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Orbital Effect on Carbyne Based Sensor

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Abstract

Carbyne material with sp-hybridized atoms has been considered as a one dimensional structure with unique properties which has been widely used in nanotechnology. In the presented work the effect of electron overlap energy in the form of electron interaction with in the unit cell and nearest neighbors is explored. In addition, the band structure variation under proposed interaction in one dimensional carbyne is investigated. The effect of overlap energy variation inside and outside the unit cell on the band gap is intended. Under proposed structure the effective mass and density of states parameters are explored. It is demonstrated that by increasing the interaction between s and p orbitals in the unit cell, the band gap increases. However, the band gap is decreased by increasing the interaction between s and p orbitals out the unit cell which can be sued as a sensing mechanism.

Keyword: Carbyne, Orbital effect, Bandgap, Effective mass, One Dimensional.

Introduction

Innovative category of carbon allotropes arranged in one dimensional chain with strong chemical action called carbyne with bulk production has been reported [1-3]. Its electrical property rarely compare to the other carbon based 1D structures such as nano-tubes and nano-ribbons has been explored [1-3]. Carbyne sp-hybridization is observed when one s and one p orbital in the same main shell of an atomic structure mixed to make two new equivalent orbitals. The new orbitals are called sp-hybridized orbitals [4] that can explain the linear structure in the molecule [5-8]. One of the factors that facilitate the overlap between two atomic orbital is the distance between the orbitals [8-9] which manipulates the energy gap and changes the specified state of the system to another. In this study, band gap variation in SP² carbyne structures [10] is as shown in figure 1 is focused.

Figure 1. SP^2 bonded carbyne atoms [10].

Model and formalism

Figure 2 depicts the chain of the unit cell, each unit cell has two atoms A and B. Note that each atom has three orbitals (SP^2) and their molecular interaction is also considered.

Figure 2. The geometry of the model.

The Hamiltonian form of two atoms in one-dimensional nanostructure is as follows:

$$\begin{aligned}
H = & E_0 \sum_{n=1}^N [|A_n S\rangle\langle A_n S| + |A_n P_x\rangle\langle A_n P_x| + |A_n P_y\rangle\langle A_n P_y| \\
& + |B_n S\rangle\langle B_n S| + |B_n P_x\rangle\langle B_n P_x| + |B_n P_y\rangle\langle B_n P_y|] \\
& + t \sum_{n=1}^N [|A_n S\rangle\langle A_n P_x| + |A_n S\rangle\langle A_n S| \langle A_n P_y| + |B_n S\rangle\langle B_n P_x| + \\
& |B_n S\rangle\langle B_n P_y| + |A_n S\rangle\langle B_n S| + |A_n P_x\rangle\langle B_n P_x| + |A_n P_y\rangle\langle B_n P_y|] \\
& + t' \sum_{n=1}^N [|B_n S\rangle\langle A_{n+1} S| + |B_n S\rangle\langle A_{n+1} P_x| + |B_n S\rangle\langle A_{n+1} P_y| + \\
& |B_n P_x\rangle\langle A_{n+1} S| + |B_n P_x\rangle\langle A_{n+1} P_x| + |B_n P_x\rangle\langle A_{n+1} P_y| + \\
& |B_n P_y\rangle\langle A_{n+1} S| + |B_n P_y\rangle\langle A_{n+1} P_x| + |B_n P_y\rangle\langle A_{n+1} P_y|]
\end{aligned}
\tag{1}$$

Each atom in the unit has S, P_x , P_y spins. Within each unit cell, the spin of any atom affects another atom. The effects of S and P spins are considered to be the same. The effects of the spins of atoms A and B on each other within each unit cell are shown with t. The effects of the atom B from first unit cell to the atom A from the second unit cell are shown by t' . Also, E_0 is on-site energies for each atom. Considering this description, we define the matrix of Hamiltonian in the form blow:

$$H = \begin{pmatrix} E_0 & t & t & t & t & t & 0 & 0 & 0 & 0 & 0 & 0 & \dots \\ t & E_0 & t & t & t & t & 0 & 0 & 0 & 0 & 0 & 0 & \dots \\ t & t & E_0 & t & t & t & 0 & 0 & 0 & 0 & 0 & 0 & \dots \\ t & t & t & E_0 & t & t & t' & t' & t' & 0 & 0 & 0 & \dots \\ t & t & t & t & E_0 & t & t' & t' & t' & 0 & 0 & 0 & \dots \\ t & t & t & t & t & E_0 & t' & t' & t' & 0 & 0 & 0 & \dots \\ 0 & 0 & 0 & t' & t' & t' & E_0 & t & t & t & t & t & \dots \\ 0 & 0 & 0 & t' & t' & t' & t & E_0 & t & t & t & t & \dots \\ 0 & 0 & 0 & t' & t' & t' & t & t & E_0 & t & t & t & \dots \\ 0 & 0 & 0 & 0 & 0 & 0 & t & t & t & E_0 & t & t & \dots \\ 0 & 0 & 0 & 0 & 0 & 0 & t & t & t & t & E_0 & t & \dots \\ 0 & 0 & 0 & 0 & 0 & 0 & t & t & t & t & t & E_0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}
\tag{2}$$

So, the general form of the Hamiltonian matrix is:

$$H = \begin{pmatrix} H_{11} & H_{12} & H_{13} & 0 & 0 & 0 & 0 \\ H_{21} & H_{22} & H_{23} & 0 & 0 & 0 & 0 \\ 0 & H_{32} & H_{33} & H_{34} & 0 & 0 & 0 \\ 0 & 0 & 0 & \ddots & \dots & 0 & 0 \\ 0 & 0 & \dots & H_{nn-1} & H_{nn} & H_{nn+1} & \dots \end{pmatrix} \quad (3)$$

We define the H_{nn-1} , H_n , H_{nn+1} matrix in the form of 6×6 matrices as follows:

$$H_{nn-1} = \begin{pmatrix} 0 & 0 & 0 & t' & t' & t' \\ 0 & 0 & 0 & t' & t' & t' \\ 0 & 0 & 0 & t' & t' & t' \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (4)$$

$$H_{nn} = \begin{pmatrix} E_0 & t & t & t & t & t \\ t & E_0 & t & t & t & t \\ t & t & E_0 & t & t & t \\ t & t & t & E_0 & t & t \\ t & t & t & t & E_0 & t \\ t & t & t & t & t & E_0 \end{pmatrix} \quad (5)$$

$$H_{nn+1} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ t' & t' & t' & 0 & 0 & 0 \\ t' & t' & t' & 0 & 0 & 0 \\ t' & t' & t' & 0 & 0 & 0 \end{pmatrix} \quad (6)$$

In accordance to Schrödinger's equation, the energy Eigen value can be calculated as:

$$H|\Psi\rangle = E|\Psi\rangle \quad (7)$$

Wave function of system is given by Eq. (4).

$$\Psi_n = \Psi_0 e^{i\vec{k} \cdot \vec{r}_n} \quad (8)$$

By solving the above equation, the following relation is obtained:

$$H_{nn-1} \Psi_{nn-1} + H_{nn} \Psi_{nn} + H_{nn+1} \Psi_{nn+1} = EI \Psi_n \quad (9)$$

Where I is the unit matrix. After solving the above equation, we get a fourth order equation as follows:

$$(E_0 - E)^4 + t^2(E_0 - E)^2 - t^3(E_0 - E) + t^2 t'^2 + t^3 t' 2 \cos(k.a) + t^4 = 0 \quad (10)$$

$$(E_0 - E)^4 + t^2(E_0 - E)^2 - t^3(E_0 - E) + t^4(2 + 2 \cos(k.a)) = 0 \quad (11)$$

After solving the fourth order equation and considering that the amount of energy in the band gap E_0 between the carbon atoms is 1 and the lattice parameter is 0.142, the energy equation is given in the form below:

$$E = \mp \left(\left((t^4 - 4t^2 - 8 \cos(71k / 500) t t' - 4t^2)^{1/2} + t^2 \right) / 2t \right) \quad (12)$$

According to above equation, the total energy is depended on the energy in the cell unit (t) and energy out of the unit cell (t'). The relation (12) is plotted for different values of t , and t' . The diagram of dispersion relation with respect to the wave vector K_x for various values of t and t' will be as follow. At first, the expression of interaction between the orbital s and p outside the unit cell (t') is fixed and equal to one, and the curves are plotted for different values of t . Figure 3 shows the band structure for $t' = 1$ and different values of t .

Figure 3. (a) Energy curves for $t = 3.01$ and $t' = 1$, (b) $t = 3.02$ and $t' = 1$, (c) $t = 3.03$ and $t' = 1$.

By comparing the curves, it is found that the increase in the interaction between the s and p orbitals inside the unit cell (t) will increase the gap between the energy strips, meaning that the energy strips go away. Since the sp -hybridization leads to the stability of the compound. These hybridization orbitals increase the electron density in the graft region to make the sigma band, and leading to a pair of hybrid springs for spin in opposite directions. According to the theory of strips, molecular orbitals differ from the atomic orbits that make them up. The allowed energy states are divided into close states and shape of the orbits changes. These split modes are continuously formed and created wide strips of energy. In orbital molecules, bonding and anti-bonding orbitals are formed and this made energy level multiplicity. Bonding and anti-bonding orbitals create valence and conductive bands. Due to the electrical conductivity, according to the filling of these bands, there are three main groups: metals, semiconductors and insulators. In metal, the band is full and the barrel of the conductive strip is also filled with electrons. But the empty part of the conduction band allows the electrons to move freely with a small amount of energy. As disadvantages, the bonding band is complete and no electron is present in the conduction band. Because the difference in energy between the highest capacity band and the lower in the bandwidth is a lot and the electrons cannot move to the conduction band and move freely. In the semiconductors, the capacity band (at 0 K°) is full, but due to the low bandwidth of the band, the electrons can travel to the conducting band and move freely by gaining a little energy (for example, through heat) [11]. According to these contents, increasing the band gap causes the material to be nonconductor. In Figures 4(a-c), t is constant and equal to 3 and the value of t' increases. This effect will be investigated as a sensing phenomenon in our time in the next research.

Figure 4. Energy curves for (a) $t=3$ and $t'=0.8$, (b) $t=3$ and $t'=0.9$, (c) $t=3$ and $t'=1$.

By examining the shapes, it is understood that energy band gap reduces by increasing of t' . The atomic orbitals are closed to each other and the bonding interaction gets strong. Consequently, the orbital width increases. According to these contents, increasing the band gap causes the material to be conductive. This section deals with calculation of the effective mass for the proposed model. The effective mass can be defined by Eq. (12) as follows:

$$m^* = \hbar \left(\frac{\partial^2 E}{\partial^2 K} \right)^{-1} = (t(8tt' \cos(ka))(t^4 - 4t^2 - 8tt' \cos(ka) - 4t^2)^{-1/2} / (-8tt' \sin(ka))(t^4 - 4t^2 - 8tt' \cos(ka) - 4t^2)^{1/2}) - 1 \quad (13)$$

As shown in figure 5 effective mass can be positive or negative based on the curvature configuration. Figure 5(a) indicates that the effective mass is large in $K_x = 0$ as $t \neq t'$ ($t' = 1$ and $t = -3$), ($t \neq t', K_x = 0 \Rightarrow m^* \rightarrow \infty$). Figures 5b and c indicate the effective mass versus wave vector for ($t' = 1, t = \pm 1$) and ($t' = 0.8, t = 3.03$), respectively. It is noteworthy that the waves are non-dispersive for large effective masses [14, 15]. The variation of energy curvature in the presence of impurities can be employed on the impurity sensing mechanism based on the capacitance measurement by voltage variation [19, 20].

Figure 5. The effective mass against wave vector (K_x) for (a) $t' = 1$ and $t = -3$, ($t \neq t'$), (b) $t' = 1$, and $t = \pm 1$, (c) $t' = 0.8$ and $t = 3.03$.

Conclusion

The behavior of matter can be determined by the basic energy calculation based on the structure investigation. In the presented work, the orbital effect on carbyne band gap is investigated based on the structure energy calculation. It is demonstrated that the increasing interaction between s and p orbitals in the unit cell, makes the band gap affected which powers impurity detection systems come to account. On the other hand, the band gap is decreased by increasing the interaction between s and p orbitals out the unit cell. Also the effective mass variation for different values of orbital interaction in one unit cell and between the different unit cells is investigated. The calculation of effective mass versus wave vector indicates that as $t \neq t'$, the non-dispersive wave is signified at Dirac point ($K_x = 0$).

Declarations

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Availability of data and material: The data that supports the findings of this study are available within the article and reference number.

Code availability: The results of software application are available within the article.

Authors' contributions: The main idea has been suggested by Dr. M.T.Ahmadi. The simulation and obtained results are discussed and supported by Z. Heidari, Dr. M. Rahmani and M. Ahmadi.

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Figures

Figure 1

SP² bonded carbyne atoms [10].

Figure 2

The geometry of the model.

Figure 3

Legend for figure 3 can be found in the manuscript file.

Figure 4

Legend for figure 4 can be found in the manuscript file.

Figure 5

Legend for figure 5 can be found in the manuscript file.