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Optical spectra of zigzag carbon nanotubes

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ABSTRACT

Density functional theory was used to calculate optical properties of (4, 0) and (8, 0) zigzag carbon nanotubes. The optical spectra such as dielectric function, optical conductivity and optical absorption coefficient were simulated for the x and the z polarization of the incident photons. The results showed that the dielectric functions of these zigzag nanotubes are anisotropic. The joint density of states indicated that the 1D singularities at the JDOS of CNTs (8, 0) with z-polarization are higher than for CNTs (4, 0). For CNTs (8, 0) with z-polarization, around about 2.8 eV, optical conductivity is equal to 2100 Ω^{-1} cm^{-1} refer to high intra-band transition. Results show that by increasing the diameter of nanotubes the static optical refractive index and dielectric constant of zigzag CNTs increase.

1. Introduction

Carbon nanotubes (CNTs) as a significant member of the fullerene-based materials are appropriate for many experimental and theoretical researches in different fields [1–3]. Single-walled carbon nanotubes can be supposed as a section of a rolled graphene sheet. Each nanotube has its own physical properties depend on the (n, m) indices called chirality [4,5]. Because the physical properties of nanotubes vary extremely with the chirality [6], CNTs show mixed characteristics lead to the some of the most promising applications limitation. Optical investigations have been very powerful tools to clarify the many interesting properties of SWNTs. In particular, optical absorption is directly correlated to the electronic sub- bands of SWNTs [7]. Optical band gaps of zigzag CNTs using golden Fermi's rule have been calculated in our previous research.

In the present study, the effect of chirality on optical properties of zigzag carbon nanotubes was investigated using first principles calculations which confirms calculated optical band gaps (see Ref. [8].) The optical spectra of carbon nanotubes have been calculated in various studies [9–11]. Several experimental and theoretical studies have considered (4, 0) [12–14] and (8, 0) [15,16] carbon nanotubes properties, but yet the simulated nanotubes in this paper had not been discussed comprehensively.

2. The simulation method

The calculations were performed on density functional theory framework as implemented in the WIEN2k code. Perdew-Burke- Ernzerhof generalized gradient approximation (GGA-PBE) was applied for the exchange correlation correction term [17–19]. The tetragonal unit cell with z-direction as the tube axis was chosen to simulate isolated nanotube model. The optimized input parameters are summarized in Table 1.

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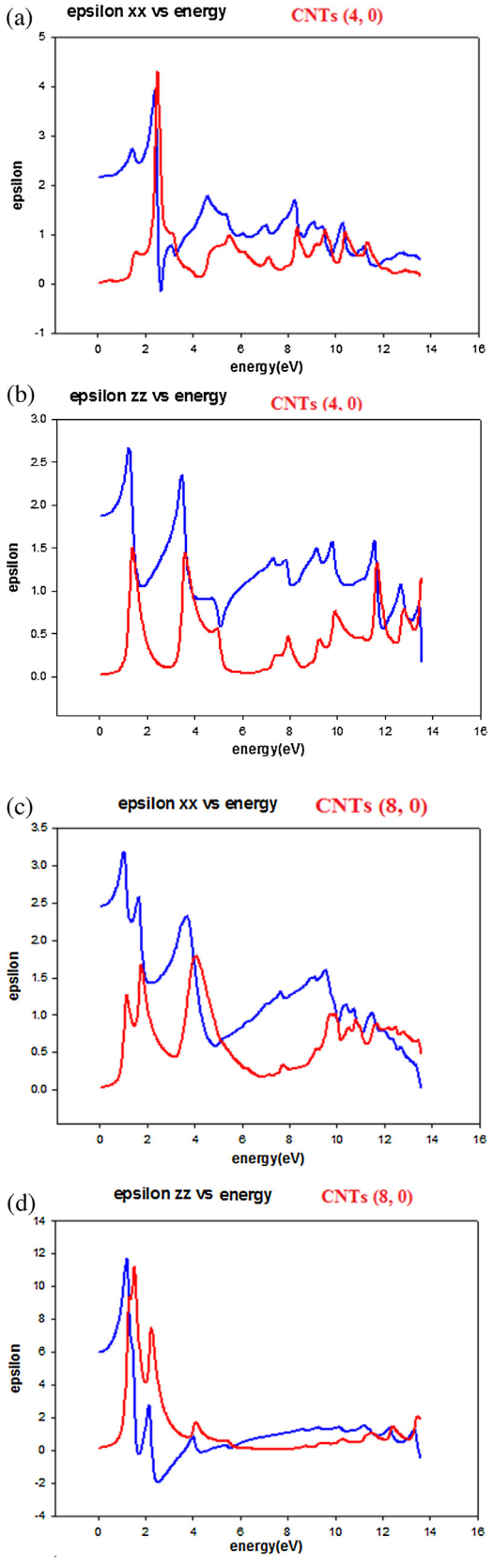

Fig. 1. Dielectric function of CNTs (4, 0) and CNTs (8, 0). The curves denote real part of dielectric function with higher and lower peaks.