Available online at: http://brsj.cepsbasra.edu.iq

ISSN -1817 -2695

Band Structure of Single-Walled Carbon Nanotubes (SWCNTs) under the influence of Elastic Deformation and Magnetic Field

[1]A. A. ALI , [2]M. J. MAJID

[1]Department of Physics, College of Science,
[2]Department of physics, College of Education for Pure Sciences,
University of Basrah IRAQ

E-mail: [1]aliphysics7806969@yahoo.com, [2]majid.jasim.nano@gmail.com

Abstract

We investigate the electronic band structure of SWCNTs exposed to the elastic mechanical deformation and external magnetic field along axis of the tubes. Our theoretical calculations were accomplished by using the dispersion relation of π-electrons in the tight binding approximation for armchair, zig-zag and chiral SWCNTs under the influence of the helical deformation and uniaxial tension in the case of the presence or absence of a magnetic field. The exponential expression has been used for the matrix element of the Hamiltonian operator, which is exponentially proportional to the distance between the carbon atoms in the SWCNT. The energy gap for armchair (10,10) SWCNT increases under the helical deformation with the absence of the magnetic field, consequently, the SWCNT will turn from conducting to semiconducting. In contrast, the energy gap for armchair (10,10) SWCNT is unchangeable under the influence of the uniaxial tension. Moreover, we have noticed the growth of the energy gap for armchair (10,10) SWCNT when the tube is exposed to an external magnetic field. We observed a different behavior for zig-zag (9,0) SWCNT, where the energy gap increases slightly when applying helical deformation and rapidly under the uniaxial tension without a magnetic field. Through our study of the band structure for chiral (10,9) SWCNT, we found that it is not significantly affected when applying the two patterns of mechanical deformation. The presence of the magnetic field in chiral (10,9) SWCNT causes a decrease in the energy gap and thus increases the electrical conductivity of this tube. The variations in the energy gap values can be practically used in the nanosystems based on carbon nanotubes such as CNT field-effect transistors, nanosensors and other practical applications in the field of nanoelectronics.

Keywords: Electronic band structure; SWCNT; Elastic mechanical deformation; Magnetic field; Tight binding approximation; Torsional deformation; Uniaxial tension; Energy gap.

1. Introduction

Carbon nanotubes (CNTs) are a source of attention for many researchers due to the physical and chemical properties they possess, where the prevailing belief for a long period of time was that crystalline carbon forms were confined to two crystalline bodies, diamond and graphite, but with the discovery of fullerene in 1985 [1] it became clear that pure carbon It has the ability to form other stable structures. In 1991, carbon nanotubes were discovered by Iijima, after which studies began to develop to include Double-walled carbon nanotubes (DWCNTs) and Multi-walled carbon nanotubes (MWCNTs)[2,3]. The electronic and mechanical properties of carbon nanotubes are unique, so they can have a major role in the field of future nanoelectronics, and therefore their properties have been extensively studied [4,5]. Many researchers have attempted to use these unique electronic properties of single-walled carbon nanotubes (SWCNTs) to develop nanoelectronics devices. Among the characteristic features of carbon nanotubes are the high elastic modulus in addition to the interdependence between electronic and mechanical properties by applying of elastic mechanical deformations [6-12]. The study of the band structure of carbon nanotubes has attracted a lot of interest in using it in nanotechnology applications.

The mechanical properties of carbon nanotubes are stronger than steel, where studies have shown that nanotubes have a strain of up to 0.3 with a tensile strength of 300 GPa. Therefore, the band structure of nanotubes is sensitive to mechanical deformations. It has been found that the energy gap of carbon nanotubes is depended on the magnitude of applied deformation, where the electronic structure of the deformed tubes depends on the chirality indices and deformation pattern [13]. Experimental and theoretical studies have been done by Tombler et al. to calculate the conductance of SWCNTs under the influence of deformation by the atomic force microscope tip. The authors found that the conductance of the metallic carbon nanotube decreased under deformation[14]. Through the study referred to in Ref. [15] it was clarified that the zig-zag (8,0) CNT is exposed to collapse process when applying the elastic mechanical deformation of the value 12%. The decreases in the conductance of the armchair and zig-zag and carbon nanotubes have been investigated experimentally through the atomic force microscope tip by opening the energy gap under the influence of torsional and tensile deformation, respectively [16]. Minot et al. presented a theoretical study on the effect of strain on the band gap, and it were found that the band gap can be opened in the metallic carbon nanotubes and tune of the band gap in the semiconducting tubes [16].

The electronic properties of carbon nanotubes have been studied by Umeno et al., and they have shown that these properties can be modified from semiconducting to metallic or vice versa depending on the magnitude of applied deformation [17]. The electronic structure and electronic transport properties of zig-zag (6,0) CNT, which is considered a conducting tube, have been investigated by using first principle calculations and Green's function techniques by Yao et al., and they found that the conductivity is sensitive to mechanical deformation and it decreases with increasing the deformation for both tension and compression [18]. Cristancho*et al.* have used ab─initio calculations to study the relationship between the mechanical and electronic properties of CNTs. They emphasized that the energy gap is increasing between the occupied and unoccupied molecular orbitals under the influence of plastic strain. The

coupling between mechanical and electronic properties can be used to control in the energy gap, which leads to improve the characteristics of electromagnetic absorption [19]. Studies have confirmed that the energy gap can be opened and changed for armchair (4,4) CNT through the application of uniaxial tension and the electric field, and it has been found that growth of the energy gap decreases with increasing diameters of carbon nanotubes [20]. The conductance behavior of SWCNTs were analyzed by S. S. Savinskii and A. V. Belosludtsev [21] at zero temperature in a magnetic field along the axis of the tube, where this study shows that the conducting tube becomes dielectric in a weak magnetic field and the energy gap depends on the magnetic field. On the other hand, the electronic energy levels of CNTs in a magnetic field perpendicular to the tube axis were studied by using the tight binding approximation, where the energy bands near to the Fermi level correspond to those calculated in the (k. P) method within a wide range of magnetic field [22]. Recently, a theoretical study showed that the electronic properties of CNTs are affected under torsional deformation and uniaxial tension by using tight binding approximation, where this study confirmed that the some types of deformation lead to change the properties of the tube from metallic to semiconducting or vice versa [23].

The present work includes studying the electronic band structure diagrams of SWCNTs under the influence of the two patterns of elastic mechanical deformation, helical deformation and uniaxial tension in the presence or absence of a magnetic field. Our results focused on studying selected samples of SWCNTs, armchair (10,10), zig-zag (9,0) and chiral (10,9).

2. Computational Details

Geometrically, the SWCNT is described as a rolled up graphene strip in the form of a hollow cylinder. The diameters of SWCNTs do not exceed several nanometers and not only have metallic properties, but also have semiconducting properties depending on the chiral vector $\vec{C}$ [24,25]. Because of the ratio between length and diameter, the carbon nanotube is a one-dimensional nanostructure. The graphene strip is rolling along the vector direction $\vec{C}$ to form a carbon nanotube, as shown in the Fig. 1. The chiral vector is defined by the relation $\vec{C} = n\,\vec{a}_1 + m\,\vec{a}_2 \equiv (n,m)$, where $\vec{a}_1$ and $\vec{a}_2$ represent the basis vectors of graphene lattice and (n,m) is the chirality indices, which are integers. The SWCNTs can be classified to three types depending on the indices (n,m), armchair and the indices are identical (i.e. $n = m$), zig-zag at$(m = 0)$ and chiral at $(n \neq m,\ m \neq 0)$ [26-29]. The condition of electrical conductivity for carbon nanotubes is determined by $|n - m| = 3i$, so all the armchair CNTs are conducting [30-32]. As a result of rolling the graphene strip and the opposite ends adhesion to each side, which leads to quantization of the wave vector in the transverse direction, a cylindrical surface will be formed with the rotational parameters $\delta\varphi_{1,2}$ and $\delta z_{1,2}$ along the transverse and longitudinal direction, respectively. The cylindrical coordinates (R,φ,z) of any point on the surface of the tube will be turned to$(R,\varphi+\delta\varphi,z+\delta z)$. The radius and the chiral angle θ (which is the angle between the vector $\overrightarrow{C}$ and the basis vector $\vec{a}_1$) of the cylindrical surface are given in terms of the chirality indices by the following relations [33],

$$R = \frac{|\vec{C}|}{2\pi} = \frac{\sqrt{\vec{C}.\vec{C}}}{2\pi} = \frac{a\sqrt{n^2+nm+m^2}}{2\pi}$$
$$\theta = \sin^{-1}\left(\frac{\sqrt{3}\,m}{2\sqrt{n^2+m^2+nm}}\right) \quad (1)$$

Where a is the length of the basis vectors and is equal to 2.46 A^0. The zig-zag CNTs

have a chiral angle $\theta = 0^0$. In the other extreme, the armchair CNTs have $\theta = 30^0$ and the chiral CNTs is between $30^0 > \theta > 0^0$ [34].

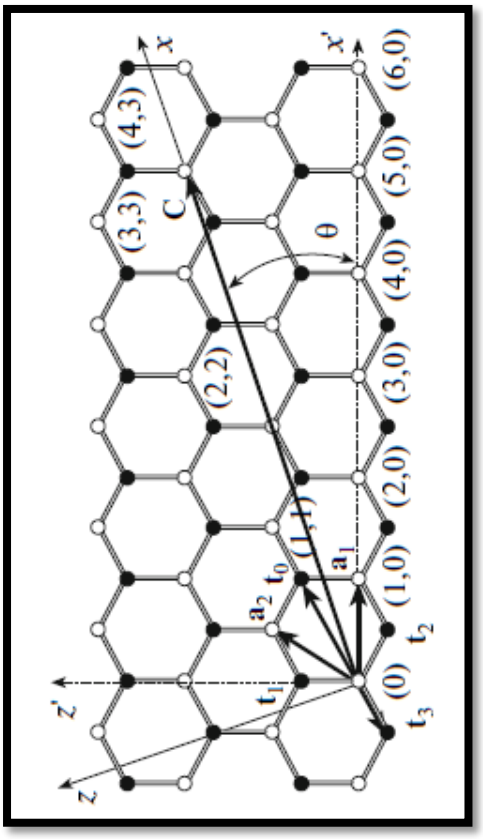


Fig. 1. Nanotube construction diagram of the basis vectors for graphene strip [6].

The rotational parameters $\delta\varphi_{1,2}$ and $\delta z_{1,2}$ of carbon nanotubes are given by (see Fig. 1),

$$\delta\varphi_1 = a\ \cos\theta\ /\ R$$

$$\delta\varphi_2 = a\ \cos(60-\theta)\ /\ R \qquad (2)$$

$$\delta z_1 = -\,a\ \sin\theta$$

$$\delta z_2 = a\ \sin(60-\theta)$$

To study the band structure of carbon nanotubes in the tight binding approximation, it is necessary to know the transition matrix elements that determine the amplitudes of electron hopping between the nearest atoms in the lattice of the SWCNT, and are based on the wave functions of π-electrons. We performed our calculations with respect to the transition matrix element (in units of eV) by using the Parametric function as shown below [35],

$$\beta_i = 2.7\left(-3.37\left(-1+\left|\vec{t_i}\right|\ /\ a_{c-c}\right)\right), \qquad (3)$$

i=1,2,3

Where a_{c-c} is the distance between the nearest neighbors to carbon atoms in pristine SWCNT and is equal to 0.142 nm and $\vec{t_i}$ is the vectors that connect the adjacent carbon atoms.

The rotational parameters are involved in the energy spectrum relation of the SWCNT, which depends on the magnetic quantum number $m_q = 0, \pm1, \pm2, \ldots..$ and it represents the band number in addition to the wave number k, so the energy spectrum relation and the derivative within the tight binding approximation can be written in the following form [6],

$$E^{\pm}_{m_q,k} = \pm\begin{vmatrix} \beta_1 e^{-i(m_q\delta\varphi_1+k\delta z_1)} + \\ \beta_2 e^{-i(m_q\delta\varphi_2+k\delta z_2)} + \\ \beta_3 e^{-im_q(\delta\varphi_1+\delta\varphi_2)-ik(\delta z_1+\delta z_2)} \end{vmatrix} \qquad (4)$$

When the SWCNT is exposed to an external magnetic field toward axis of the tube, the energy spectrum relation shown by the formula (4) does not change, but the quantum magnetic number m_q is turned to $m_q + \Phi/\Phi_0$, where $\Phi = \pi R^2 B$ represents the magnetic flux which penetrates the cross section of the SWCNT, $\Phi_0 = 2\pi c\hbar\ /\ e$ is the magnetic quantum flux, c is the light velocity and B is the magnetic flux density [36]. As the magnetic field changes, the allowed states within the k values in the Brillouin zone will move, and thus the physical properties of the tube will change.

Therefore, the energy of π-electrons for the SWCNTs under the influence of a magnetic field is given in the expression below,

$$E_{m_q,k}^{\pm} = \pm \begin{vmatrix} \beta_1 e^{-i\left(\left(m_q+{}^{\Phi}/_{\Phi_0}\right)\delta\varphi_1+k\delta z_1\right)} + \\ \beta_2 e^{-i\left(\left(m_q+{}^{\Phi}/_{\Phi_0}\right)\delta\varphi_2+k\delta z_2\right)} + \\ \beta_3 e^{-i\left(m_q+{}^{\Phi}/_{\Phi_0}\right)(\delta\varphi_1+\delta\varphi_2)-ik(\delta z_1+\delta z_2)} \end{vmatrix} \quad (5)$$

The positive and negative signs in the energy spectrum formula refer to the conduction and valence bands, so the total number N of the sub-bands and the equivalent to the number of carbon atoms of the overall SWCNT unit cell is calculated as follows [37],

$$N = \frac{4(n^2+m^2+nm)}{d_R} \quad (6)$$

Where,

$$d_R = \begin{Bmatrix} q & if & n-m \neq 3qi \\ 3q & if & n-m = 3qi \end{Bmatrix} \quad (7)$$

Here i represents an integer number and q is the greatest common divisor (gcd) between the chirality indices (n,m). The number of sub-bands is usually less than N because of the degeneracy that occur to them.

In the case of the zig-zag SWCNTs (n, 0), the gcd is equal to n ($q = n$) and ($d_R = q$), so $N = \frac{4n^2}{n} = 4n$, while the gcd for the armchair SWCNTs (n, n) is also equal to n ($q = n$), but ($d_R = 3q$), i.e. $N = \frac{12n^2}{3n} = 4n$.

The geometric representation of the uniform mechanical deformation of carbon nanotubes is $(R, \varphi, z) \rightarrow (R', \varphi', z')$, where (R, φ, z) represent the cylindrical coordinates before deformation and (R', φ', z') are the cylindrical coordinates after deformation. We have [6]:

$$\varphi' = \varphi + z \times \gamma_1/R,\ z' = z \times (1+\gamma_2),$$
$$R' = R \times (1+\gamma_3) \quad (8)$$

Where γ_1, γ_2 and γ_3 represent the dimensionless deformation parameters applied to the nanotube. Therefore, the rotational parameters will change under the influence of elastic mechanical deformation. According to the relation (8), the rotational parameters can be expressed,

$$\delta\varphi'_{1,2} = \delta\varphi_{1,2} + \delta z_{1,2} \times \gamma_1/R\ ,$$
$$\delta z'_{1,2} = \delta z_{1,2} \times (1+\gamma_2) \quad (9)$$

The first pattern of elastic deformation can be represented by helical (twist) deformation corresponding to parameters, $\gamma_2 = 0$, $\gamma_3 = 0$ and γ_1 is the twist angle. Whereas the second pattern of the deformation is uniaxial tension, in this case we assume the values of the parameters $\gamma_1 = 0$ and $\gamma_3 = -v \times \gamma_2$, where v is called the Poisson ratio and it is fixed in all the graphitic components (v =0.165) [38]. By applying the elastic mechanical deformation, the distance between the carbon atoms in the pristine SWCNT $|\vec{t_l}|$ shown in the analytical formula (3) is defined as [39],

$$\vec{t_l'} = |\vec{t_l}| \cdot \left[u(\vec{r} + \vec{t_l}) - u(\vec{r})\right] \quad (10)$$

Where $u(\vec{r})$ represent the displacement vector.

3. Results and discussion

In this study, calculations were carried out the electronic band structure of pristine and deformation SWCNTs in the presence or absence of an external magnetic field along axis of the tubes. The band structure of the CNTs is symmetric around the Fermi level in the tight binding approximation. Consequently, half of the sub-bands will be above the Fermi level and the other half of the sub-bands will be below

the Fermi level. We have used the energy spectrum relations represented by formulas (4) and (5), these relations have been used to reveal on the effect of elastic mechanical deformation and magnetic field on the band structure of SWCNTs.

Figs. 2 (a-f) show the electronic band structure of armchair (10,10) SWCNT under the effect of the helical deformation and uniaxial tension in the presence or absence of a magnetic field. We notice from the Fig. 2 that the upper sub-bands in the band structure represent the conduction bands, while the lower sub-bands are the valence bands. Each one of these sub-bands in the energy spectrum of carbon nanotubes corresponds to a quantum magnetic number m_q. By the electronic band structure, we can calculate the energy gap (E_g), which represents the energy difference (in units of *eV*) between the lowest sub-band of the conduction band and the highest sub-band of the valence band (it can be called the fundamental band) and we assume that the Fermi level in the middle (i.e. at energy E = 0).

The calculated band structure when the magnetic flux is equal to zero Φ/Φ_0=0 for pristine, under helical deformation and under uniaxial tension armchair (10,10) SWCNT is illustrated in Fig. 2(a), (b) and (c), respectively. Fig. 2(a) shows us that the energy gap value is zero (E_g =0 *eV*) in the band structure due to the convergence of the lowest sub-band of the conduction band with the highest sub-band of the valence band (metallic tubes) with observation that the number of sub-bands in each band (conduction or valence) is equal to N = 11. In the case of the helical deformation for armchair (10,10) SWCNT, as shown in the Fig. 2(b), it is found that the energy gap increases in order of 0.68 *eV* at the fundamental band that corresponds to the quantum magnetic number m_q=10 when the value of deformation parameter up to γ_1=0.05. The band structure behavior for armchair (10,10) SWCNT such as Fig. 2 (c) indicate that there is no energy gap when applying uniaxial tension deformation by γ_2=0.05, so the armchair SWCNT remains conducting. These results correspond to the results of Ref. [22], where they emphasized that the armchair SWCNTs do not change under the uniaxial tension. For a magnetic flux of Φ/Φ_0=0.5, the energy gap is increasing by 0.85 *eV* without deformation $\gamma_1 = \gamma_2 = 0$ as it appears in the Fig. 2(d). We also see from this the figure that the number of sub-bands in each band is equal to N = 10, and this means that effect of the magnetic field on armchair (10,10) SWCNT reduces the number of sub-bands in the energy spectrum due to the fact that the energy values at the sub-bands corresponding to a quantum magnetic numbers m_q = 9 and 10 will be identical. It is evident that a small energy gap of 0.17 *eV* will appear under the effect of helical (twist) deformation at γ_1=0.05 with the presence of magnetic flux as we see in Fig. 2(e). Meanwhile, the computed energy gap for armchair (10,10) SWCNT under the effect of uniaxial deformation is plotted in Fig. 2(f), where we find that the value of the gap is equal 0.92 *eV*.

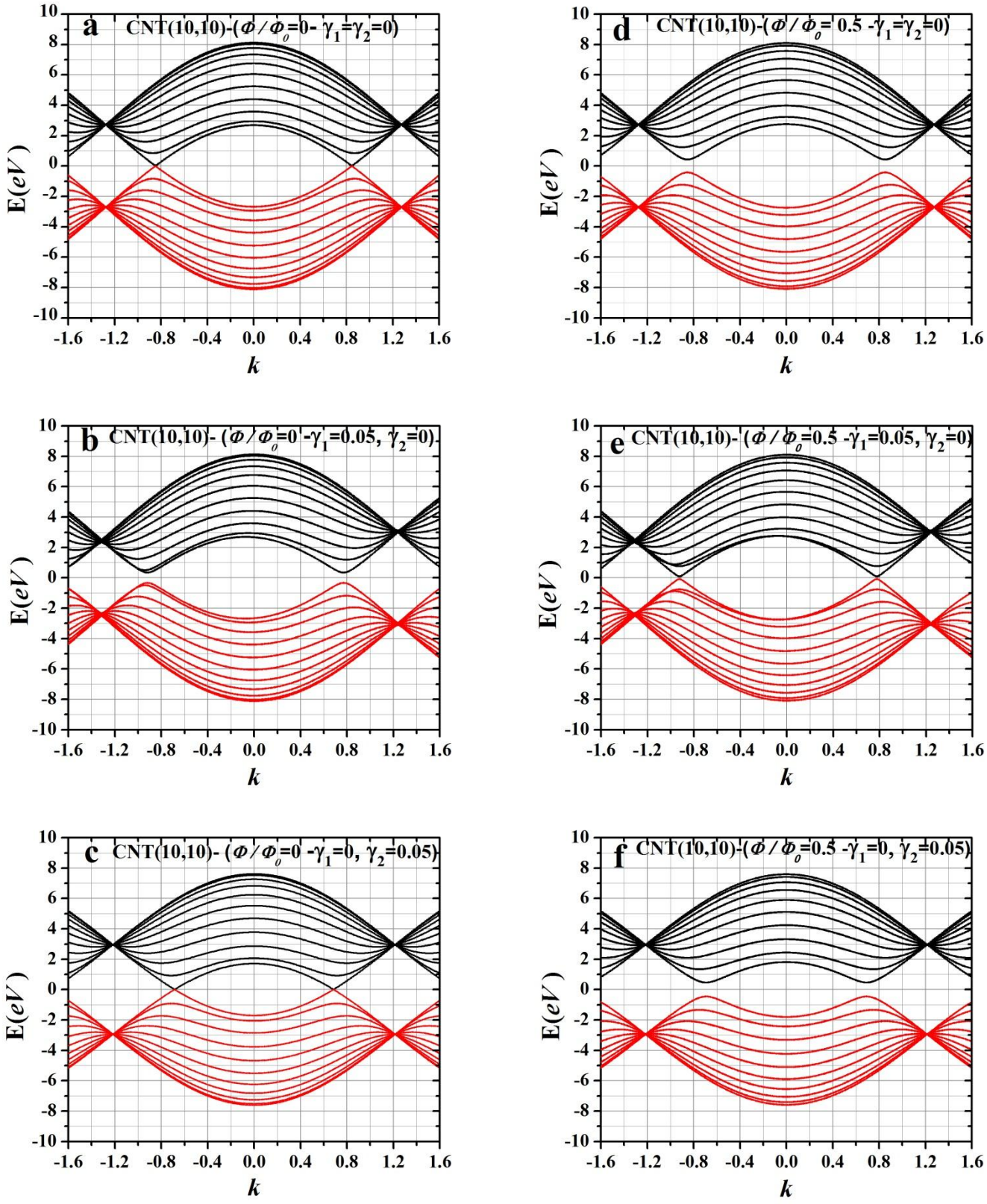
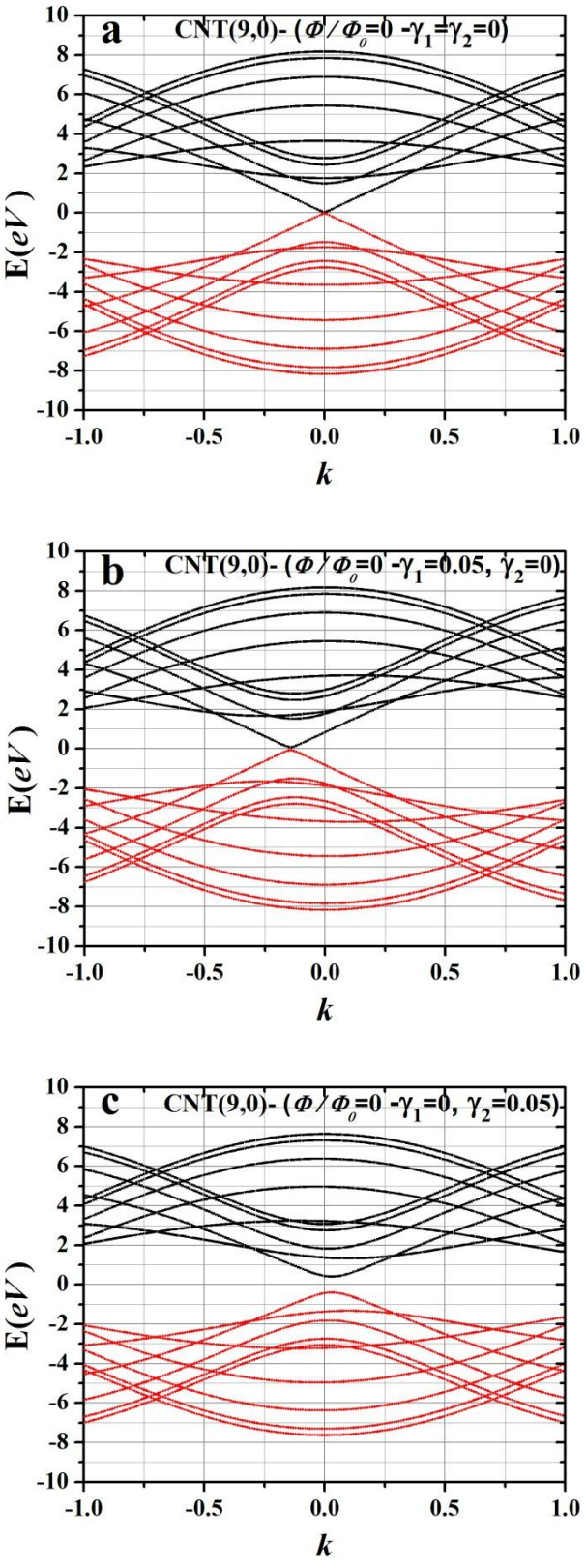


Fig.2. Band Structure of armchair (10,10) SWCNT under the influence of twist deformation and uniaxial tension in the presence or absence of a magnetic field.

The zig-zag (9,0) SWCNT has been studied under the influence of elastic mechanical deformation and the magnetic field toward axis of the tube. Fig. 3(a) shows the metallic property of pristine zig-zag (9,0) SWCNT according to the conductivity condition of carbon nanotubes, where we notice the absence of the energy gap at the fundamental band that corresponds to the magnetic quantum number m_q = 6. Fig. 3(b) displays the plot of the band structure dependence on the twist deformation for zig-zag (9,0) SWCNT, and it is noticeable that the energy gap appears at 0.15 eV when the value of the twist parameter γ_1 =0.05 and the nanotube becomes semiconducting. Correspondingly, the energy gap increases by 0.80 eV when applying tension deformation in the longitudinal direction as apparent in Fig. 3(c). Our results are consistent with the results of the study presented in Ref. [40], where they studied the effect of helical deformation on the increase and decrease of the energy gap. At magnetic flux of Φ/Φ_0=0.5, there we see a great change in the energy spectrum of the tube. In the absence of deformation, as in Fig. 3(d), the energy gap appears at 1.63 eV. We observe that the number of sub-bands has become N = 9 in each band and m_q = 5 for the lowest band in the band structure; this is due to the energy values are equivalent at m_q = 8 and 9. Whereas the number of sub-bands at zero magnetic field of zig-zag (9,0) SWCNT is N=10. Figs. 3(e) and (f) illustrate the band structure for zig-zag (9,0) SWCNT at the values corresponding to (5%) of rotational (helical) and uniaxial deformation, respectively and in the presence of the magnetic field. We note that the energy gap when applying the deformation patterns is 1.55 eV and 0.88 eV, respectively. Through Figs. 3(a, b) and Figs. 3(d, e), we show a slight difference in the band structure behavior for this type of the tubes with a slight change also in the energy gap and we see also that the Dirac points are shifted from the equilibrium positions.



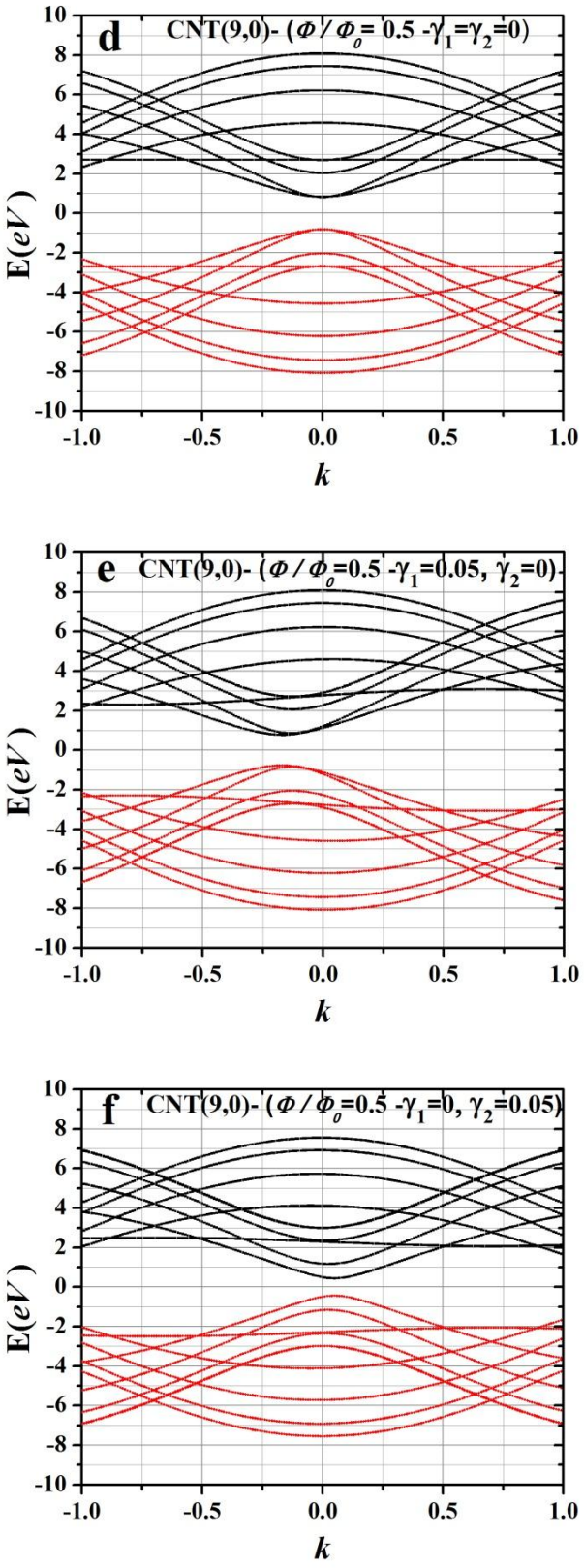
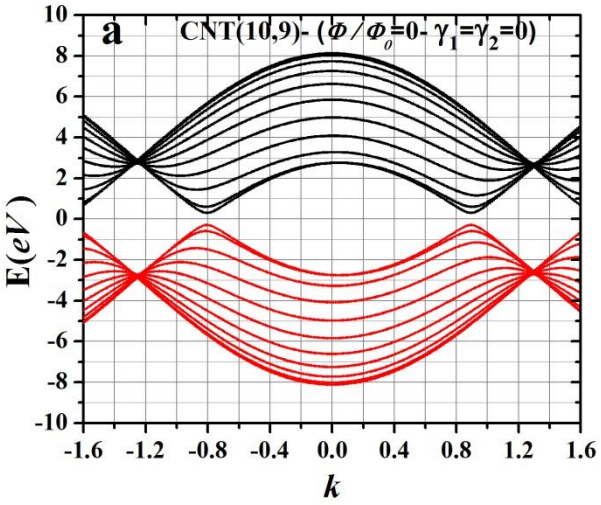


Fig.3. Band Structure of zig-zag (9,0) SWCNT under the influence of twist deformation and uniaxial tension in the presence or absence of a magnetic field.

Fig. 4 shows the band structure of chiral (10,9) SWCNT with the two patterns of deformation and the magnetic field. At zero magnetic flux and the deformation parameters are $\gamma_1 = \gamma_2 = 0$, the chiral (10,9) SWCNT is semiconducting with an energy gap of 0.6 *eV* in Fig. 4(a) at the quantum magnetic number $m_q = 9$. Specifically, when $\gamma_1 = \gamma_2 = 5\%$ [Figs. 4(b) and (c)], the energy gap is about 0.5 *eV* and 0.72 *eV*, respectively. In the absence of deformation, the energy gap will decrease to half of its value under the influence of magnetic flux by $\Phi/\Phi_0=0.5$, so it becomes about 0.3 *eV* as it appears in Fig. 4(d). When applying torsional deformation in Fig. 4(e), it was found that there is a slight increase in the energy gap under the same value of the magnetic flux for chiral (10,9) SWCNT, as it is about 0.38 *eV*, while the energy gap is equal to 0.25 *eV* under the tension deformation of the axial direction of this tube is as shown in Fig. 4(f).



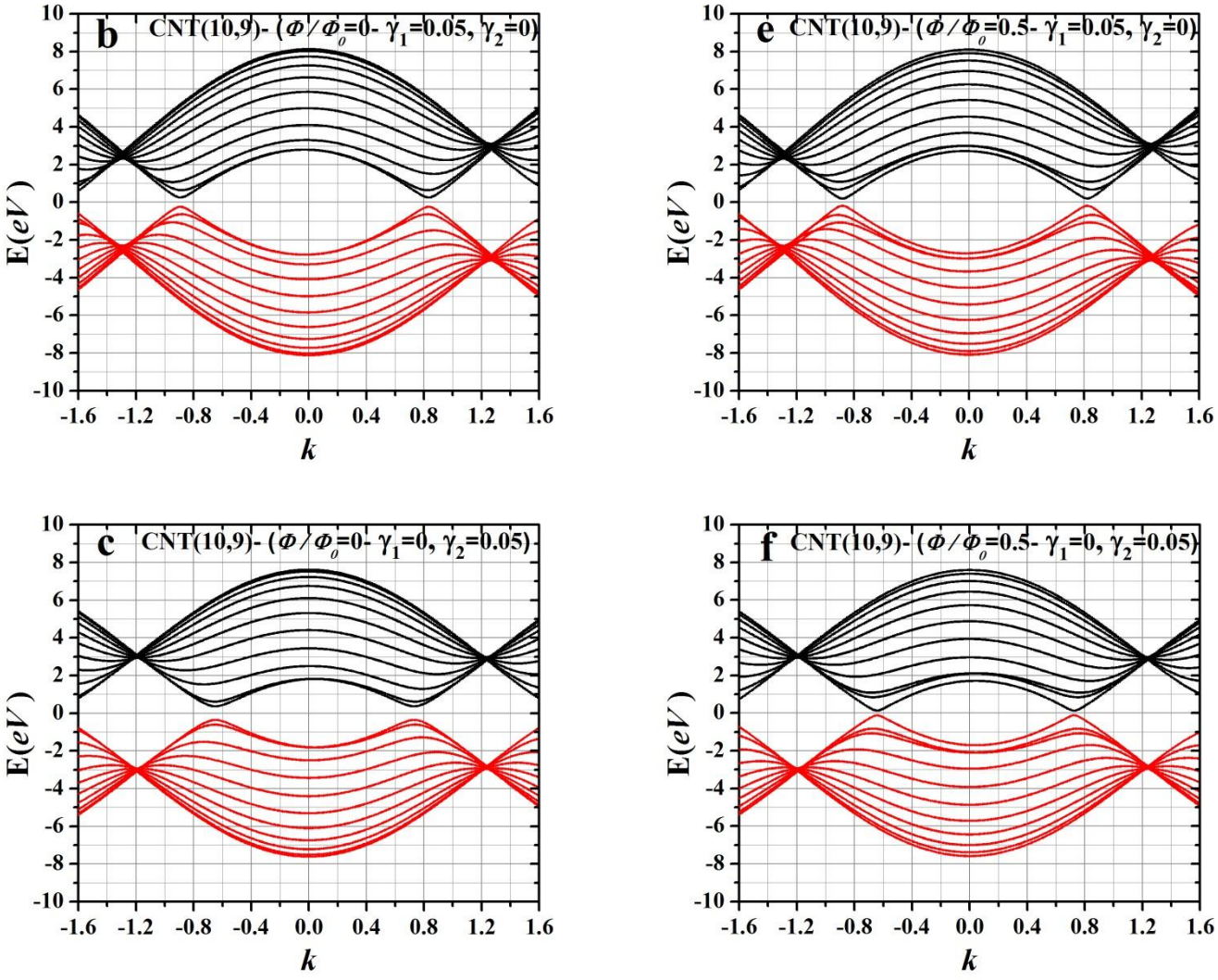


Fig.4. Band Structure of chiral (10,9) SWCNT under the influence of twist deformation and uniaxial tension in the presence or absence of a magnetic field.

4. Conclusion

In this paper, we presented a detailed study about the affected of the electronic properties of SWCNTs by the process of elastic mechanical deformation and the axial magnetic field. We performed the calculations to the electronic band structure of selected samples of SWCNTs, armchair, zig-zag and chiral. The values of the deformation parameters of the SWCNTs have been adopted in our calculations of 0.05, which are considered within the elastic limits of mechanical deformations to ensure

their practical application and avoid of the lattice fracture in the SWCNTs. We notice from the results obtained in our theoretical calculations that the structure band of SWCNTs is completely dependent on the chirality indices, deformation pattern and the value of the magnetic field. It appears clear that the electronic properties of armchair (10,10) SWCNT are affected under the helical (torsional) deformation, then the tube becomes semiconducting. Furthermore, our numerical calculations have emphasized that the band structure for armchair (10,10) SWCNT is unchangeable under the effect of uniaxial deformation due to the maintaining of the mirror symmetry. We also conclude from this study that the helical deformation at the value γ_1 =0.05 does not significantly affect the behavior of the energy spectrum of zig-zag (9,0) SWCNT. In contrast, the electronic properties of zig-zag (9,0) SWCNT are affected under the uniaxial tension at γ_2 =0.05**.** Our study of zig-zag (9,0) SWCNT shows that the energy gap grows under the influence of the elastic mechanical deformation patterns and the magnetic field, which means that the electronic properties of the tube can be controlled. When comparing the results of the energy gap that we obtained from the band structure, it appears to us that the energy gap values under the influence of magnetic flux of Φ/Φ_0=0.5 with the two deformation patterns on the SWCNTs are reversed with their values before the magnetic flux effect. This means that when there is an increase in the energy gap with one of the deformation patterns without magnetic flux, the value of the energy gap itself will decrease when using the same deformation pattern with the presence of magnetic flux and vice versa.

The physical interpretation for the increase or decrease of the energy gap under the influence of elastic mechanical deformations in the case of the presence or absence of a magnetic field is the result of the increase or decrease in the distance between the atoms in the lattice. It can be said that the energy gap is directly proportional to the distance between the carbon atoms. The electronic properties of chiral (10,9) SWCNT are not significant effect under the helical and uniaxial deformations at the parameters $\gamma_1 = \gamma_2$= 0.05. The influence of the magnetic field is evident on the arrangement of sub-bands in the valence or conduction bands for zig-zag (9,0) SWCNT and the arrangement of sub-bands remains in both the armchair (10,10) SWCNT and chiral (10,9) SWCNT. Finally, we have demonstrated in this research that the electronic properties of the SWCNTs can be improved by applying elastic mechanical deformation and the longitudinal magnetic field.

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تركيب النطاق للأنابيب النانوية الكربونية الأحادية الجدران (SWCNTs) تحت تأثير التشويه المرن والمجال المغناطيسي

علي عبد الرزاق عبد الحسين1 و ماجد محمد جاسم2

[1] قسم الفيزياء, كلية العلوم, جامعة البصرة, العراق

[2] قسم الفيزياء, كلية التربية للعلوم الصرفة, جامعة البصرة, العراق

الخلاصة :

درسنا تركيب النطاق الإلكتروني للأنابيب النانوية الكربونية أحادية الجدران (SWCNTs) المعرضة الى التشويه الميكانيكي المرن والمجال المغناطيسي الخارجي على طول محور الأنابيب. أُنجزت حساباتنا النظرية باستخدام علاقة التشتت لإلكترونات-π في تقريب الربط المحكم للأنابيب النانوية الكربونية أحادية الجدران ذراع الكرسي (Armchair)، المتعرجة (Zig-Zag) و اللاانطباقية (Chiral) تحت تأثير التشويه الحلزوني والشد أحادي المحور في حالة وجود أو عدم وجود مجال مغناطيسي. لقد تم استخدام الصيغة الأسية لعنصر مصفوفة المؤثر الهاملتوني، الذي يتناسب أسياً مع المسافة بين ذرات الكربون في الأنبوب النانوي الكربوني أحادي الجدران (SWCNT). تزداد فجوة الطاقة للأنبوب النانوي الكربوني ذراع الكرسي armchair (10,10)SWCNT تحت تأثير التشويه الحلزوني مع غياب المجال المغناطيسي, وبالتالي، سوف يتحول الأنبوب

النانوي الكربوني أحادي الجدران (SWCNT) من موصل إلى شبه موصل. في المقابل, فإن فجوة الطاقة للأنبوب armchair SWCNT (10,10) لا تتغير تماماً تحت تأثير الشد أحادي المحور. من ناحية أخرى، لاحظنا نمو فجوة الطاقة للأنبوب النانوي الكربوني أحادي الجدران armchair (10,10) SWCNT عندما يتعرض الأنبوب إلى مجال مغناطيسي خارجي. تمت ملاحظة تصرف مختلف للأنبوب النانوي الكربوني أحادي الجدران المتعرج Zig-Zag (9,0) SWCNT، حيثُ تزداد فجوة الطاقة قليلاً عند تطبيق التشويه الحلزوني وبسرعة تحت تأثير الشد أحادي المحور بدون مجال مغناطيسي. من خلال دراسة تركيب النطاق للأنبوب النانوي الكربوني أحادي الجدران اللاانطباقي Chiral (10,9) SWCNT، تبين لنا أنه لا يتأثر كثيراً عند تطبيق نمطي التشويه الميكانيكي. إنّ وجود المجال المغناطيسي في الأنبوب Chiral (10,9) SWCNT يسبب انخفاض في فجوة الطاقة وعليه تزداد التوصيلية الكهربائية لهذا الأنبوب. يمكن استخدام الاختلافات الحاصلة في قيم فجوة الطاقة عملياً في الأنظمة النانوية القائمة على الأنابيب النانوية الكربونية مثل ترانزستورات تأثير المجال، المتحسسات النانوية وغيرها من التطبيقات العملية في مجال الإلكترونيات النانوية.

الكلمات المفتاحية: تركيب النطاق الإلكتروني، الأنبوب النانوي الكربوني الأحادي الجدران، التشويه الميكانيكي المرن، المجال المغناطيسي، تقريب الربط المحكم, التشويه الحلزوني، الشد أحادي المحور، فجوة الطاقة.