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Theoretical Investigation of Diameter Effects and Edge Configuration on the Optical Properties of Graphdiyne Nanotubes in the Presence of Electric Field

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Abstract

In this research, the structural, electronic and optical properties of the armchair (ant) and zigzag (znt) Graphdiyne nanotubes (GDY-NT) with different diameters were studied based on density functional theory (DFT). The computations were done using SIESTA code, based on linear combination of localized atomic orbitals (LCAO) method and the generalized gradient approximation (GGA). The results from the band structure analysis show that all these nanotubes are semiconductors with direct band gap at gamma point. The band gap of the nanotubes is clearly dependent on the nanotube diameter, and by increasing the nanotube diameter, the band gap is decreased. Optical properties such as dielectric function; absorption coefficient, optical conductivity and refractive index were examined and calculated for all samples. The results show that all these functions have an inverse relationship with the nanotube diameter and a direct relationship with the band gap. The effect of applying the external electric field with intensity of 0.1 V/Å, 0.2 V/Å in the direction of x-axis (perpendicular to the nanotube axis) on the structural and electronic features of these nanotubes has been studied and calculated.

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1. Introduction

Unlike natural structures of carbon that often have two stable allotropes of diamond and graphite, and sp^3 and sp^2 hybridized carbon atoms, respectively, a wide range of synthetic carbon allotropes have been synthesized or theoretically predicted. This has made the present day become known as the era of carbon allotropes [1]. As the most prominent and most notable achievements, the discovery of Fullerenes [2], carbon nanotubes [3], and Graphene [4-6] represents the prominent and novel types of zero-, one- and two-dimensional carbon structures that have the carbon structures with sp^2 hybridization. In addition, the tendency of carbon to form the three types of sp^1, sp^2 and sp^3 hybridization states allows for the creation of multiple combinations of carbon allotropes by linking the carbon atoms with different hybridizations [7-9].

One of the most interesting families of carbon allotropes introduced in recent years is the Graphyne family [8]. This car-

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bon allotrope has a flat structure with a one atom thick single-plate lattice that is made by replacing some $= C = C =$ bonds in Graphene with -C≡C- acetylene bonds. These structures have two non-equivalent types of carbon atoms: sp^2 hybridized carbon atoms with three identical bonds and sp hybridized carbon atoms with two identical bonds [10].

In Graphdiyne, a member of the Graphyne family, there are also two sp and sp^2 hybrids of carbon atom [11]. The sp^2 hybridized carbon atoms form a hexagonal ring, which are connected together by di-acetylene sp connections. Compared to Graphene, Graphdiyne has many interesting properties such as uniformly distributed holes, strong π bonding, controllable electronic features, lower density, high electrical conductivity excellent hardness and high temperature resistance that these properties are due to the sp and sp^2 hybrids and the natural holes in its structure [11].

These plane carbon lattices with high number of π bond, density lower than that of Graphene, and modifiable electronic properties are the promising materials in the nano-electronics industry. It is also believed that various forms of Graphyne with multiple functionalities can compete with the older carbon structures such as Fullerenes, carbon nanotubes or Graphene and respond positively to the increasing need for carbon nanostructures.

2. Computational Method

The atomic structure of nanotubes has been investigated by density functional theory (DFT) approach and using SIESTA computational code based on LCAO method and the GGA-PBE approximation for the exchange-correlation functional of e-e interaction [12-13].

Brillouin zone (BZ) division was done by Monkhorst–Pack method. The optimum number of k points selected for the armchair Graphdiyne nanotubes was $1 \times 1 \times 7$ and for the zigzag Graphdiyne nanotubes, it was $1 \times 1 \times 11$. In the computations, the optimal cutoff energy used for the armchair Graphdiyne nanotubes was 300 Ry and for the zigzag Graphdiyne nanotubes, it was 400 Ry. A large enough vacuum layer (10 Å and 12 Å for the armchair and zigzag nanotubes, respectively) is considered for all nanotubes to avoid interacting with adjacent structures. All these nanotubes are relaxed until the total atomic force value reaches less than 0.01eV/Å. The optimized lattice constant obtained for the armchair and zigzag nanotubes were 16.71Å and 9.46Å, The dimeter of znt2, znt3, znt4, ant2, ant3 and ant4 after relaxation is obtained equal to 10.25, 15.56, 20.81, 6.42, 9.08 and 12.04, respectively.

In order to perform the optical computations, the energy range in which the optical properties are investigated was selected from zero to 40eV. In the optical computations, the spin-orbit interaction is neglected because it will not have much impact on the results. In this section, one of the important parameters is the kind of the optical polarization. In all structures studied, the polarized light and its propagation along the x direction were considered. The optical properties such as the real part of the dielectric function, absorption coefficient, refractive

Table 1. The Optimized Bond Lengths of the znt and ant Graphdiyne Nanotubes after Relaxation

Optimized bonding length (Å)	Bonding type
1.40	$=C - C \equiv$
1.43	$=C = C =$
1.35	$= C - C \equiv$
1.24	$- C \equiv C - -$

index and reflection coefficient were calculated using the imaginary part of the dielectric function and the Kramers–Kronig relations [14].

In the final step, the efficacy of applying the electric field in the direction of x-axis, with the sizes of 0.1 V/Å, 0.2 V/Å on the structural and electronic features of the zigzag and armchair Graphdiyne nanotubes was studied.

3. Results and discussion

3.1. Investigating the Structural Properties

Similar to carbon nanotubes, Graphdiyne nanotubes are produced by rolling the Graphdiyne sheet (plate). Similar to carbon nanotubes, the denomination (n, m) can be used for Graphdiyne nanotubes. However, unlike carbon nanotubes, (n, n) represents the zigzag type and (n, 0) represents the armchair type. Nanotube Maker software was used to obtain the coordinates of points forming nanotubes [14]. In the study, the zigzag (2, 2), (3, 3), (4, 4) and armchair (2, 0), (3, 0), (4, 0) Graphdiyne nanotubes were investigated. Figures 1 and 2 show the structure of the znt and ant nanotubes examined after optimization, respectively. The bond lengths of nanotubes after the structural relaxation are presented in Table 1. The values obtained are in agreement with the results of other researchers [15]. The length of carbon-carbon bonds in the hexagonal ring and the di-acetylene bonds are not the same, indicating the existence of different hybrids in the carbon bonds of Graphdiyne nanotubes. This difference leads to more structural flexibility for Graphdiyne nanotubes compared to carbon nanotubes [16-17]. Another important difference between Graphdiyne nanotubes and carbon nanotubes is that GDY-NT have the uniformly distributed holes in their walls, which facilitates the electron transport in the nanotube wall and it is important for the applications such as hydrogen storage.

3.2. Electronic Properties of GDY-NT

The band structure of the znt and ant Graphdiyne nanotubes is shown in Figures 3 and 4, respectively. The Fermi energy was selected at the zero point. All these GDY-NT are semiconductors with the direct band gap at gamma point of the first BZ. The values of band gap and diameter of the zigzag and armchair nanotubes are presented in Table 2. Similar to carbon nanotubes, the diameter of Graphdiyne nanotubes can be obtained from the following relationship:

$$d = \frac{a}{p} \sqrt{n^2 + nm + m^2}$$
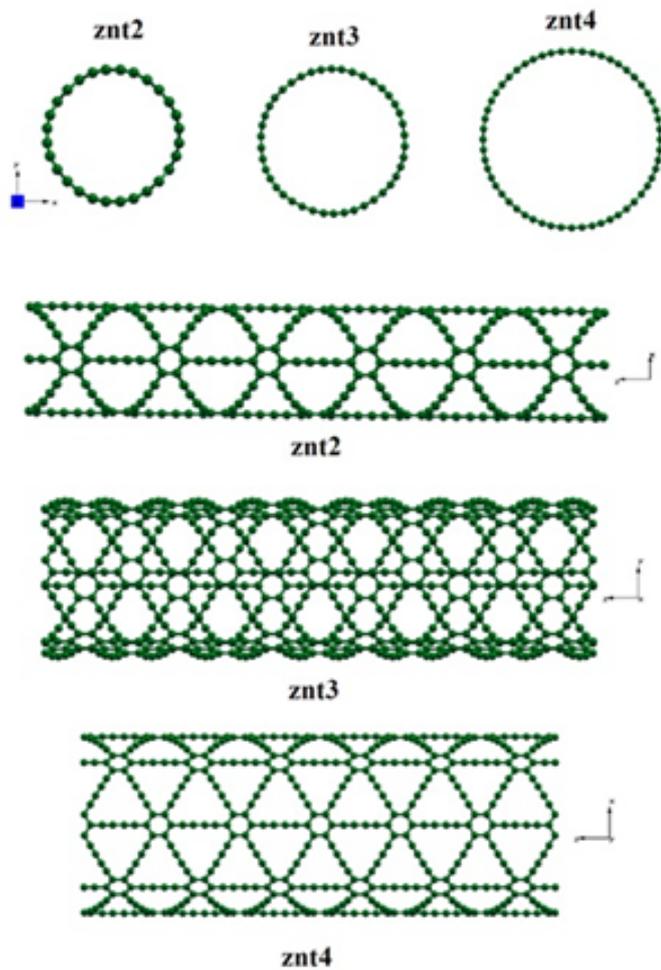
Figure 1. Structure of the Zigzag Graphdiyne Nanotubes after Relaxation
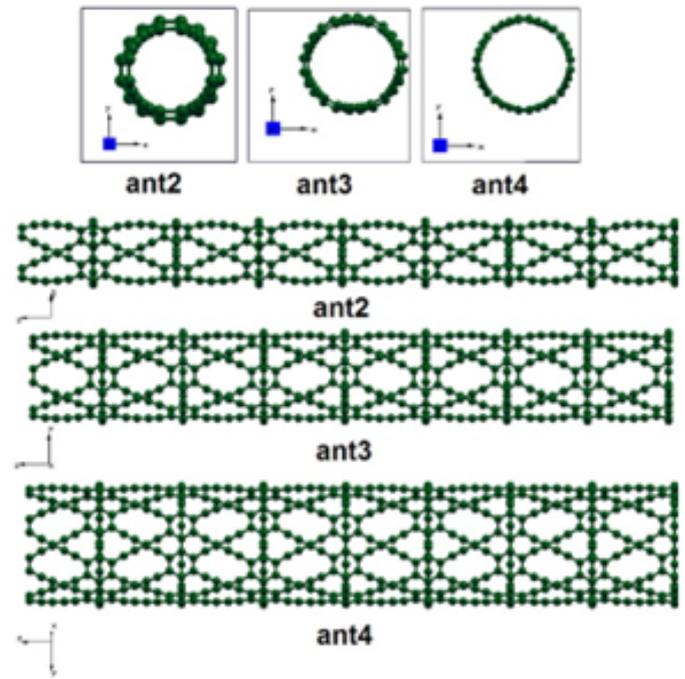
Figure 2. Structure of the Armchair Graphdiyne Nanotubes (Double wall) after Relaxation

Table 2. The Value of Band Gap and Diameter of the znt and ant Graphdiyne Nanotubes

Nano tube diameter (Å)	Band gap (eV)	Structure
10.25	0.65	znt2
15.56	0.55	znt3
20.81	0.50	znt4
6.42	0.95	ant2
9.08	0.65	ant3
12.04	0.55	ant4
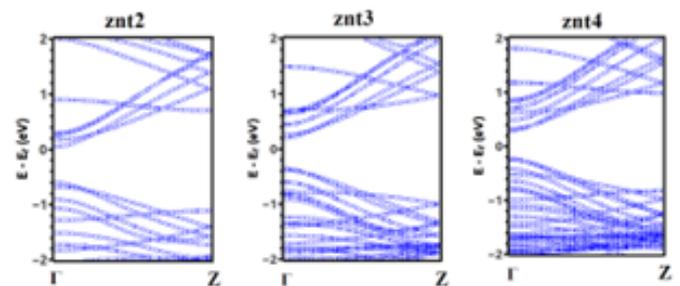
Figure 3. Band Structure of the znt Graphdiyne Nanotubes

that a is the lattice constant of GDY-NT [5].

As shown in these Figures, because of the quantum confinement effect, the band gap value of the znt and ant nanotubes is obviously dependent on the nanotube diameter, and decreases with increasing the nanotube diameter. In addition, the armchair nanotubes have a smaller diameter and the larger band gap than the zigzag nanotubes.

Figures 5 and 6 show the density of the total states (DOS) of the znt and ant Graphdiyne nanotubes, respectively. The DOS at Fermi energy is zero, which confirms the semiconducting behavior of GDY-NT. Examining the band structure and the DOS, we observe that as the diameter of the GDY-NT increases, the band gap decreases and the DOS increases.

3.3. Optical Properties of Nanotubes

3.3.1. Dielectric Function

The complex dielectric function describes the optical properties of solids. This function is used to describe the crystal response to electromagnetic fields, which depends on the band structure of crystal [18]. In Figures 7 and 8, the diagrams of the real and imaginary parts of the dielectric function of the Graphdiynenanotubes are plotted for the polarized incident light in the direction of x-axis (perpendicular to the axis of Graphdiynenanotubes), respectively. The imaginary part of the dielectric function partly reflects the actual transfers between occupied and unoccupied states. We also know that the interband transition is due to excitation at the absorption edges, and the intra-band transition is the result of volumetric plasmons (absorption by free electrons). Therefore, in diagram 7, the relatively high increase in energy values less than 5eV in the
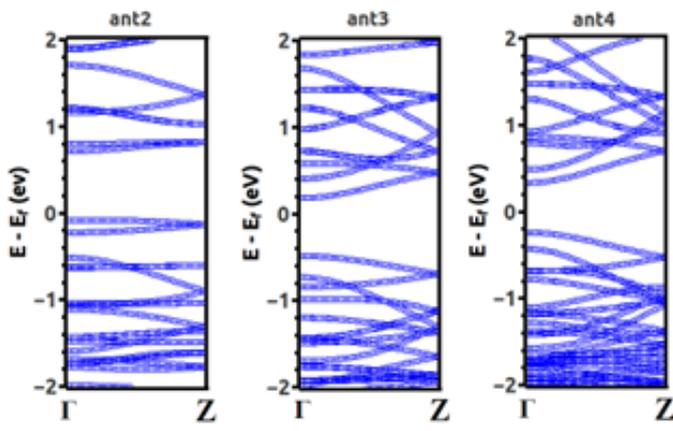
Figure 4. Band Structure of the Armchair Graphdiyne Nanotubes

Figure 5. DOS of the Zigzag GDY-NT

Figure 6. DOS of the Armchair GDY-NT
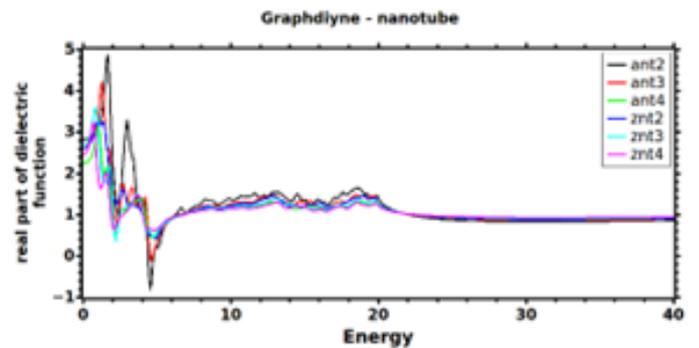
Figure 7. Real Part of the Dielectric Function of GraphdiyneNanotubes for the Polarized Light in the Direction of X-Axis

imaginary part of the dielectric function, as well as the almost constant behavior at energies above 30eV confirm these absorption approaches.

Comparison among different nanotubes with various diameters shows that the highest dielectric function intensity is related to AGDYNT (2, 0) nanotube which has the smallest diameter and the largest gap, and the lowest dielectric function intensity is related to ZGDYNT (4, 4) nanotube that has the largest diameter and the smallest gap. The results show that the dielectric function intensity is inversely related to the diameter of the nanotubes and there is a direct relationship between the dielectric function intensity and the band gap.

3.3.2. Optical Absorption

The absorption spectrum of GDY-NT with different diameters is illustrated in Figure 9. The Figure shows the permitted optical transitions of the electron between the empty states of the conduction band and the full states of the valence band. The threshold energy for transition in the absorption spectrum corresponds to the gap size in the band structure of Graphdiyne-nanotubes and it means that the electrons are excited and make a transient by receiving the least energy greater than the band gap value.

The comparison between different nanotubes with various diameters also shows that the highest absorption is related to
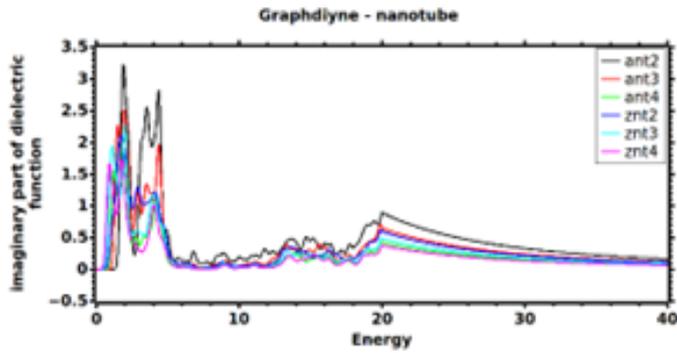
Figure 8. Imaginary Part of the Dielectric Function of GraphdiyneNanotubes for the Polarized Light in the Direction of X-Axis
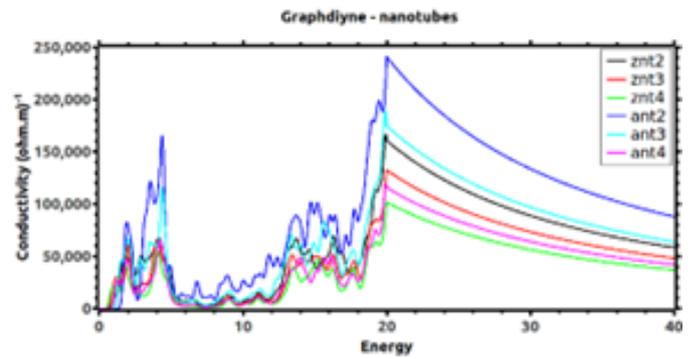
Figure 10. The Diagram of Optical Conductivity of GDY-NT with Different Diameters for the Polarized Light in the Direction of X-Axis
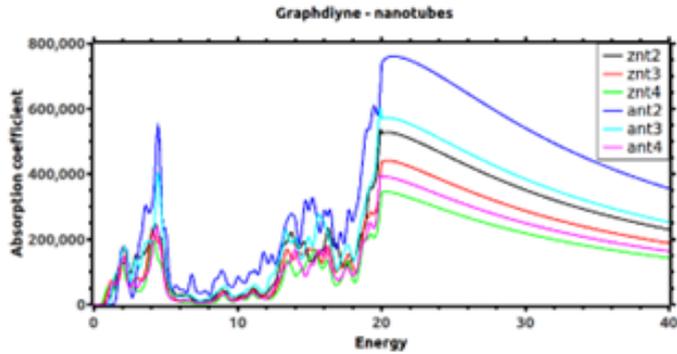
Figure 9. The Diagram of Absorption Spectra of GraphdiyneNanotubes with Different Diameters
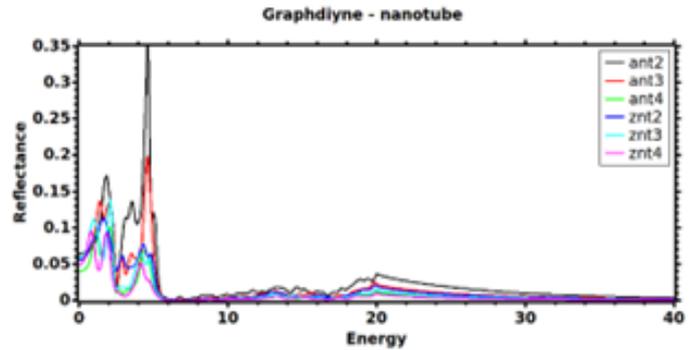
Figure 11. Reflection Diagram of GraphdiyneNanotubes with Different Diameters

AGDYNT (2, 0) nanotube which has the smallest diameter and largest gap, and the lowest absorption is related to ZGDYNT (4, 4) nanotube which has the largest diameter and the smallest gap. The results show that the optical absorption coefficient is inversely related to the diameter of the nanotubes and is directly related to the band gap.

3.3.3. Optical Conductivity

Figure 10 shows the changes of optical conductivity of Graphdiynenanotubes with different diameters compared to the incident photon energy. As can be seen, the diagram of optical conductivity is proportional to the imaginary part of the dielectric function. Generally, at the energies that present in the imaginary part of the peak dielectric function, these peaks are also seen in the real part of the optical conductivity. In this spectrum, the conductivity increases up to 20eV and then decreases, and at energies with the highest absorption, we have the optical conductivity maximum. The results show that the optical conductivity has an inverse relationship with the diameter of the nanotubes and a direct relationship with the band gap.

3.3.4. Reflection

The reflection diagram of GDY-NT with different diameters is plotted in Figure 11. According to this diagram, we find that the magnitude of the reflection is generally very small at the energies above 6eV. We also have the maximum reflection at the

energies where the highest absorption occurs. Here, a comparison of the reflection coefficient of the nanotubes with different diameters shows that the reflection coefficient is inversely related to the diameter of the nanotubes and directly related to the band gap.

3.3.5. Refractive Index

The value of the refractive index at zero energy is called the static refractive index, which is equal to the static dielectric constant. The static refractive index of the znt and ant Graphdiyne-nanotubes with different diameters is reported in Table 3. If, by increasing the frequency, the refractive index increases, this behavior is called the normal dispersion, which is the usual behavior of all transparent materials. In areas where the slope of the diagram of refractive index is negative, it is related to absorption. In this area, when passing through the material, longer - wavelength light breaks more than short - wavelength light, which this behavior is called the anomalous dispersion. The diagram of refractive index and extinction coefficient of GDY-NT with different diameters are shown in Figures 12 and 13, respectively. As you can see in these diagrams, the refractive index reaches its lowest value at the energies between 4eV and 6eV, so the reflection increases, which is consistent with Figure 13.

Table 3. Static Refractive Index of GraphdiyneNanotubes

ant2	ant3	ant4	znt2	znt3	znt4
1.68	1.64	1.5	1.62	1.64	1.57
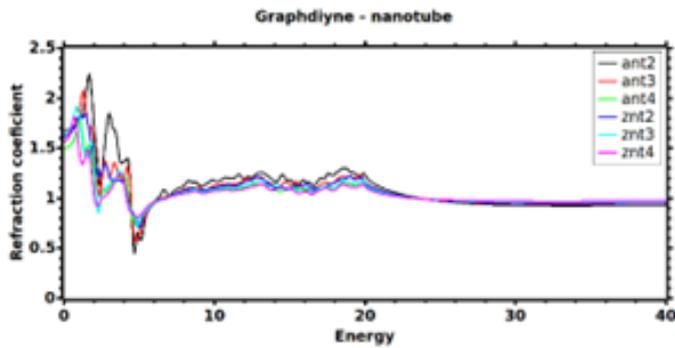
Figure 12. Diagram of Refractive Index of GDY-NT with Different Diameters
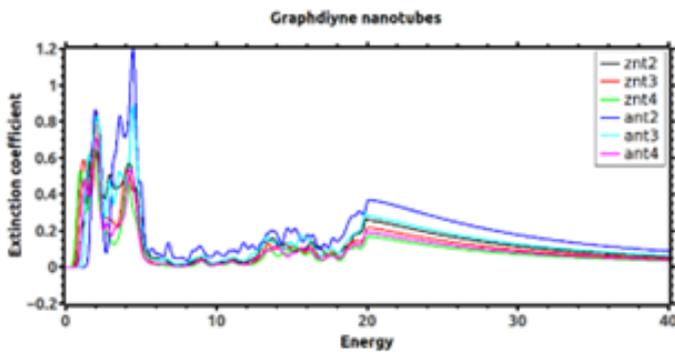
Figure 13. The Diagram of Extinction Coefficient of GDY-NT with Different Diameters

3.4. Effect of Applying the External Electric Field

In the final step, the electric field along the x-axis with the sizes of 0.1V/Å and 0. 2V/Å was applied to the znt and ant Graphdiynenanotubes with different diameters. The geometric structure and band structure of the Graphdiyne nanotubes were compared in the absence and presence of the external electric field.

The results show that by applying the electric field in the direction of the x-axis and with different sizes to the ant2 nanotube, its geometric structure and band structure is not changed (Figure 14). For the ant3 nanotubes, as shown in Figure 15, there is little change in the energy bands in the presence of the electric field of 0.1V/Å, and only slight shift (about 0.02 to 0.05eV) is seen in the energy bands. In addition, the size of the band gap is not changed. But by applying the electric field of 0.2V/Å, the band structure is completely changed and the size of the band gap increased (Figure 15). In addition, by increasing the external electric field, the diameter of ant3 nanotube is also increased.

Figure 16 shows the band structure of ant4 nanotubes in the presence and in the absence of the external electric field. In the presence of the electric field of 0.1V/Å, the size of band gap is not changed. But greater shift is seen in the energy bands com-
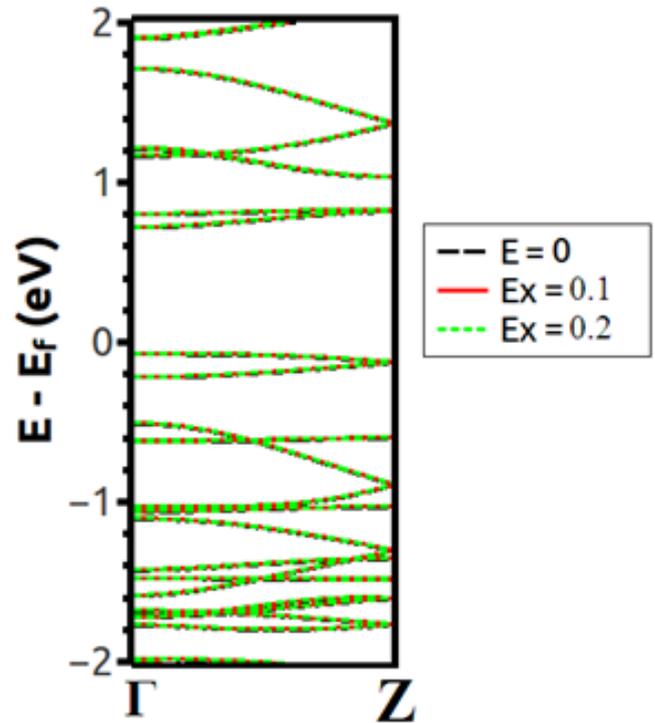
Figure 14. Comparison of the Band Structure of ant2 Nanotubes in the Absence (E=0) and Presence of Electric Field (E=0.1 and 0.2V/Å) along the X-Axis
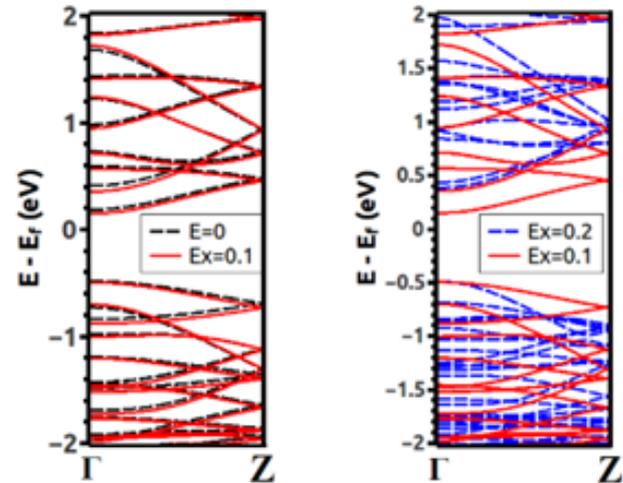
Figure 15. Comparison of the Band Structure of ant3 Nanotubes in the Absence (E=0) and Presence of Electric Field (E=0.1 and 0.2V/Å) along the X-Axis

pared to the ant3 nanotube (about 0.1eV). By applying the electric field of 0.2V/Å, the band structure is completely changed and the size of band gap increased. The diameter of ant4 nanotube is also increased by applying the electric field. The results are summarized in Table 4.

The band structure of znt2 nanotubes in the absence and presence of the external electric field is compared in Figure 17. As can be seen in the Figure, by applying the electric field of 0.1V/Å, there is little change in the energy bands. The size of the band gap and the nanotube diameter also show a slight

Table 4. The Size of Band Gap (E_g), Shift of Energy Bands and Diameter (d) of the Armchair Graphdiyne Nanotubes with Different Diameters in the Presence of the External Electric Field in the Direction of X-Axis and with the Sizes of 0.1V/Å and 0.2V/Å

Shift (eV)		d (Å)			E_g (eV)			structure
E=0.2	E=0.1	E=0.2	E=0.1	E=0	E=0.2	E=0.1	E=0	
0	0	5.8	5.8	5.8	0.78	0.78	0.78	ant2
				6.42[3,4]			0.95[3,4]	
Structure changed	0.02- 0.05	9.2	9.07	9.04	0.87	0.66	0.66	ant3
				9.08[3,4]			0.65[3,4]	
Structure changed	0.1	12.94	11.94	11.65	0.65	0.57	0.57	ant4
				12.04[3,4]			0.55[3,4]	
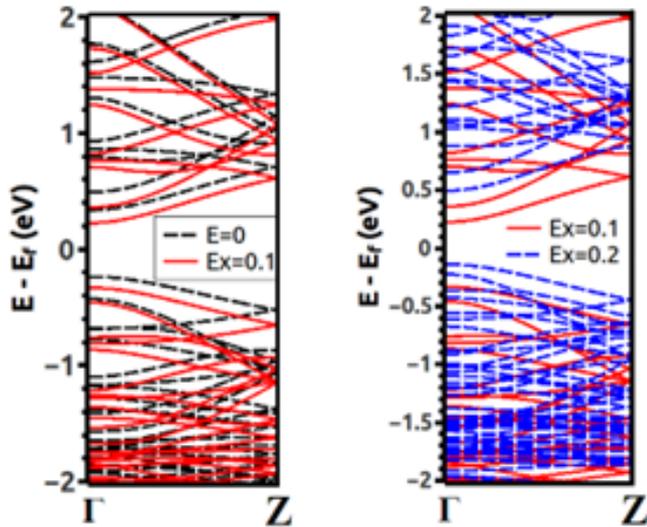
Figure 16. Comparison of the Band Structure of ant4 Nanotubes in the Absence (E=0) and Presence of Electric Field (E=0.1 and 0.2V/Å) along the X-Axis

Figure 17. Comparison of the Band Structure of znt2 Nanotubes in the absence (E=0) and presence (E=0.1 and 0.2V/Å) of the Electric Field along the X-Axis

decrease. As the external electric field intensity increases, the band structure is changed and the band gap is also decreased, but the nanotube diameter is slightly increased.

The band structure of znt3 nanotube in the presence and in the absence of the external electric field is plotted in Figure 18. Applying the electric field of 0.1V/Å, there is little change in the energy bands. The size of the band gap and the nanotube diameter also show a slight decrease. As the intensity of the external electric field increases, there is a slight shift in the band structure (0.04eV). The size of the band gap and the nanotube diameter is also slightly decreased.

In Figure 19, the band structure of znt4 nanotube is plotted in the absence and presence of the external electric field. By applying the electric field of 0.1V/Å, a shift of about 0.02eV is seen in the energy bands. The band gap value and the nanotube diameter also show a slight decrease. Applying the electric field of 0.2V/Å, the geometric structure and band structure of the nanotubes are completely changed. As shown in Figure 20, the shape of zn4 nanotube has become oval and the size of its band gap has decreased in the presence of E= 0.2V/Å. The results are summarized in Table 5.

Given that the electric field is applied perpendicular to the axis of nanotubes, the atoms in the wall of the nanotubes have the different potentials. The larger the nanotube diameter, the potential difference is also greater. Therefore, we expect that the geometric structure and band structure of nanotubes that are larger in diameter undergo more changes compared to nanotubes that are smaller in diameter, which this is consistent with the results obtained. The znt4 nanotube, which has the largest diameter among all nanotubes investigated, exhibits the most changes in the geometric structure and band structure [19-20].

No research was conducted to study the effect of applying the external electric field on GDY-NT for comparison. The results on other carbon nanostructures show that the effect of applying the external electric field on the armchair Graphdiynenano-ribbons with various widths is different. Small width does not change the size of band gap. In larger widths (N> 13), by increasing the electric field intensity, the size of band gap is decreased. By applying the electric field to the (10, 5) carbon nanotube in the direction of x-axis, the size of band gap is first increased and then decreased [21-22].

4. Conclusion

In the study, the zigzag (2, 2), (3, 3), (4, 4) and armchair (2, 0), (3, 0), (4, 0) Graphdiyne nanotubes were investigated. The results from the investigating the carbon-carbon bond lengths in Graphdiyne nanotubes are in agreement with those of other researchers on Graphdiyne nano-ribbons and nanotubes. All these nanotubes are semiconductors with direct band gap at gamma point of the first Brillouin zone. Because of the quantum confinement effect, the value of band gap of the znt and

Table 5. The Size of Band Gap (E_g), Shift of Energy Bands and Diameter (d) of the Zigzag Graphdiyne Nanotubes with Different Diameters in the absence and presence of the External Electric Field along the X-Axis and with the Sizes of 0.1V/Å and 0.2V/Å

Shift (eV)		d (Å)			E_g (eV)			structure
E=0.2	E=0.1	E=0.2	E=0.1	E=0	E=0.2	E=0.1	E=0	
Structure changed	0.0	10.33	10.286	10.287 10.25[3,4]	0.42	0.63	0.64 0.65[3-5]	**znt2**
0.04	0.0	15.6	15.542	15.541 15.56[3,4]	0.53	0.54	0.55 0.55[3,4]	**znt3**
Structure changed	0.02	12.4*24.93	20.803	20.808 20.81[3,4]	0.34	0.50	0.51 0.50[3,4]	**znt4**
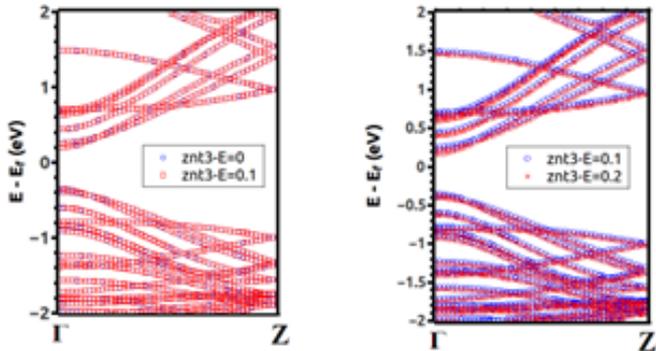
Figure 18. Comparison of the Band Structure of znt3 Nanotubes in the absence (E=0) and presence (E=0.1 and 0.2V/Å) of the Electric Field along the X-Axis
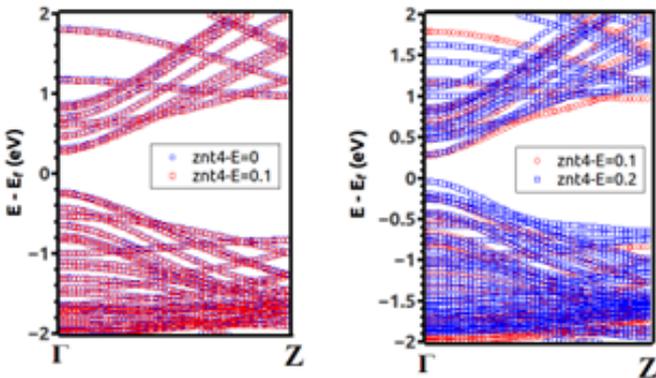
Figure 19. Comparison of the Band Structure of znt4 Nanotubes in the absence (E=0) and presence (E=0.1 and 0.2V/Å) of the Electric Field along the X-Axis

Figure 20. Geometric Structure of Zigzag Graphdiyne Nanotube (znt4) in the Presence of the Electric Field of 0.2V/Å after Relaxation

ant nanotubes is obviously dependent on the nanotube diameter, and by increasing the nanotube diameter, it decreases. In addition, the armchair nanotubes have a smaller diameter and the larger band gap compared to the zigzag nanotubes. As the diameter of the nanotubes increases, the band gap decreases and the DOS increases around the Fermi level. This means that the electrons require less energy to transition from the valence band to the conduction band.

The optical properties of all nanotubes above-mentioned were calculated and investigated using SIESTA package and based on the Kramers–Kronig relations. Dielectric function, absorption coefficient, optical conductivity, reflection, refractive index and extinction coefficient of all samples were calculated. The results show that all these functions are inversely related to the diameter of the nanotubes and are directly related to the band gap, so that the highest intensity is related to the armchair (2, 0) nanotubes and the lowest intensity is to the zigzag (4, 4) nanotubes.

In addition, the effect of external electric field on the geometric structure and band structure of the ant and znt Graphdiyne nanotubes with different diameters is also studied. The results show that by applying the electric field of 0.1 V/Å along the x-axis to the armchair and zigzag Graphdiyne nanotubes, there is little change in the geometric structure and band structure. But, in the presence of the electric field of 0.2 V/Å, the band structure of the zigzag GDY-NT is changed and the size of band gap also dramatically decreased, with the most change seen in the znt4 nanotube, which becomes oval. In the presence of the electric field of 0.2 V/Å in the armchair nanotubes, the size of band gap and diameter of ant3 and ant4 nanotubes are increased and the band structure of these nanotubes also completely changed.

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