and mechanical properties that can potentially be exploited in a wide range of applications such as energy storage and nanoelectronics [1]. The electronic structure and dielectric properties of the tubes are two key areas to study. We present a first principle calculation of the electronic structure, energy loss function, optical constants and dielectric function of single walled zigzag (13-0) carbon nanotube by using density functional theory method (DFT) [2]. For the expansion into the wave function, the full-potential linearized augmented plane-wave (FP-LAPW) method is used as implemented in the Wien2k code [3]. Also we have treated the exchange and correlation effects by the generalized gradient approximated (GGA) potential presented by Perdew and Wang [4,5]. It is found that zigzag (13-0) nanotube is semiconductor with the value of 0.6 eV band gap at  $\Gamma$  point. The optical spectra of (13-0) carbon nanotubes have been calculated for both electric field polarizations, parallel and perpendicular to the tube axis. The dielectric function was found highly anisotropic being much larger when the electric field is aligned along the tube axis than when it is aligned perpendicular to the tube axis. The calculated static dielectric constant for polarization parallel to the tube axis is 11 while for the polarization perpendicular to the tube axis it is obtained 4. Optical properties are calculated within the random phase approximation (RPA).

*Key words:* DFT, Carbon nanotube, Optical spectra, Dielectric function.

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