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Original Research Article

Investigating the Role of Chirality on the Physical Properties of Boron Nitride and Carbon Nanotubes with Small Diameter

Nafiseh Gerivani

Islamic Azad university, Science and Research Branch of Tehran, Iran, ORCID: 0000-0001-5882-5465

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ABSTRACT

In this research, the electronic structure and optical properties such as dielectric function and optical constants of boron nitride and carbon nanotubes (0,5), (3,3) and (2,4), which all have a small diameter of about 4Å, it has been studied with the help of density functional theory and using first principles. The calculated band structure of these nanotubes shows that carbon nanotubes with a small diameter can have metallic or semiconducting properties depending on the chirality of the nanotube, while boron nitride nanotubes are semiconducting with a high gap regardless of the chirality. In addition, the results of optical calculations indicate that, unlike boron nitride nanotubes, the absorption spectrum of carbon nanotubes with a small diameter strongly depends on the chirality of the nanotube. The results of this research are reported in good agreement with theoretical and experimental data. The emergence of nanotechnology has caused a huge revolution in all aspects of human life, including electronics, medicine, the military, and space industries

Keywords: Chirality, Electronic structure, Carbon nanotube, Boron nitride, Density functional theor

***Corresponding Author E-mail:** *industrial.mr6@gmail.com*

Introduction

The emergence of nanotechnology has caused a huge revolution in all aspects of human life, including electronics, medicine, the military, and space industries [1]. Reducing the size and dimensions of electronic components in recent years has had tremendous consequences in terms of reducing the price and increasing the power of computers and electronic devices [2] in transferring information. Several nanometer materials have the potential to be used in micro-Nano systems, but nanotubes have particular advantages. Interesting properties of nanotubes include high conductivity [3], mechanical strength, low density, etc.

The high stability has caused them to receive a lot of attention from researchers in recent years. One of the most widely known and widely used nanotubes is single-walled nanotubes [4], which have been widely used in all aspects of human life due to their interesting electrical, optical, mechanical [5], and thermal properties. Due to the effects of high curvature, small-diameter nanotubes show interesting and unique electrical properties compared to larger nanotubes [6].

Therefore, a complete understanding of the microscopic properties of these nanotubes is important [7]. All possible forms of single-walled nanotubes, which include three zigzag groups (0, n), chiral (m,n), and armchair groups (n,n), can be obtained using chiral vectors (m,n). Carbon nanotubes with a smaller diameter can have both metallic properties and semiconductor properties [8], whose degree of conductivity depends on their chiral vector [9]. The difference in the conductivity properties is related to their molecular structure [10], which leads to a different band and gap structure. While the nanotube Boron nitrides are stable at room temperature, independent of nanotube chirality.

Semiconductor nanotubes are high-gap and therefore widely used in the nanoelectronics industry. The structural and vibrational properties of boron nitride nanotubes with a small radius have been investigated by the functional theory method. In this method, with preliminary calculations, they showed that the zigzag nanotube (0.5) is the smallest stable boron nitride nanotube. They have also calculated the frequency of vibration modes and phonon scattering for boron nitride nanotubes. In this article, the electronic and optical properties of boron nitride nanotubes with a small diameter have been calculated by the density functional theory method, and the effect of chirality on the physical properties of these nanotubes has been investigated [11].

Calculation method

The calculations of this article using the first principles and with the generalized gradient approximation (GGA) by the full potential method of linearly amplified plane waves (LAPW-FP) in the framework of DFT density functional theory [7-8] Hohenberg, Cohen sham with Wien2k software To achieve proper accuracy in the calculations and to minimize the total energy [12], we have used the number of 100 K points in the first Brillouin zone. Because in the Wien2K code, the primary cell must be a single cell.

defined in three dimensions, here the primary cell for all the nanotubes investigated in this research is considered as a tetragonal primary cell [13]. Of course, it should be noted that the periodicity of the nanotubes is along the x-axis. By optimizing the volume, we found that about 8 angstroms of moles in the line axes perpendicular to the nanotube are necessary to prevent innertube interaction [14]. An example of the primary cell and also the zigzag boron nitride nanotube supercell (5 and 0) is shown in Figure 1.

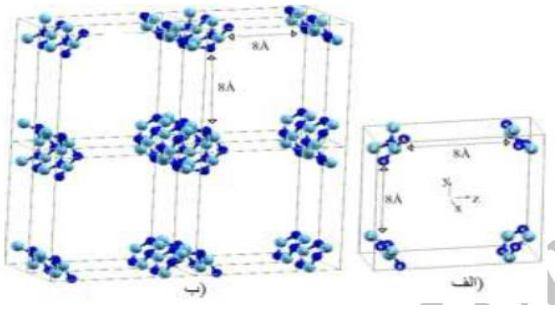

Figure 1. An example of the primary cell and also the zigzag boron nitride nanotube supercell (0,5)

Discussion and results

Electronic structure

The band structure of single-walled carbon nanotubes with a diameter of about 4Å is shown in Figure 2. According to Figure 1, the nanotubes studied in this study alternate along the x-axis. Depending on the chirality of the nanotube, small-diameter carbon nanotubes may exhibit metallic or semiconducting properties. A nanotube with a gap of 0/24eV has metallic properties, while a nanotube with a gap of 0,5 and 3,3 has semiconducting properties. For all types of single-walled carbon nanotubes, we calculated the X-point and the energy gap of about 1.2 eV.

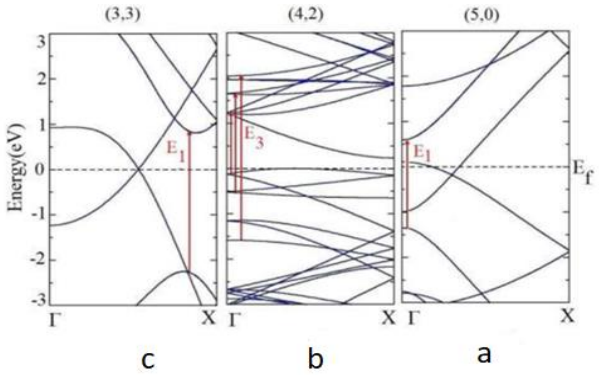

Figure 2. Calculated band structure for carbon nanotubes with a small diameter of about 4Å a): (5,0), b): (4,2) c): (3,3)

Calculations show that zigzag nanotubes with chirality multiples of three are semiconductors with a narrow gap of less than 0/1eV, whereas the model relies on curvature effects. In nanotubes with small diameter, the effects of curvature are more and as a result, it leads to more hybridization between σ *and* π orbitals and changes the band structure [15]. In Figure 2, the arrows indicate the optical transitions between the occupied capacitance band states and the empty conduction band states. As a result of these transitions, peaks appear in the imaginary part of the dielectric function, as shown in Figure 5. In Figure 3, you can see band structures calculated for boron nitride nanotubes with diameters such as 0,5 and 3,3. Calculated band structures [16] indicate that boron nitride nanotubes (0.5) and (3.3) are semiconductors with gap values of 1.7 and 4eV. Figure 4 shows the band structure calculated for boron nitride nanotubes with different chirality and larger diameter. Due to the thigh gap, boron nitride nanotubes are semiconductors independent of their chirality, unlike carbon nanotubes.

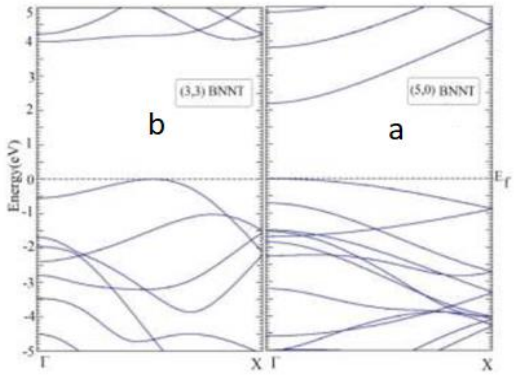

Figure 3. Calculated band structure for boron nitride nanotubes with a diameter of 4 Å a) :(0,5), b) :(3,3)

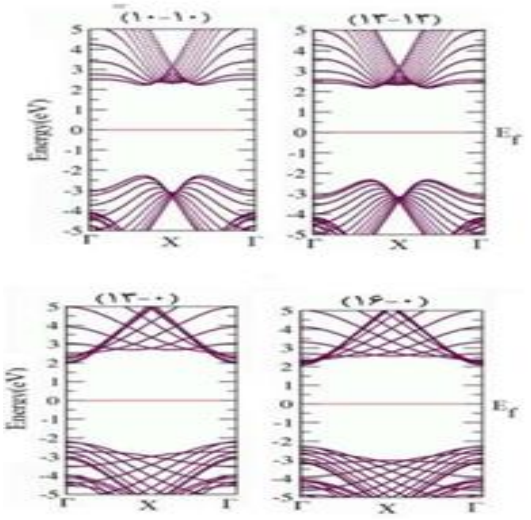

Figure 4. Calculated band structure for boron nitride nanotubes with different chirality and larger diameter.

Optical properties

Dielectric function expresses the response of a material to the electromagnetic field applied to it. In the last decade [18], optical spectroscopy has been used as the most important experimental tool to determine the band structure. The mixed dielectric tensor is calculated using the following equations: The real and imaginary parts of this tensor are obtained from the following relations:

$$\varepsilon'_{\alpha\beta}(\omega) = Re\varepsilon_{\alpha\beta}(\omega) = \delta_{\alpha\beta} + \frac{2}{\pi} P \int_0^{\infty} \frac{\omega IM\ \varepsilon_{\alpha\beta}(\omega')}{\omega'^2 - \omega^2} d\omega'$$

$$\varepsilon_{\alpha\beta}(\omega) = \varepsilon'_{\alpha\beta}(\omega) + i\varepsilon''_{\alpha\beta}(\omega)$$

$$\varepsilon''_{\alpha\beta}(\omega) = IM\varepsilon_{\alpha\beta}(\omega) = \frac{4\pi e^2}{m^2\omega^2}$$

$$\sum_{c,v} \int dk < c_k|p^{\alpha}|v_k >< v_k|p^{\beta}|c_k > \delta(\varepsilon_{ck} - \varepsilon_{vk} - \omega)$$

Where P represents the Cauchy part of the integral and $|c_k > and\ |v_k >$ represents the state of the electron in the capacity band and conduction band. The imaginary part of the dielectric function calculated in this research for single-walled (0,5), (3,3) and (2,4) carbon and boron nitride nanotubes in the case of an applied field parallel to the nanotube axis are shown in Figures 5 and 6, respectively.

it has been shown. The observed peaks in the imaginary part of the dielectric function indexed by Ei indicate the allowed optical transitions between bands. The first peak of the imaginary part of the dielectric function of the chair handle nanotube (3,3) has been observed at an energy of about 3eV, which is in good agreement with the previously reported experimental and theoretical results. This peak is mainly due to interbond optical transitions from the 1-HOMO level to LUMO or HOMO to 1+LUMO, because interbond transitions from the HOMO to LUMO level are symmetrically prohibited in armchair nanotubes [19, 20]. We have compared the optical gap calculated in this research for carbon nanotubes with a small diameter with the theoretical and experimental results reported by others in Table 1.

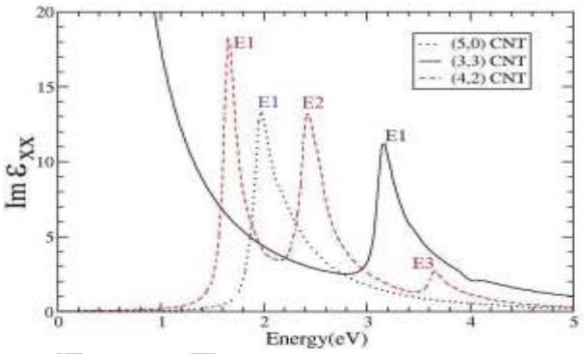

Figure 5. Imaginary part of the dielectric function for single-walled carbon nanotubes a): (5,0), b): (3,3) and c): (4,2) for an applied field parallel to the axis of the nanotube.

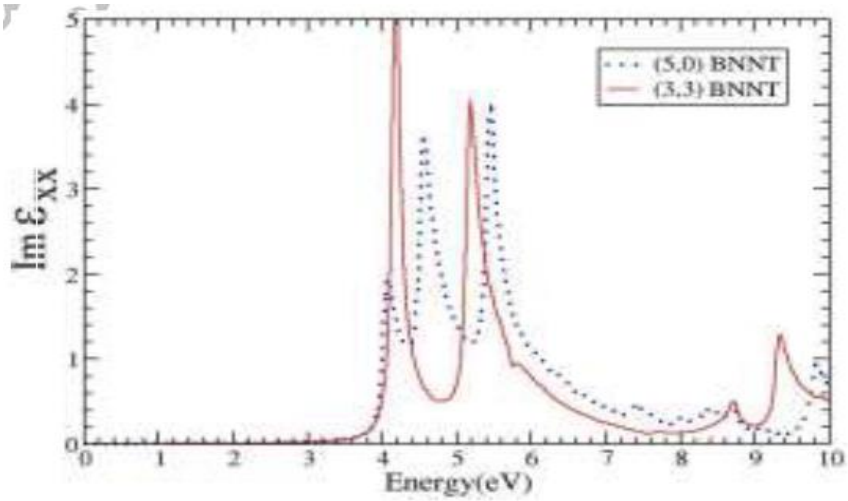

Figure 6. Imaginary part of the dielectric function for external nitride nanotubes (5,0) (dashed point) and (3,3) for an applied field parallel to the axis of the nanotube

The real part of the dielectric function for carbon nanotubes and for the applied field parallel to 4Å boron nitride with a diameter around the axis of the nanotube is shown in Figures 7 and 8, respectively. Table 2 shows the optical constants calculated by the method for carbon nanotubes and boron nitride studied by GGA in this research. According to the optical functions calculated (figures 5 to 8) and tables 1 and 2, it is concluded that unlike boron nitride nanotubes and carbon nanotubes with a large diameter, the absorption spectrum and optical constants of carbon nanotubes with a small diameter strongly depend on the chirality of the nanotube.

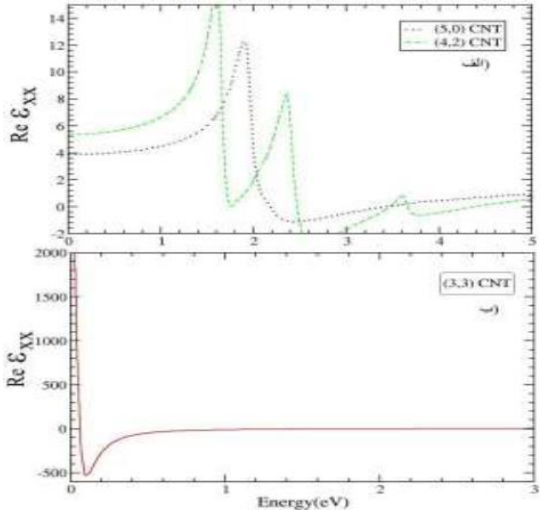

Figure 7. The real part of the dielectric function for single-walled carbon nanotubes a): (dashed point), (2,4) and b): (3,3) for an applied field parallel to the axis of the nanotube.

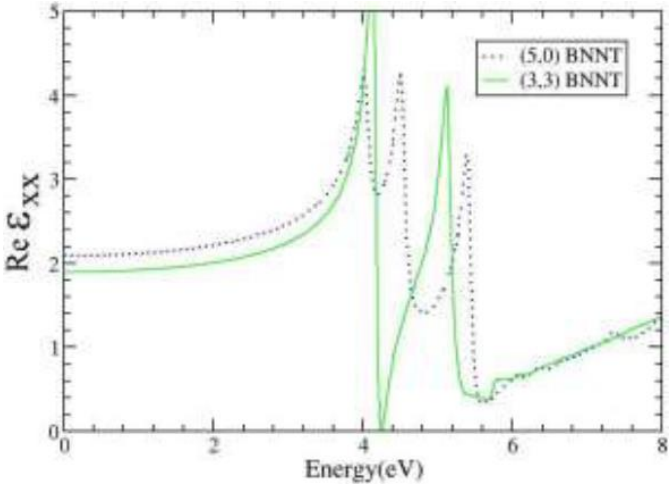

Figure 8. The real part of the dielectric function of boron nitride nanotubes (5,0) (dashed point) and (3,3) for an applied field parallel to the axis of the nanotube.

Table 1. Comparison of the first optical transition (optical gap) of carbon nanotubes with a diameter of 4Å calculated in this research with the results of others in terms of eV

(Å) electrical properties	(Å) Pitch nanotube	The length of the nanotube (Å)	experimental	BS	GW	LDA	LDA	These LDA calculations	Chirality (n,m)
Metal	4.07	2.46	3.1	3.17	3.26	2.83	2.8	3	3)،(3
Semiconductor	4.15	11.28	2.1	-	-	-	1.9	1.8	2)،(4
Metal	3.92	4.26	1.37	1.33	1.30	1.13	1.2	1.6	0)،(5

Table 2. Comparison of the band gap and calculated optical constants of carbon nanotubes and boron nitride with a diameter of about 4Å by GGA method

tape gaffe Eg(eV)	Dielectric constant $\varepsilon_0(X)$	Optical gaffe E11x(eV)	Chirality (n,m)
4	1.9	4.2	(3,3) boron nitride
1.7(2.1)	2.1(3.55)	4.1	(0.5) Boron Nitride
0	∞	3	(3،3) carbon
0	3.9	1.6	(5،0) carbon
0.24	5.4	1.8	(2،4) carbon

Conclusion

Optical properties such as dielectric function, optical constants, and also the band structure of carbon nanotubes and boron nitride with a diameter of 4 mm have been studied in this study. Kramers-Kronic transformations were used to calculate mixed optical properties. As a result of the results, carbon nanotubes with a small diameter may have metallic or semiconducting properties depending on their chirality, whereas boron nanotubes. In contrast, nanotubes. In contrast, semiconductors are dented because of their chirality.

According to our results, carbon nanotubes (5.0) and (3.3) have metallic properties, while carbon nanotube (4.2) is semiconducting with gaps of about 0.24eV at point X and 1.2eV at point G. GAF value is zero for the zigzag carbon nanotube (5,0) as a result of high curvature, but it is semiconducting according to the strong dependence model. The difference between Our results and the strong dependence theory is due to curvature effects. Since carbon nanotubes with small diameters have more curvature effects, they lead to more hybridization between σ and π orbitals, which changes the band structure.

The results show that unlike nanotubes Boron nitride absorption spectrum of carbon nanotubes with a small diameter strongly depends on the nanotube's chirality.

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