First-Principles Study on Electronic and Optical Properties of Single-Walled Carbon Nanotube Under an External Electric Field

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Abstract

In this study, the electronic and optical properties of one-dimensional (1D) Single-Walled Carbon Nanotube (SWCNT) nanostructures, under an external electric field (E_{ext}) effects applied in z direction, are investigated using density functional theory (DFT) calculations. The Visualizer module of Material Studio software used to construct single-layer nanotube. Then, we use the CASTEP code for optimize and calculate the band structure, density of states and optical properties of carboxyl group substitution on Single-Walled Carbon Nanotube (SWCNT/Carboxyl). The E_{ext} effects lead to modulate the band gap and change the total density of states (TDOS), partial density of states (PDOS), absorption coefficient, dielectric function, optical conductivity, refractive index and loss function. The application of an E_{ext} effect on SWCNT/Carboxyl structure, lead to close its band gap. The peaks of TDOS around the fermi level are very weak. The absorption coefficient increases in visible range and decreases in ultraviolet (UV) domain, by reason of increased an E_{ext} effects. It is found that electronic structures and optical properties of SWCNT/Carboxyl, could be affected by the E_{ext} effects. All these results provide the important information for understanding and controlling the electronic and optical properties of 1D-crystals by an E_{ext} effects. This study can provide certain theoretical basis for our future experimental work of optoelectronic properties of SWCNT/Carboxyl material.

Keywords: External electric field, Optical property, First-principle calculation, electronic structure, absorption spectrum.

1. Introduction

Electronic states of graphene, are well described by the tight binding Hamiltonian of π electrons in carbon atoms [1]. In graphene, the carbon atoms have four valence electrons, occupy 2s and 2p orbitals ($2s^2\ 2p^2$). As carbon atoms form graphene, three atomic orbitals 2s, $2p_x$ and $2p_y$ are hybridized to form three sp^2 hybrid orbitals in the same plane, while $2p_z$ orbital remains perpendicular to other orbitals. The hybridized orbitals are responsible for three σ bonds between adjacent carbon atoms, and $2p_z$ orbital

results in π bonds out of the plane of graphene sheet [2]. Graphene, a semimetal with zero band gap energy, is the representative members of 2D-family that have been receiving much attention in many fields, due to their remarkable physical properties. Its band structure shows zero gap at the Dirac point, which can be opens by an external perturbations such as the application of an E_{ext} effects [3].

Graphene can be considered the mother of three carbon allotropes (buckyball - carbon nanotubes - graphite). Folding graphene into a cylinder produces the nanotubes. In recent years, carbon nanotubes have been intensively studied, due to their importance as building block in nanotechnology. Three different types of carbon nanotubes are experimentally observed: armchair, zigzag and chiral [4]. Due to their cylindrical shape and high specific surface, the CNTs are strongly interact with light and possess interesting physical properties [5]. Electronic and optical properties of SWCNT structure, are largely depend on their curvature and chirality, which offer great potential applications fields, including nanoelectronic devices and energy storage [6]. The electronic properties of CNTs are due to the sp^2-hybridized carbon atoms and delocalized π network, perpendicular to the nanotube surface [7]. With large surface area, all carbon atoms could be direct contact with the external exposed molecules. Thus, they are very sensitive to the surrounding environment, and could be suitable for storing molecules adsorbed on the surface. The carboxyl unit substitution on the surface form the specific group (-C(=O)OH) with sp^3 carbon regions [8].

In many cases, the E_{ext} effects, lead to change the carrier concentration in a semiconductor material and consequently modified the electric current. The E_{ext} effects also modify the electronic and optical response of 1D-SWCNT. The E_{ext} effects applied on electronic and optical properties of SWCNT/Carboxyl structure, have received great interest for fundamental and application research. Applying an E_{ext} on material can cause an electro-optical effects and change their optical properties [9,10].

In this research, an influence of an E_{ext} applied in z direction on SWCNT/Carboxyl tube. The electronic structure and optical properties of this 1D-material, are studied using first-principles calculations [11]. Including band gap energy, TDOS, PDOS and optical properties. In the case of applied an E_{ext}, a perturbation in the form of electrostatic potential to the Hamiltonian of π-electrons in SWCNT/Carboxyl structure is expected. The homogeneous E_{ext} effects, lead to modifies the Hamiltonian of SWCNT/Carboxyl structure:

$$H = H_0 - eE_z \quad (1)$$

Where H_0 is the Hamiltonian of system in equilibrium conditions.

Our paper is outlined as follows: In section 2, we briefly present the Computational Methods. Section 3 is devoted to discuss the numerical results and give our interpretations. Finally, the conclusions of our study is included in Section 4.

2. Computational methods

The electronic and optical properties of SWCNT/Carboxyl structure, are determined based on DFT calculations, using CASTEP code by OTFG ultrasoft pseudopotentials [12,13]. Only the valence electrons (C $2s^2 2p^2$ and O $2s^2 2p^4$) are considered using ultrasoft pseudopotentials. In this study, the exchange-correlation energy employed using Perdew-Burke-Ernzerhof (PBE) functional, within the generalized gradient approximation (GGA) [14]. A plane-wave energy cut-off was set to 500 eV for all calculations.

The K-point of the Brillouin zone sampled using 5×5×1 gamma-centered Monkhorst-Pack grid, during the geometry optimizations of SWCNT/Carboxyl structure [15]. However, during all structural relaxations, the convergence tolerance criteria for the geometry optimization was set to $2x10^{-6}$ eV/atom for energy. During the atomic relaxations, the positions of atoms are optimized until convergence of the force on each atom was less than 0.05 eV/Å, and 0.03 Å for the displacement. The self-consistent field (SCF) convergence tolerance was set to $2x10^{-6}$ eV/atom. The maximum stress was set to 0.1 GPa.

In the present simulations, the SWCNT/Carboxyl structure was investigated using CASTEP code. In this model, we have considered that a supercell contains 49 C, 1 H and 2 O atoms, are coordinates as shown in Tab1. In these atomic structure, the C(=O)OH group was distributed randomly on the side of SWCNT sheet. The E_{ext} effects values 0 V/Å, 0.1 V/Å, 0.2 V/Å and 0.3 V/Å are applied in z direction of SWCNT/Carboxyl layer, lead to obtain the electronic and optical properties. We construct an armchair carbon nanotube SWCNT with m = n = 6, bond length 1.42 Å and diameter d = 8.14 Å, with supercell range (A=1, B=1, C=2) substituted by the carboxyl group as shown in Fig 1. The SWCNT/Carboxyl structure was placed inside a unit cell parameters a= 11.483001 Å, b= 11.483001 Å, c= 4.919024 Å and α= β= 90°, γ= 120° for an optimization calculation.

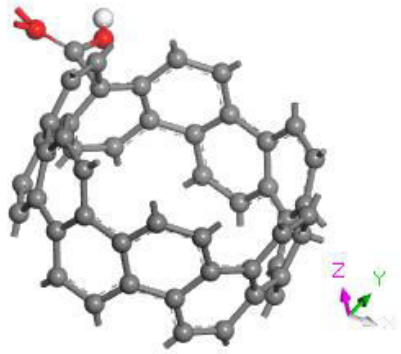

Fig 1. Crystal structure of SWCNT/Carboxyl, the biggest gray sphere represents the carbon atom, the second biggest blanch and red spheres represent hydrogen and oxygen atoms respectively.

Tab 1. The coordinates of C, O and H atoms in supercell of SWCNT/Carboxyl.

Element	Atom Number	Fractional coordinates of atoms		
		u	v	w
H	1	0.162102	0.897179	0.679921
C	1	0.895224	0.745306	0.028855
C	2	0.883075	0.799970	0.278983
C	3	0.781359	0.907277	0.028214
C	4	0.827413	0.883450	0.278549
C	5	0.380584	0.770624	0.027299
C	6	0.659727	0.907520	0.027909
C	7	0.590962	0.887789	0.277744
C	8	0.255630	0.649089	0.027011
C	9	0.201505	0.583472	0.274499
C	10	0.450718	0.817891	0.278651
C	11	0.107381	0.375798	0.027601
C	12	0.127060	0.444867	0.279282
C	13	0.228969	0.106038	0.028185
C	14	0.098115	0.251095	0.027715
C	15	0.111753	0.197796	0.279038
C	16	0.348496	0.101989	0.028017
C	17	0.416145	0.116000	0.277964
C	18	0.179113	0.125093	0.278442
C	19	0.626180	0.221797	0.028044
C	20	0.556040	0.175612	0.277917
C	21	0.886289	0.619684	0.028531
C	22	0.750202	0.340995	0.028072
C	23	0.798824	0.410187	0.278505
C	24	0.864908	0.549978	0.278740
C	25	0.893132	0.744341	0.529432
C	26	0.884771	0.801280	0.779139
C	27	0.781338	0.907443	0.528775
C	28	0.828476	0.884753	0.778699
C	29	0.384150	0.774621	0.527574
C	30	0.660150	0.908430	0.527963
C	31	0.590889	0.888253	0.777890
C	32	0.235762	0.666170	0.526780
C	33	0.197509	0.585155	0.781174
C	34	0.450752	0.818689	0.776371

C	35	0.096970	0.372993	0.528969
C	36	0.123324	0.444763	0.777488
C	37	0.227984	0.104169	0.528125
C	38	0.092138	0.247991	0.528556
C	39	0.109873	0.196270	0.777207
C	40	0.348806	0.102033	0.528038
C	41	0.416362	0.116085	0.778188
C	42	0.178281	0.124146	0.777957
C	43	0.625868	0.221718	0.528114
C	44	0.556033	0.175150	0.778145
C	45	0.883737	0.618565	0.529399
C	46	0.749679	0.340953	0.528677
C	47	0.800518	0.409699	0.778450
C	48	0.867623	0.550459	0.779002
C	49	0.176142	0.761312	0.498568
O	1	0.195279	0.834852	0.722148
O	2	0.131492	0.773809	0.284933

3. Results and discussions

3.1 Electronic structure

3.1.1 Optical gap

Applying an E_{ext} effects on a material, is a method for controlling its band gap. In the case of SWCNT/Carboxyl material, the band structures are calculated along the high symmetry directions in the Brillouin zone, as plotted in Fig 2. The band structures show that the conduction band minimum and the valence band maximum, are located at various points of the Brillouin zone, which indicate that the SWCNT/Carboxyl structure has a direct band gap Fig 2. The band gap of SWCNT/Carboxyl decrease from 0.384 eV, 0.384 eV, 0.215 eV and 0.119 eV, by reason of an E_{ext} effects applied in z direction, from 0 V/Å, 0.1 eV, 0.2 eV and 0.3 V/Å respectively, as shown in Fig 3. These results, show the closing band gap by the effects of E_{ext}. The response of the band gap of SWCNT/Carboxyl under an $E_{ext} - field$ applied in z direction, facilitate the modulation of this electronic property.

It is clear from Fig 3, the SWCNT/Carboxyl structure exhibit a decreases of band gap energy by the effects of E_{ext}, which indicate the semiconducting property of this 1D-material. The effects of an E_{ext} on the band gap closer to fermi level can be summarized as follows: The both conduction and valence bands are fixed for an $E_{ext} = 0.1\ \mathrm{V/Å}$, which indicates that this value of E_{ext} doesn't influence the valence electrons of SWCNT/Carboxyl structure. The both conduction and valence bands moves upward and closing for an $E_{ext} = 0.2\ \mathrm{V/Å}$. The conduction band moves downward and the valence band remains almost fixed, for closing the band gap under an $E_{ext} = 0.3\ \mathrm{V/Å}$. The presence of perturbing potential

bigger than 0.1 V/Å, can lead to mixing the states of energies and breaking the symmetry of SWCNT/Carboxyl. This results makes SWCNT/Carboxyl material an semiconductor with band gap modulated by an E_{ext} effects. Exploiting these results, for developing the photodetectors devices based on SWCNT material.

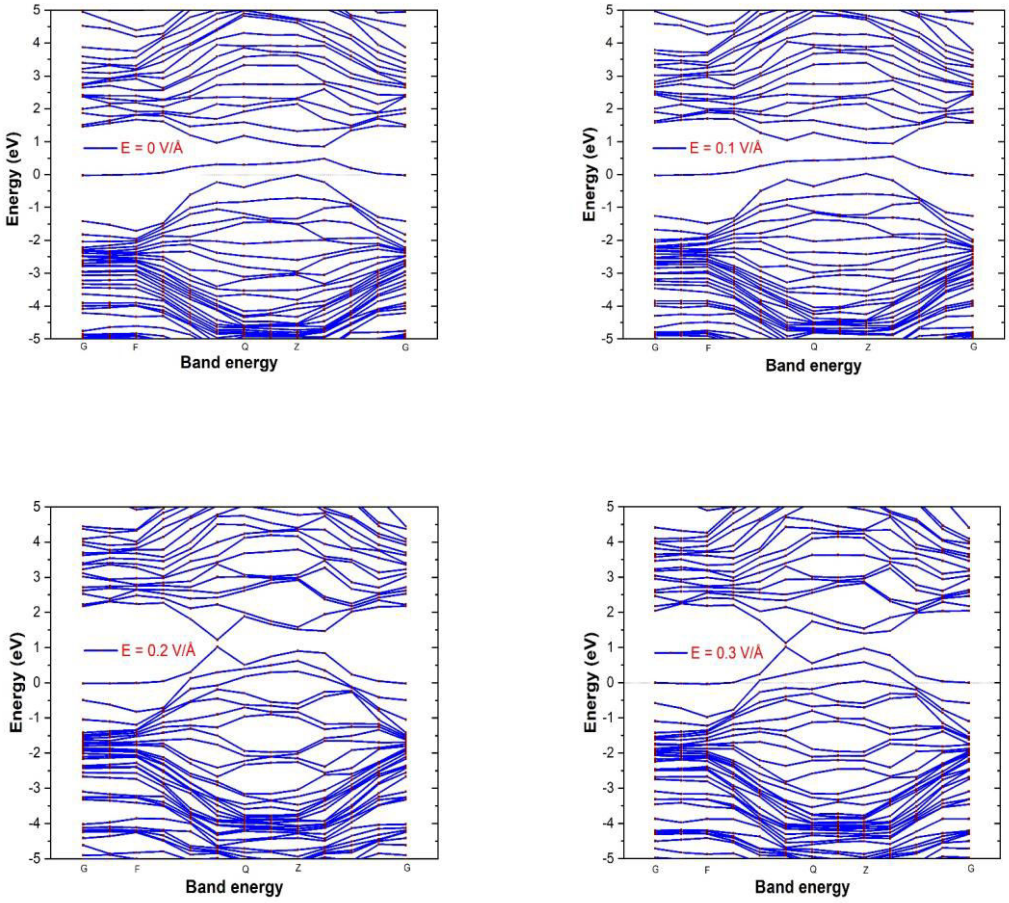

Fig 2. Band gap energies of SWCNT/Carboxyl structure, under an E_{ext} effects applied in z direction.

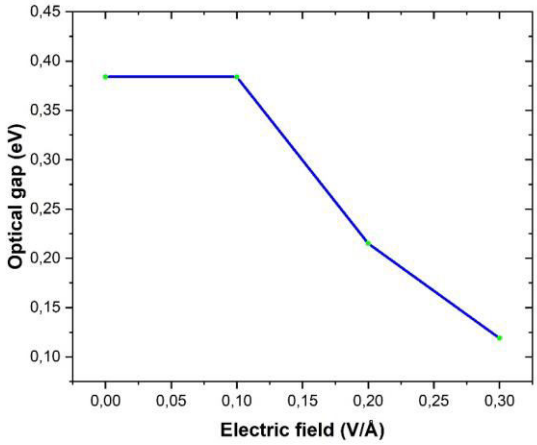

Fig 3. The variation of band gap energy as a function of the E_{ext} effects.

3.1.2 Density of stats

The concept of density of states, corresponds to the number of allowed electron energy states per unit energy interval around an energy E. The TDOS and PDOS of SWCNT/Carboxyl structure, under an E_{ext} effects values 0 V/Å, 0.1 V/Å, 0.2 V/Å and 0.3 V/Å applied in z direction, are plotted in Fig 4 and Fig 5, respectively. The TDOS near the Fermi level exhibits low population, by reason of the semiconducting characteristic of SWCNT/Carboxyl material. The probability of occupation the electronic states, increases for the electrons and decreases for the holes, around the Fermi level, by an E_{ext} effects applied on SWCNT/Carboxyl Fig 4. which confers the reduction of band gap energy by the effects of E_{ext}.

The PDOS which is essentially the local DOS for each individual atom in SWCNT/Carboxyl, can provide additional insight into any observed changes in electronic structure Fig 5. The states of all atoms around the Fermi level, primarily originate from the valence electron orbitals of SWCNT/Carboxyl structure. So, we focused on them for plotting the PDOS. The peaks of PDOS-s increase around the Fermi level by the effects of E_{ext}, which indicates an increases of the probability for being occupied 2p orbitals by the electrons of 2s shell.

The carbon atom of SWCNT gains the electrons, while the oxygen atoms of the carboxyl group lost the electrons, by the E_{ext} effects. The loss of electrons by oxygen atoms comes from O 2p orbitals, and the gain of electrons by carbon atoms is attributed to C 2p orbitals under the E_{ext} effects. The electrons number lost by oxygen atoms or gained by carbon atoms of SWCNT/Carboxyl increases by the E_{ext} effects. The electron transfer behavior can be characterized by electron density difference Fig.5. The results clarify the strong effect of the E_{ext} on electronic properties of SWCNT/Carboxyl material.

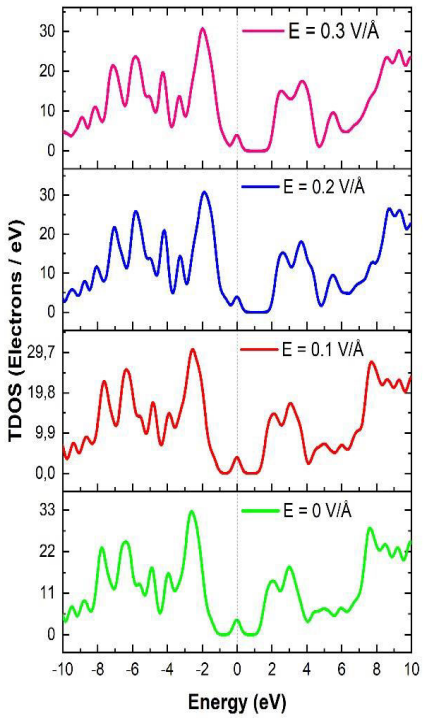

Fig 4. Calculated TDOS as a function of frequency of SWCNT/Carboxyl under the E_{ext} .

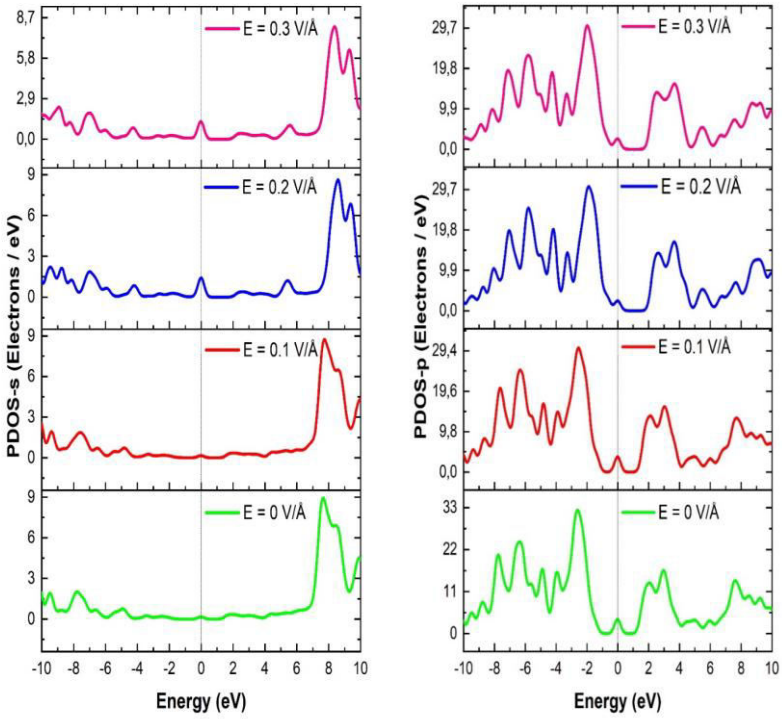

Fig 5. Calculated PDOS-s and PDOS-p as a function of frequency of SWCNT/Carboxyl under the E_{ext}.

3.2 Optical properties

3.2.1 Absorption

In the present study, we have presented the variation of the absorption coefficient of SWCNT/Carboxyl structure, under an E_{ext} effects applied in z direction and plotted in 0 - 8 eV range, as shown in Fig 6. The absorption spectrum without the effects of E_{ext}, consist of two peaks with different intensities. A first peak at 1.735 eV, and the second peak with height intensity located at 4.411 eV. The origin of these peaks arises from two important transitions, that occur between the electronic states. The first peak, corresponds to the transition of electrons from occupied states, n to unoccupied states, n* in the conduction band. The second broad peak, corresponds to the electrons transition of C-C bonds in sp^2 hybrid regions, from π-π* states close to the Fermi level. According to these two peaks, the SWCNT/Carboxyl exhibits strong light absorption in both UV and visible ranges. The intensity of absorption peaks in UV range, decreases by reason of an increases of interaction between the valence electrons and nucleus in SWCNT/Carboxyl material, under the E_{ext} effects. On the other hand, the peaks of the absorption coefficient increases in the visible range, due to the decreases of band gap energy and by reason of electrons number displace from the valence band to the conduction band, increases under the effects of E_{ext}.

The application of an E_{ext} effects of the SWCNT/Carboxyl in z direction, leads to a redshift of the absorption edge. This result, is confirmed by a decreases of band gap energy. These results demonstrate that the E_{ext} effects, can be effectively used to modify the absorption of SWCNT/Carboxyl. Finally, the effects of the E_{ext} enables us to increase the strong light absorbing capacity of SWCNT/Carboxyl material, which is essential for the photo-induced applications, such as the solar cells.

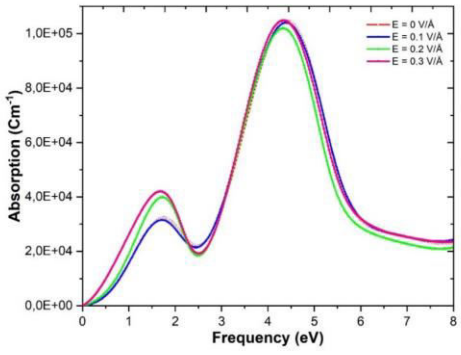

Fig 6. The absorption coefficient of SWCNT/Carboxyl structure under an E_{ext} applied in z direction.

3.3.2 Dielectric function

The complex frequency dependent the dielectric function, $\varepsilon(\omega)$ can be used to descript the optical properties of 1D-material. It determines the dispersion effects by its real part $\varepsilon_1(\omega)$ and the absorption by its imaginary part $\varepsilon_2(\omega)$. The complex dielectric function $\varepsilon(\omega)$ is the sum of real and imaginary part:

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) \quad (2)$$

In the present work, the $\varepsilon(\omega)$ of SWCNT/Carboxyl under an E_{ext} effects applied in z direction, was calculated in 0 - 8 eV range and presented in Fig 7. At low energies, $\varepsilon(\omega)$ associated of electronic intraband transitions in the conduction band. In this spectral range, the optical response dominated by the free electron behavior. But, at higher energies, $\varepsilon(\omega)$ reflects the electronic interband transitions. The application of an E_{ext} effects in z direction of SWCNT/Carboxyl, lead to decreases the peaks of $\varepsilon_1(\omega)$ in the visible range, by reason of the increases of interaction between the electrons and the incident photons, which decreases the dispersion of visible light in this material. The $\varepsilon_2(\omega)$ part has two peaks in 0-8 eV range, are always related to the electron excitation. Additionally, the peaks of $\varepsilon_2(\omega)$ increases in visible range, by the effects of E_{ext} applied in z direction. These results show the remarkable enhanced abilities to absorb the photons by SWCNT/Carboxyl material, in the visible area under an E_{ext} effect applied in z direction. So, we can introduce the SWCNT/Carboxyl material in the transparent conducting films and photovoltaics devices.

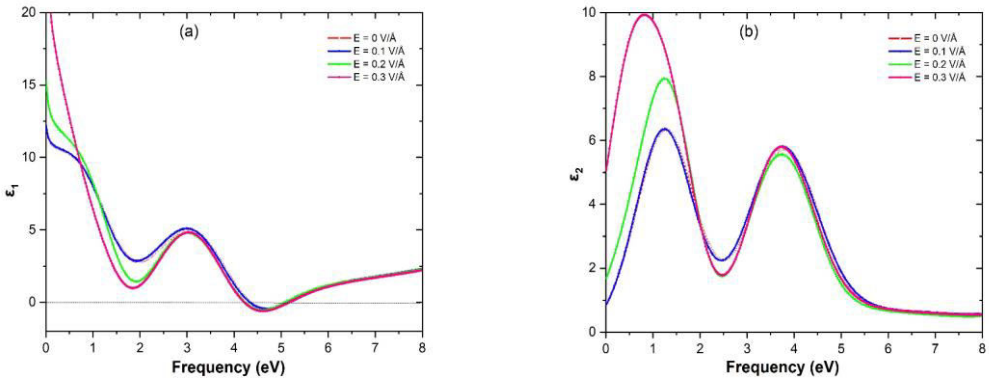

Fig 7. Calculated $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ of SWCNT/Carboxyl under an E_{ext} effects applied in z direction.

3.3.3 Refractive index

Propagation in absorbing materials can be described using a complex-value of refractive index

$n^*(\omega)$, The imaginary part, $k(\omega)$ then handles the attenuation while the real part, $n(\omega)$ accounts for refraction by [16]:

$$n^*(\omega) = n(\omega) + ik(\omega) \tag{3}$$

$$n(\omega) = \sqrt{\frac{|\varepsilon(\omega)| + \varepsilon_1(\omega)}{2}} \tag{4}$$

$$k(\omega) = \sqrt{\frac{|\varepsilon(\omega)| - \varepsilon_1(\omega)}{2}} \tag{5}$$

The variation of refractive index, $n(\omega)$ and extinction coefficient, $k(\omega)$ of SWCNT/Carboxyl under an E_{ext} effects applied in z direction, as a function of frequency are calculated using CASTEP code and plotted in Fig 8. The both values $\varepsilon_1(0)$ and $n(0)$ validate the relation $n = \sqrt{\varepsilon_1}$ Tab 2. The $n(\omega)$ part was varied as a function of frequency under an E_{ext} applied on SWCNT/Carboxyl structure. Hence, this material is a dispersive medium, and its dispersion was influenced by the E_{ext} effects.

The refractive index of SWCNT/Carboxyl under an E_{ext} applied in z direction is greater than 0.846, by reason of the energy of photons incident $E = h\nu > 5.251$ eV, lead to create a reflexion of light on the particles inside the SWCNT/Carboxyl. The increases of the E_{ext} on the SWCNT/Carboxyl, lead to decrease $n(\omega)$ part in the visible range, by reason of the increase of the interaction and the collision between the incident photons and electrons inside the SWCNT/Carboxyl, which lead to increases the velocity of electrons $(v = \frac{c}{n})$. In addition, the $k(\omega)$ part increases in the visible region, by reason of the decreases of band gap energy under the E_{ext} effects Fig 8. When we analyse the graphs of $\varepsilon_2(\omega)$ and $k(\omega)$ parts, a similar physical behavior is observed in Fig 7 and Fig 8. These two physical quantities give the information of the absorption light by SWCNT/Carboxyl material.

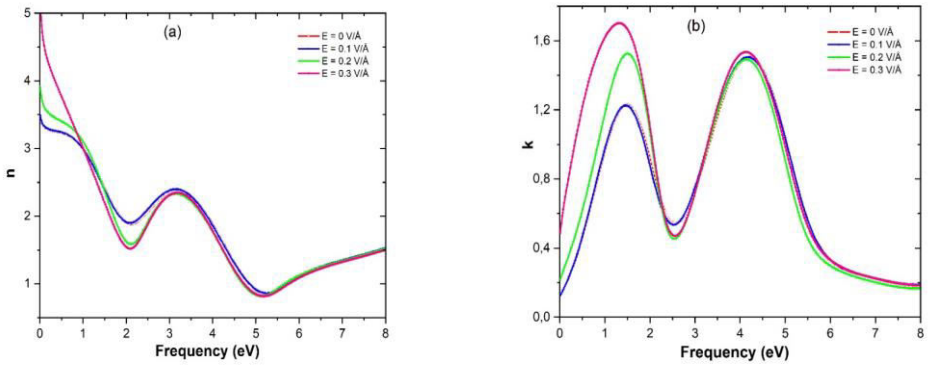

Fig 8. Calculated $n(\omega)$ and $k(\omega)$ of SWCNT/Carboxyl under the E_{ext} effects.

Parameters	$E_{\perp}$			
E (V/Å)	0	0.1	0.2	0.3
$n(0)$	3.485	3.493	3.913	5.217
$\varepsilon_1(0)$	12.130	12.189	15.271	26.981

Tab 2. Static dielectric constant $\varepsilon_1(0)$ and refractive index $n(0)$ of SWCNT/Carboxyl.

3.3.4 Conductivity

It is interesting to know the complex optical conductivity $\sigma(\omega)$ of SWCNT/Carboxyl material, because we can derive valuable physic information's from it. The conductivity $\sigma(\omega)$ is given by following relation [17]:

$$\sigma(\omega) = \sigma_1(\omega) + i\sigma_2(\omega) \tag{6}$$

$$\sigma_1(\omega) = 2nk\left(\frac{\omega}{4\pi}\right) \tag{7}$$

$$\sigma_2(\omega) = [1 - (n^2 - k^2)]\left(\frac{\omega}{4\pi}\right) \tag{8}$$

The real $\sigma_1(\omega)$ and imaginary $\sigma_2(\omega)$ parts of optical conductivity are calculated of SWCNT/Carboxyl structure, under an E_{ext} effects applied in z direction, and are plotted in Fig 9. The first peak of $\sigma_1(\omega)$ appear at 1.536 eV which corresponds to the fundamental band gap, by reason of the interband transitions of the valence electrons. The application of an E_{ext} on the SWCNT/Carboxyl structure in z direction, lead to increases the $\sigma_1(\omega)$ part in the visible range, by reason of the increases of electrons number, and by the decreases of energy difference between valence band and conduction band. The $\sigma_2(\omega)$ part has two peaks in 0-8 eV range. The first peak has a negative value in the visible range, by reason of well-distributed charge in SWCNT/Carboxyl material. The application of the E_{ext} effects increase the $\sigma_2(\omega)$ peaks in the visible range, by reason of the increases radiation scattering, such as the visible light.

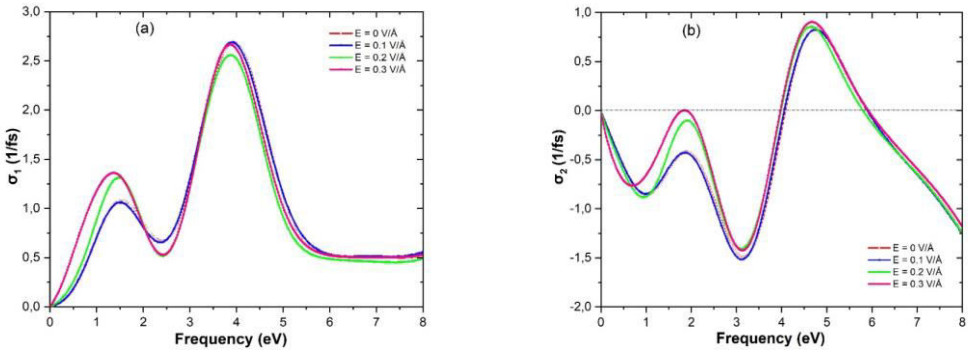

Fig 9. Calculated σ of SWCNT/Carboxyl structure under an E_{ext} applied in z direction.

3.3.5 Loss function

The loss function $L(\omega)$ describes the energy loss of a fast electron traversing a material. From the real and imaginary parts of complex dielectric function, $L(\omega)$ can easily be obtained by [18]:

$$L(\omega) = -Im\left(\frac{1}{\varepsilon(\omega)}\right) = \frac{\varepsilon_2(\omega)}{\varepsilon_1^2(\omega)+\varepsilon_2^2(\omega)} \quad (9)$$

Calculated $L(\omega)$ function of SWCNT/Carboxyl structure, under an E_{ext} effects applied in z direction, as shown in Fig 10. The origin of several peaks of $L(\omega)$ are due to the collective excitations for various frequency of the incident photons. The $L(\omega)$ function has two peaks approximately at 2.044 and 5.406 eV respectively, which are associated of the plasma frequency. These peaks indicate the maximum energy lost inside SWCNT/Carboxyl material, by reason of the interaction of radiation (incident photons) with matter (different particles in SWCNT/Carboxyl). In the visible range, the energy loss increases under the E_{ext} effects, for the reason that the increases of absorption of photons by this material. A peak in the $L(\omega)$ function corresponds to a dip of the real part of dielectric function Fig 7 and Fig 10.

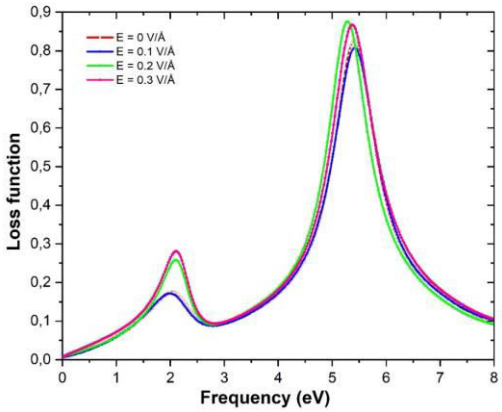

Fig 10. Calculated $L(\omega)$ of SWCNT/Carboxyl structure under an E_{ext}.

4 Conclusions

In conclusion, we have studied the electronic and optical properties of SWCNT/Carboxyl structure, under an E_{ext} effects applied in z direction, by using the DFT calculations. The application of an E_{ext} produces deferent results, in both band structure and optical properties of this 1D-material. We have shown that the structure is a semiconductor, and the band gap can be significantly modified by the

E_{ext} effects. We observed the changes in dielectric function, by reason of a decreases of band gap energy. The intensity of absorption peak increases, by the E_{ext} effects applied in z direction of SWCNT/Carboxyl. We have explored the possibility to control electronic and optical properties of SWCNT/Carboxyl material, using the E_{ext} effects. This study is more important in the interpretation of experimental results of 1D-materials field. These results, lead to include the SWCNT/Carboxyl in many application, such as the optoelectronic devices.

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Contribution statement

The authors have approved the manuscript and agree with submission to your esteemed journal. There are no conflicts of interest to declare. All authors have participated in (a) conception and design, or analysis and interpretation of the data; (b) drafting the article or revising it critically for important intellectual content; and (c) approval of the final version.

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