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Optical Properties of Peapods

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Abstract: Optical and nonlinear optical properties of materials are important because they are used for the development of electronic and photonic technologies. Development of these technologies depends heavily on the important and effective factors that can lead to a substantial increase in polarization . We investigate the first-order polarization with using SSH method , for open and close peapod study and we have shown that the polarization of the open peapod far larger close peapod that can be used in making these types of technologies.

Key words: Optical properties · Peapods · Polarization · SSH method

INTRODUCTION

In recent years structural and properties of fullerenes and also peapods has attracted attention of many scientists in physics and chemistry to research electronic, optical, mechanical properties and other properties. Due to the unique structure of fullerenes, this material in various sciences such as the construction of optical components, electronic equipment, medical and pharmaceutical, etc. have been used [1-3]. Single - wall carbon nanotubes (SWCNTs) encapsulating fullerenes say peapod that have new nanostructures . Fullerene peapods, discovered by Smith *et al* [4]. Fullerene encapsulating SWCNTs have attracted considerable interest after the discovery of C60 @SWCNT peapods [5]. Peapod have nanotubes and fullerenes with C_{60} or C_{60} @SWCNT two sides open are and 330 molecules of carbon , it is known that the open peapods (Fig. 1), close peapods are like open peapods but is closed on both sides with carbon molecules to the number of carbon atoms in its molecules to reach 540 (Fig. 2).

In this regard and given the importance of these materials in various sciences, in the electron transport properties of peapods we will consider. Since the development of these technologies is depends heavily on the advances made in materials Nonlinear Optical (NLO), therefore , considerable research efforts have been made to make this type of technology development , including the design and synthesis of molecular-level processors and so on.

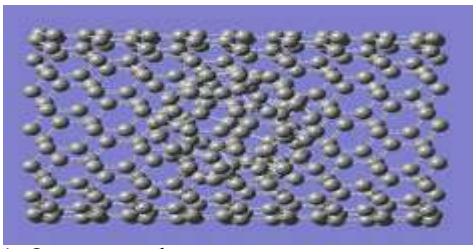
Fig. 1: Open peapod

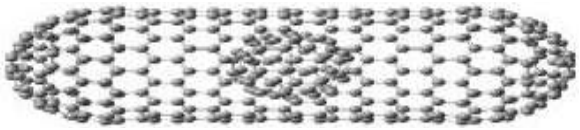
Fig. 2: Close peapod

As recently by researchers in the field of nanotechnology is mentioned a lot of attention peapod capsule form [6-8]. In addition , researchers and scientists working on this issue has been so important and effective factors which led to a substantial increase in polarization is to .In this way we will calculate the polarization of the first- order and use the SSH model, we have calculated the optical properties open and close peapod .

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Theoretical Methods: In the way without Coulomb interaction SSH, approximate Hamiltonian model SSH (Su - Schrieffer - Heeger), model based on the interaction of electrons-phonon with strong techniques in the formulation Hamiltonian C_{60} molecule lack presence of magnetic field can be written as :

$$H_{ssh} = \sum_{(ii)}\left[-t_0 - \alpha y_{i,j}\right]\left(C_i^{\dagger}C_i + H.C\right) + \frac{1}{2}K\left(y_{ij}\right)^2 \quad (1)$$

Here t_0 mutation rate (hopping integral) in the channel region of the C- C bond between the two carbons. α fixed coupling of electron - phonon (electron-phonon coupling constant), K factor, spring constant, $C_{i,s}$ and $C_{i,s}^{\dagger}$ operators of creation and annihilation operator electrons π at ith carbon atoms with spin s and length Change $y_{i,j}$ bond between carbon atoms i and j are location and is close to the <i,j>summation on neighbors. Finally phrase, the elastic energy of the phonon system with spring constant k is a constant factor. Hamiltonian eq. (1) can be approximated by the standard method without adiabatic, the Schrödinger equation may be solved for π electrons [9-12]:

$$\varepsilon_k Z_{ks}(i) = \sum_{(i,j)}\left(-t_0 - \alpha y_{i,j}\right)Z_{ks} \quad (2)$$

In particular ϵ_k values of k th mode Z_{ks}electron wave function is related to it. The total energy C_{60} molecule as a function of $y_{i,j}$obtained from the following equation:

$$E_T\left(y_{ij}\right) = 2\sum_k^i \varepsilon_k + \sum_{(i,j)}\frac{k}{2}y_{ij}^2 \quad (3)$$

Primed sign indicates that summation is only over the occupied levels. Using the equation Schrödinger For the total energy we have:

$$E_T\left(y_{ij}\right) = 2\sum_{k,s}^{i} + \sum_{(i,j)}\left(-t_0 - \alpha y_{i,j}\right)Z_{ks}(i) + \sum_{(i,j)}\frac{k}{2}y_{ij}^2 \quad (4)$$

The minimization of the total energy E_T of all y_{ij} and Lagrange undetermined coefficients $\Psi = \sum_{(i,j)} y_{ij}$ that the constraint is satisfied, the Lagrange equations can be written as follows:

$$\frac{\partial E_T}{\partial y_{ij}} + \lambda\frac{\partial \psi}{\partial y_{i,j}} = 0 \quad (5)$$

We have:

$$2\sum_{k,s}^{i} + \sum_{(i,j)} -\alpha Z_{ks}(i)Z_{ks}^{*}(i) + \sum_{(i,j)} ky_{i,j} + ?\sum_{(i,j)} 1 = 0 \quad (6)$$

considering $\sum_{(i,j)} 1 = N$, where N is the total number of nearest neighbor bonds.We have:

$$\lambda = \frac{1}{N}\sum_{k,s}^{i}\sum_{(i,j)} -\alpha Z_{ks}(i)Z_{ks}^{*}(i)) \quad (7)$$

Put the equation in (3-6) we have:

$$\sum_{(i,j)}\begin{bmatrix}\sum_{k,s}^{i} -\alpha Z_{ks}(i)Z_{ks}^{*}(i) + \sum_{(i,j)} Ky_{ij} + \lambda\frac{1}{N} \\ \sum_{(i,j)} -\alpha Z_{ks}(i)Z_{ks}^{*}(i)\end{bmatrix} = 0 \quad (8)$$

In view of the above equation to reach a series of self- equations for y_{ij} follows:

$$y_{ij} = \frac{2\alpha}{k}\sum_{k,s}^{i} Z_{ks}(i)Z_{ks}^{*}(i) - \Delta y \quad (9)$$

That:

$$\Delta y = \frac{1}{N}\sum_{(i,j)}\frac{2\alpha}{K}\sum_{k,s}^{i} Z_{ks}(i)Z_{ks}^{*}(i) \quad (10)$$

Here N =220 total number of bonds π is in the open peapod molecule and N =360 total number of bonds π in the close peapod molecule. Coupled equations (2) and (9) and (10) can be solved to replicate .These values, have in good agreement with other methods like methodology LDA and strong correlation method [13-17].

(t_0) value jumps between nearest neighbor carbon atoms C-C bonds the molecule put equal 2.5 ev. Size of the binding constant of electron - phonon is considered $\alpha_0 = 3031\frac{ev}{A^o}.(V_0)$ the quantity of Coulomb force intensity

between nearest neighbors and the positions i and j equal t_0 and value Coulomb repulsion force in any situation (U_0) doubled t_0 choose form $U_0 = 2V_0 = 2t_0$ .The amount of heat that is selected in the Fermi function comes T = 300k . The connection between nearest the atomic positions of the electrodes t_0 and between the molecule and the electrodes t' consider[18-21].

RESULT AND DISCUSSION

According to calculations done by polarization diagrams, we draw real and imaginary parts of the polarization and peapod mean that the results are as follows. The following Table (1) and first-order polarization properties of the real and imaginary parts of the polarization open and close peapod for the two higher peaks were collected. The first-order linear polarization curves for open and close peapod in directions X, Y, Z is plotted are observed first-order polarization in directions y, z for the real and imaginary parts of the spectrum for open and close peapod are equal.

According to the cylindrical shape of peapod result could be due to the symmetry in the Y, Z and also it can be related to isotropic molecules open and close peapods[22-25].

As shown in Table (1) and figures in above the peaks seen for open and close peapods, value of the polarization and average of energy real and imaginary parts of open peapods the are larger close peapods . Here we open and close peapods curves in the same directions (directions of X open and close peapods etc.), both for the real and imaginary parts are compared . However these cases peapods moreover , the same will happen again.

If we compare the polarization of open and close peapod real part, we find that peak of energy for open peapod 0.98ev and peak close peapod 0.48ev be seen in the far polarization of open peapod is higher than close peapod .

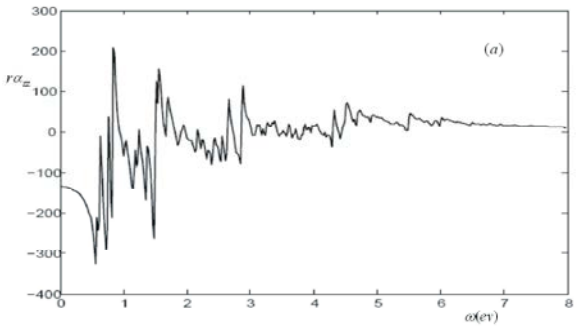
The imaginary part also the peak of energy open peapod 0.86ev and close peapod 0.46ev is that open peapod polarization is larger close peapod .With respect to the polarization relations, because energy transfer at denominator impact , then the is an important factor affecting there upon the optical properties of open peapod is older close peapods [26-27].

Furthermore , open peapod average polarization larger is of close.

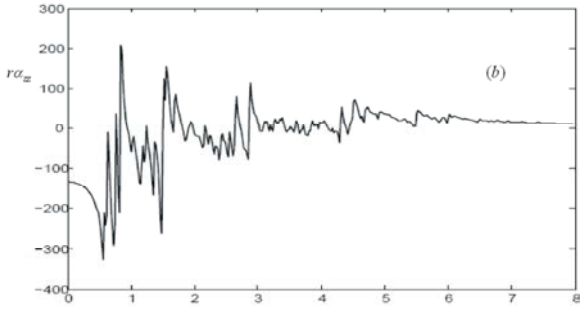
Charts rα_{zz} and rα_{yy} and rα_{xx} and mean in terms of energy (ev) is drawn. Should be noted that r = real and I = imaginary

Table 1: First-order polarization real and imaginary parts for open and close peapod

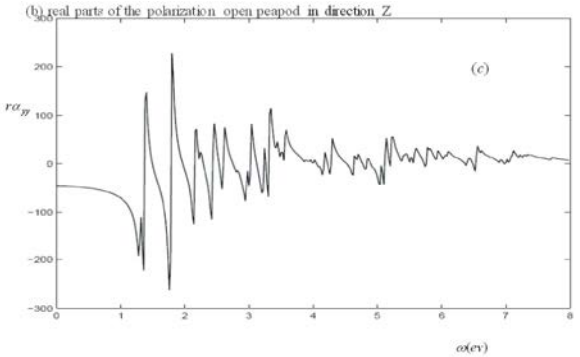
			Peapod-close				
a/E	ra_{xx}	ra_{yy}	ra_{zz}	ia_{xx}	ia_{yy}	ia_{zz}	$\overline{V}$
α_1/E_1	0.24	0.86	0.86	0.22	0.76	0.86	0.22
α_2/E_2	0.48	1.58	1.58	0.46	1.52	1.52	0.46
			Peapod-open				
a/E	ra_{xx}	ra_{yy}	ra_{zz}	ia_{xx}	ia_{yy}	ia_{zz}	$\overline{V}$
α_1/E_1	0.08	1.82	1.82	0.06	1.4	1.4	0.04
α_2/E_2	0.98	1.42	1.42	0.98	1.8	1.8	0.96



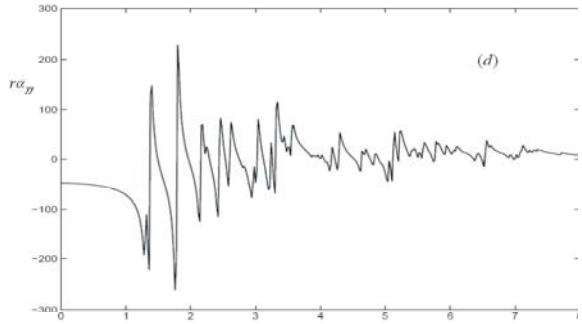
(a): Real part of the polarization chose peapod in direction Z



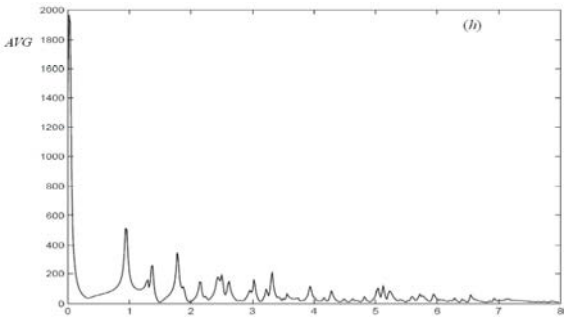
(b): Real part of the polarization open peapod in direction Z



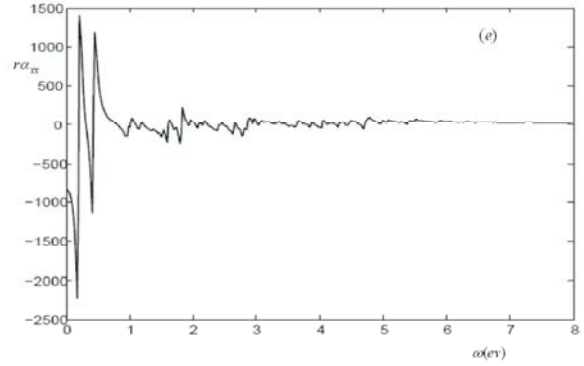
(c): Real part of the polarization chose peapod in direction Y



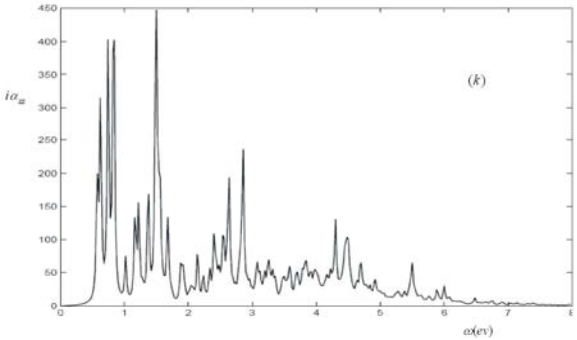
(d): Real part of the polarization open peapod in direction Y



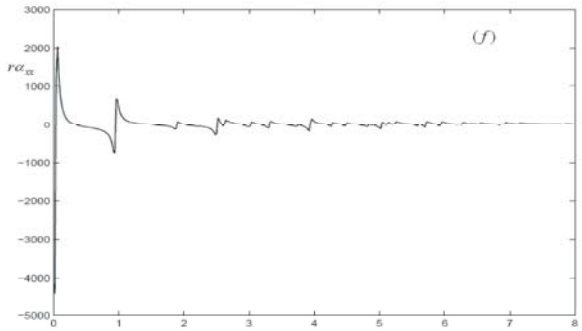
(h): Arerage part of the polarization open peapod



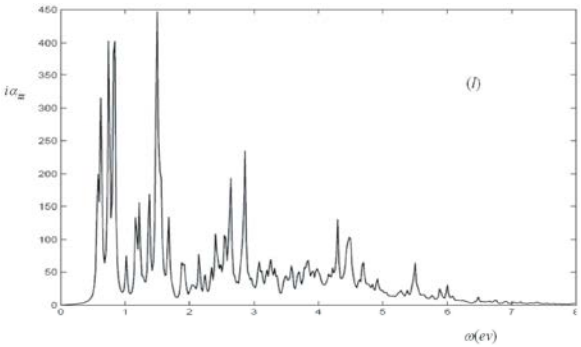
(e): Real part of the polarization chose peapod in direction X



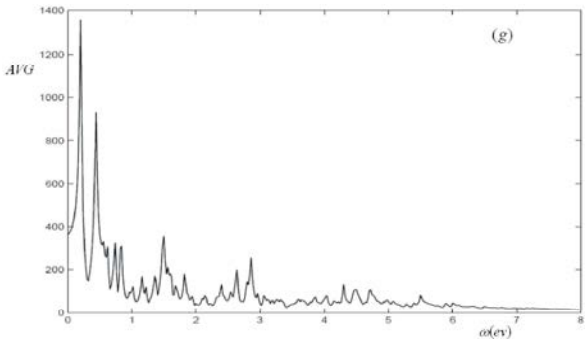
(k): Imaginary part of the polarization close peapod in direction Z



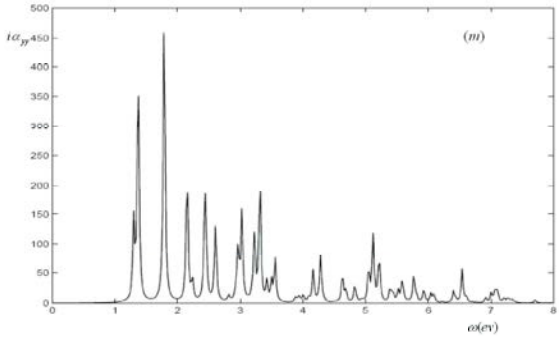
(f): Real part of the polarization open peapod in direction X



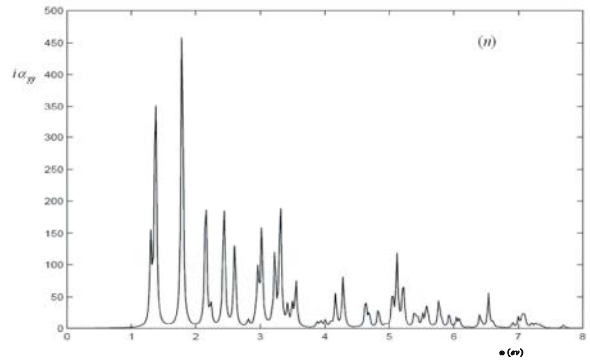
(I): Imaginary part of the polarization open peapod in direction Z



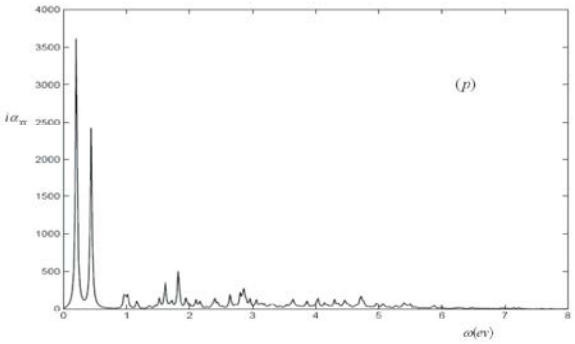
(g) Arerage part of the polarization close peapod



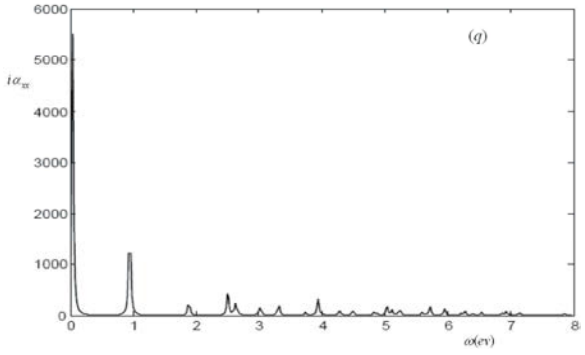
(m): Imaginary part of the polarization colse peapod in direction Y



(n): Imaginary part of the polarization open peapod in direction Y



(p): Imaginary part of the polarization colse peapod in direction X



(q): Imaginary part of the polarization open peapod in direction X

The following forms the charts $r\alpha_{zz}$ and $r\alpha_{yy}$ and $r\alpha_{xx}$ and average in terms of energy (ev) for open peapod, both for the real and imaginary parts are plotted.

CONCLUSION

Because for the development of technologies photon and electron in clouding its design at the molecular level synthesis ,process or sand so the development of these technologies is highly dependent upon advances made in materials Nonlinear Optical NLO, so considerable effort in research for this type of technology development is occurring.

We plan on using the polarization properties peapod SSH method opened and closed without and with Coulomb interactions were evaluated computation . As noted increased polarization and its many applications are in the field of optics . peapod results show that the polarization is much larger than peapod close (both the real and imaginary parts) can be considered to researchers peapod open win could open peapod interesting properties for electronic and optical parts and etc. Used, then the best option would be peapod.

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