

Review Article

A Review of Electronic Band Structure of Graphene and Carbon Nanotubes Using Tight Binding

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The electronic band structure variations of single-walled carbon nanotubes (SWCNTs) using Huckle/tight binding approximation theory are studied. According to the chirality indices, the related expressions for energy dispersion variations of these elements are derived and plotted for zigzag and chiral nanotubes.

1. Introduction

Carbon nanotubes (CNTs) are graphene sheets rolled up into cylinders with diameter of the order of a nanometer varying from 0.6 to about 3 nm [1]. Depending on their chirality (the direction along which the graphene sheets are rolled up), they can be either metallic with no bandgap, or semiconducting with a distinct bandgap [2].

Because of their extremely desirable properties of high mechanical and thermal stability, high thermal conductivity, and unique electrical properties such as large current carrying capacity [3–7], CNTs have aroused a lot of research interest in their applicability as VLSI interconnects of the future.

Semiconducting CNTs are being extensively studied as the future channel material for ultrahigh performance and scaled field-effect transistors (FETs) and are expected to be the successors of silicon transistors. Interconnect technology has to be commensurately scaled to reap the benefits of these novel transistors. Metallic CNTs have been identified as possible interconnect material of future technology generations and the heir to aluminum (Al) and Cu interconnects [8].

2. The Energy Variations of Graphene

Graphite is a 3D (three-dimensional) layered hexagonal lattice of carbon atoms and a single layer of graphite forms

a 2D (two-dimensional) material, called 2D graphite or a graphene layer [9, 10]. Figure 1 shows the lattice of a graphene sheet in which the two fundamental carbon atoms 1 and 2 are the basic elements of overall lattice and form a unit cell. Thus, the lattice of unit cells is periodic.

Each point on the periodic lattice of Figure 1 can be described by $\vec{R} = m\vec{a}_1 + n\vec{a}_2$ where m and n are two integers, a_1 and a_2 are the two unit vectors which are defined as

$$\begin{aligned}\vec{a}_1 &= a\left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right), \\ \vec{a}_2 &= a\left(\frac{\sqrt{3}}{2}, -\frac{1}{2}\right),\end{aligned}\tag{1}$$

where $a = 2.46 \text{ \AA}$ is the lattice constant of graphene [11]. The tight binding theorem implies that [11]

$$\phi = c_1\phi_1 + c_2\phi_2,\tag{2}$$

where ϕ is the wave function due to the unit cell, and ϕ_1 and ϕ_2 are the wave functions related to the $2p_y$ atomic orbitals of atoms 1 and 2 in Figure 1, respectively, and c_1 and c_2 are two constants. We will be using Bloch's theorem [11]

$$\psi(x) = \sum_R e^{i\vec{k}\cdot\vec{R}} \phi(x - R),\tag{3}$$

where $\psi(x)$ is the total wave function of lattice, \vec{K} is the wave vector, and R is the lattice vector. With considering the overlap between the two above-mentioned orbitals, we will have

$$\begin{aligned}\langle \phi_1(x)|H|\psi(x)\rangle &= \varepsilon\langle \phi_1(x) | \psi(x)\rangle, \\ \langle \phi_2(x)|H|\psi(x)\rangle &= \varepsilon\langle \phi_2(x) | \psi(x)\rangle,\end{aligned}\quad (4)$$

where H is the Hamiltonian operator [11] and ε is the energy dispersion of graphene lattice. Also using the previously mentioned relations, we can write

$$\begin{aligned}\langle \phi_1(x)|H|\psi(x)\rangle &= \varepsilon c_1, \\ \langle \phi_2(x)|H|\psi(x)\rangle &= \varepsilon c_2.\end{aligned}\quad (5)$$

With noticing Huckel/tight binding approximation and the previous relations, we will have

$$\begin{aligned}\langle \phi_1(x)|H|\psi(x)\rangle &= c_1\alpha + c_2\beta\left(1 + e^{-i\vec{K}\cdot\vec{a}_1} + e^{-i\vec{K}\cdot\vec{a}_2}\right), \\ \langle \phi_2(x)|H|\psi(x)\rangle &= c_2\alpha + c_1\beta\left(1 + e^{i\vec{K}\cdot\vec{a}_1} + e^{i\vec{K}\cdot\vec{a}_2}\right).\end{aligned}\quad (6)$$

By substituting (4)–(5) in (6), we can obtain

$$\begin{aligned}c_1(\alpha - \varepsilon) + c_2\beta\left(1 + e^{-i\vec{K}\cdot\vec{a}_1} + e^{-i\vec{K}\cdot\vec{a}_2}\right) &= 0, \\ c_1\beta\left(1 + e^{i\vec{K}\cdot\vec{a}_1} + e^{i\vec{K}\cdot\vec{a}_2}\right) + c_2(\alpha - \varepsilon) &= 0.\end{aligned}\quad (7)$$

For having nonzero responses for the homogenous equation (7), the following condition should be established

$$\begin{vmatrix}\alpha - \varepsilon & \beta\left(1 + e^{-i\vec{K}\cdot\vec{a}_1} + e^{-i\vec{K}\cdot\vec{a}_2}\right) \\ \beta\left(1 + e^{i\vec{K}\cdot\vec{a}_1} + e^{i\vec{K}\cdot\vec{a}_2}\right) & \alpha - \varepsilon\end{vmatrix} = 0.\quad (8)$$

With solving (8), we obtain the total energy dispersion variations as

$$\varepsilon = \alpha \pm \beta\sqrt{3 + \cos(\vec{K}\cdot\vec{a}_1) + 2\cos(\vec{K}\cdot\vec{a}_2) + 2\cos[\vec{K}\cdot(\vec{a}_1 - \vec{a}_2)]}.\quad (9)$$

With considering that

$$\begin{aligned}\vec{K}\cdot\vec{a}_1 &= (k_x + ik_y) \cdot a\left(\frac{\sqrt{3}}{2} + i\frac{1}{2}\right) = \frac{a}{2}(\sqrt{3}k_x + k_y), \\ \vec{K}\cdot\vec{a}_2 &= (k_x + ik_y) \cdot a\left(\frac{\sqrt{3}}{2} - i\frac{1}{2}\right) = \frac{a}{2}(\sqrt{3}k_x - k_y), \\ \vec{K}\cdot(\vec{a}_1 - \vec{a}_2) &= (k_x + ik_y) \cdot (ia) = ak_y,\end{aligned}\quad (10)$$

where $\vec{K} = (k_x + ik_y)$, which k_x and k_y are the wave numbers related to the reciprocal lattice. Therefore, the energy dispersion variations versus k_x and k_y will be obtained as

$$\varepsilon = \alpha \pm \beta\sqrt{3 + \cos\left(\frac{a}{2}(\sqrt{3}k_x + k_y)\right) + 2\cos\left(\frac{a}{2}(\sqrt{3}k_x - k_y)\right) + 2\cos(ak_y)}.\quad (11)$$

In Figure 2, the energy dispersion variations ε in (11) has been plotted versus k_x and k_y in the range of $[-2\pi/a, 2\pi/a]$, using MATLAB [12].

In Figure 3, the primitive unit cell and the Brillouin zone, related to the graphene lattice and the reciprocal lattice of graphene, respectively, have been shown. In this figure \vec{a}_1 and \vec{a}_2 are the unit vectors of the graphene lattice, respectively, and \vec{b}_1 and \vec{b}_2 are the unit vectors of the reciprocal lattice of graphene, respectively.

We can express the reciprocal lattice vectors \vec{b}_1 and \vec{b}_2 versus the lattice vectors \vec{a}_1 and \vec{a}_2 as

$$\begin{aligned}\vec{b}_1 &= 2\pi\frac{\vec{a}_2 \times \vec{z}_0}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{z}_0)}, \\ \vec{b}_2 &= 2\pi\frac{\vec{z}_0 \times \vec{a}_1}{\vec{a}_2 \cdot (\vec{z}_0 \times \vec{a}_1)},\end{aligned}\quad (12)$$

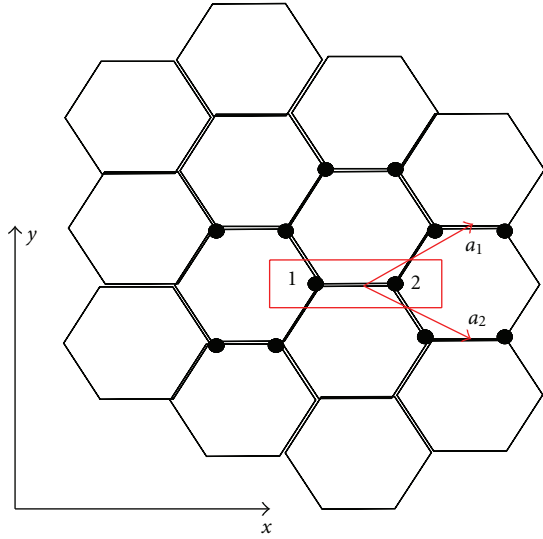


FIGURE 1: The periodic lattice of graphene consisting of the unit cell of two carbon atoms.

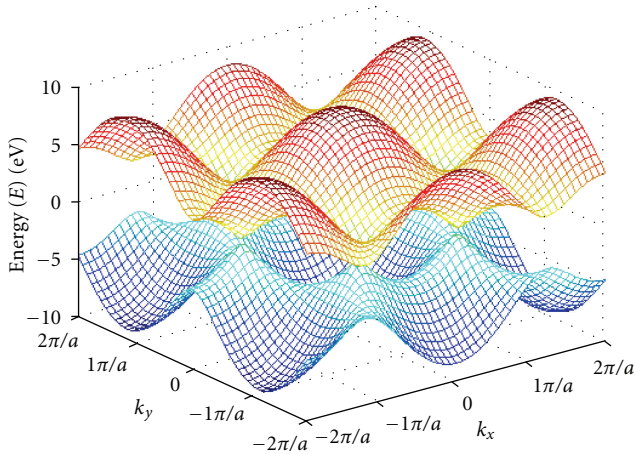


FIGURE 2: The energy dispersion variations of graphene lattice.

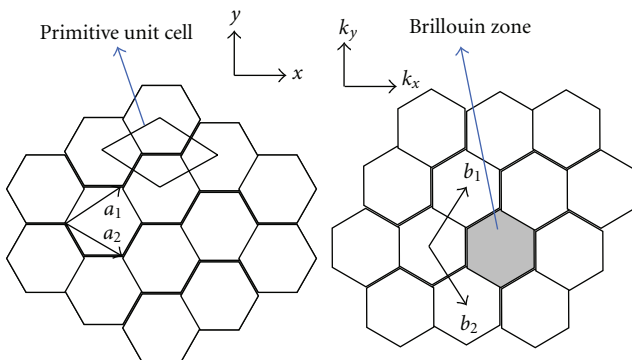


FIGURE 3: The primitive unit cell and the Brillouin zone in graphene.

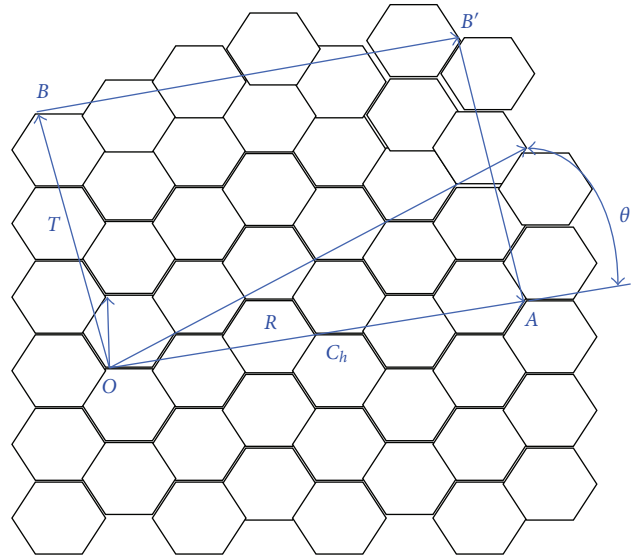


FIGURE 4: Vectors definition of graphene for converting to a carbon nanotube.

where \vec{z}_0 is the unit vector along the z -axis, which will play no important role in our discussion since we talk about the electronic states in the x - y plane assuming that different planes along the z -axis are isolated [9]. By substituting (1) in (12) we will have

$$\begin{aligned} \vec{b}_1 &= \left(\frac{2\pi}{\sqrt{3}a}, \frac{2\pi}{a} \right), \\ \vec{b}_2 &= \left(\frac{2\pi}{\sqrt{3}a}, -\frac{2\pi}{a} \right). \end{aligned} \quad (13)$$

3. The Energy Dispersion Variations of an SWCNT

In Figure 4, the vectors definition of graphene plane for converting to a carbon nanotube has been shown where \vec{C}_h , θ , and \vec{T} are the chirality (circumference) vector, the chirality angle, and the translational vector, respectively. With considering that $OA = |\vec{C}_h|$ and $OB = |\vec{T}|$ we can express \vec{C}_h versus the unit vectors \vec{a}_1 and \vec{a}_2 as

$$\vec{C}_h = n\vec{a}_1 + m\vec{a}_2, \quad (14)$$

where n and m are two integer numbers and are defined as carbon nanotube indices [11, 13]. Also, we can express the diameter of carbon nanotube versus a , n , and m as [11, 13]

$$d_t = \frac{|\vec{C}_h|}{\pi} = \frac{a\sqrt{n^2 + m^2 + nm}}{\pi}. \quad (15)$$

On the other hand, the vector \vec{T} can be defined versus the unit vectors \vec{a}_1 and \vec{a}_2 as [11]

$$\vec{T} = t_1\vec{a}_1 + t_2\vec{a}_2, \quad (16)$$

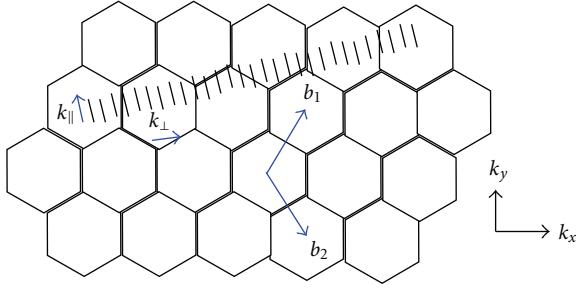


FIGURE 5: Vectors definition for the reciprocal lattice of graphene.

where

$$\begin{aligned} t_1 &= \frac{2m+n}{d_R}, \\ t_2 &= -\frac{2n+m}{d_R}, \end{aligned} \quad (17)$$

$$d_R = \text{GCD of } (2m+n), (2n+m),$$

which we can express d_R easier as

$$d_R = \begin{cases} 3d, & \text{if } (n-m) \text{ is multiple of } 3d, \\ d, & \text{if } (n-m) \text{ is not multiple of } 3d, \end{cases} \quad (18)$$

where

$$d = \text{GCD of } n, m. \quad (19)$$

Figure 5 shows the vectors of reciprocal lattice of graphene. In this figure, \vec{k}_\perp and \vec{k}_\parallel are the reciprocal lattice vector related to \vec{C}_h and the reciprocal lattice vector related to \vec{T} , respectively. With considering that \vec{C}_h and \vec{T} are orthogonal to each other, we have $\vec{C}_h \cdot \vec{k}_\perp = 2\pi$, $\vec{C}_h \cdot \vec{k}_\parallel = 0$, $\vec{T} \cdot \vec{k}_\parallel = 2\pi$, and $\vec{T} \cdot \vec{k}_\perp = 0$.

For obtaining \vec{k}_\perp and \vec{k}_\parallel versus the other parameters, we have $|\vec{C}_h \times \vec{T}|$ equal to the area of CNT unit cell, and $|\vec{a}_1 \times \vec{a}_2|$ equal to the area of primitive unit cell (as in Figure 3). Thus the number of primitive unit cells per CNT unit cell will be as

$$N = \frac{|\vec{C}_h \times \vec{T}|}{|\vec{a}_1 \times \vec{a}_2|}. \quad (20)$$

It should be noted that in above relations, “ \times ” and “ \cdot ” are the outer product and the inner product representations, respectively. Therefore the vectors \vec{k}_\perp and \vec{k}_\parallel can be expressed as

$$\begin{aligned} \vec{k}_\perp &= \frac{1}{N}(-t_2 \vec{b}_1 + t_1 \vec{b}_2), \\ \vec{k}_\parallel &= \frac{1}{N}(m \vec{b}_1 - n_1 \vec{b}_2). \end{aligned} \quad (21)$$

The energy dispersion relation of an SWCNT (single-walled carbon nanotube) can be obtained from the energy relation

of graphene sheet, which the related nanotube is made up of. With considering the periodic boundary conditions on \vec{C}_h , we find that the wave vector \vec{k}_\perp associated with \vec{C}_h (circumference) direction is quantized [11]. On the other hand, for a one-dimensional nanowire such as a carbon nanotube with the length ℓ , the wave vector associated with \vec{T} (translational) direction is discrete with

$$\Delta k = \frac{2\pi}{\ell}. \quad (22)$$

It should be noted that for a carbon nanotube of infinite length, as cleared from (22), the wave vector along the nanotube axis can be assumed continuous. Since in carbon nanotube which is a one-dimensional material, only \vec{k}_\parallel is a reciprocal lattice vector and \vec{k}_\perp gives discrete k values in the direction of \vec{C}_h .

Since an SWCNT is a rolled-up sheet of graphene, the energy band structure can be obtained simply from that of two-dimensional graphene. This work can be done easily by imposing appropriate boundary conditions in the circumferential direction around the SWCNT [11, 14]. As shown in Figure 6, the one-dimensional band structure of SWCNTs can be obtained from cross-sectional cutting of the energy dispersion of two-dimensional graphene.

For the continuous wave vector \vec{k} along the nanotube axis, we can write the energy dispersion variations for one-dimensional carbon nanotube, using the two-dimensional graphene relation (11) as [11]

$$E_S(\vec{k}) = \varepsilon \left(s \vec{k}_\perp + \frac{\vec{k}_\parallel}{|\vec{k}_\parallel|} k \right), \quad (23)$$

where $S = 0, 1, \dots, N-1$ and $-\pi/a < k < \pi/a$. This means that the N pairs of energy dispersion curves given by (23), correspond to the cross-sections of the two-dimensional energy dispersion given by (11) and shown in Figure 2. These cross-sections are made on $[s \vec{k}_\perp + (\vec{k}_\parallel / |\vec{k}_\parallel|) k]$ lines.

For a zigzag carbon nanotube with $n = 0$ and $m = 6$, we can obtain the parameters d_R , d , t_1 , and t_2 using (17)–(19) equal to 6, 6, 2, and -1 , respectively. Also \vec{C}_h and \vec{T} can be obtained using (14), (16) equal to $6a_2$ and $(2\vec{a}_1 - \vec{a}_2)$, respectively. Thus using (20), N can be obtained equal to 12. Using (21), the parameters \vec{k}_\perp and \vec{k}_\parallel will be calculated as $\vec{k}_\perp = (\vec{b}_1 + 2\vec{b}_2)/12$ and $\vec{k}_\parallel = \vec{b}_1/12$, respectively. Therefore, the argument in (23) will be

$$s \vec{k}_\perp + \frac{\vec{k}_\parallel}{|\vec{k}_\parallel|} k = \left(\frac{s}{12} + \frac{k}{|\vec{b}_1|} \right) \vec{b}_1 + \frac{s}{6} \vec{b}_2. \quad (24)$$

Using (13) for \vec{b}_1 and \vec{b}_2 , (24) will be obtained as

$$s \vec{k}_\perp + \frac{\vec{k}_\parallel}{|\vec{k}_\parallel|} k = \left(\frac{s}{2\sqrt{3}} \frac{\pi}{a} + \frac{k}{2} \right) + i \left(-\frac{s}{6} \frac{\pi}{a} + \frac{\sqrt{3}}{2} k \right), \quad (25)$$

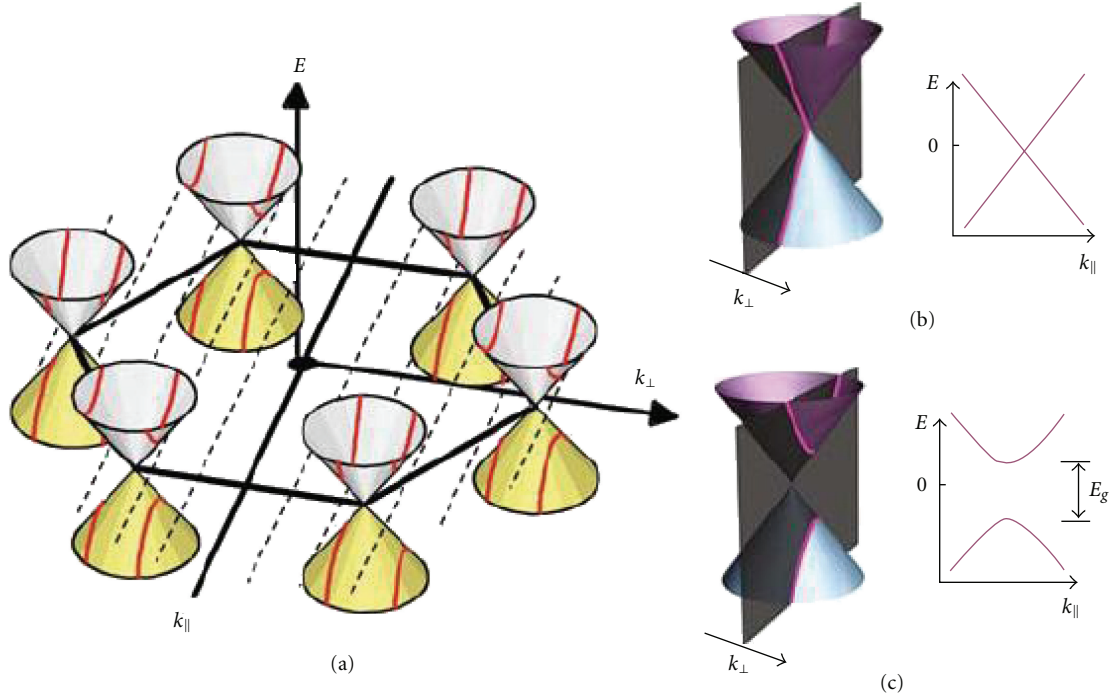


FIGURE 6: The 1D band structure of an SWCNT is obtained by cross-sections of 2D energy dispersions for (b) a metallic SWCNT and (c) a semiconducting SWCNT [14].

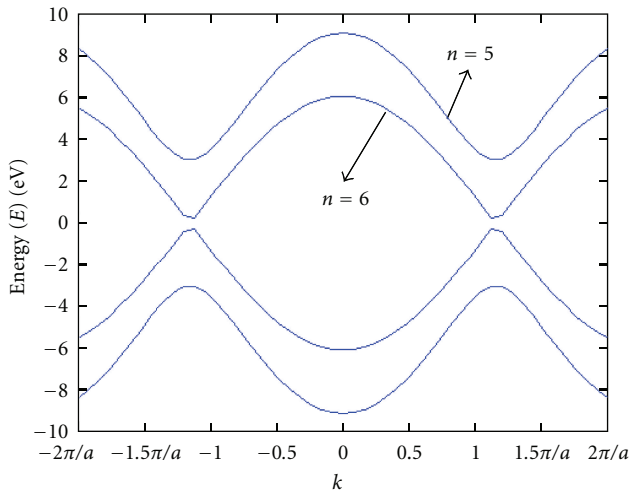


FIGURE 7: The energy dispersion variations of zigzag carbon nanotubes. One nanotube is metallic with $n = 0$ and $m = 6$, and the other is semiconductive with $n = 0$ and $m = 5$.

where i presents the imaginary part. Recall that $\vec{K} = k_x + ik_y$, (25) implies that for calculating the energy dispersion variations of CNT, it is adequate to replace k_x and k_y in (11) with the real part and the imaginary part of (25), respectively, as

$$\begin{aligned} k_x^{(0,6)} &= \frac{s}{2\sqrt{3}} \frac{\pi}{a} + \frac{k}{2}, \\ k_y^{(0,6)} &= -\frac{s}{6} \frac{\pi}{a} + \frac{\sqrt{3}}{2} k. \end{aligned} \quad (26)$$

With a similar way as described above, we can obtain k_x and k_y for the case that $n = 0$ and $m = 5$, as

$$\begin{aligned} k_x^{(0,5)} &= \frac{3s}{5\sqrt{3}} \frac{\pi}{a} + \frac{k}{2}, \\ k_y^{(0,5)} &= -\frac{s}{5} \frac{\pi}{a} + \frac{\sqrt{3}}{2} k. \end{aligned} \quad (27)$$

In Figure 7, the energy dispersion variations versus k have been plotted for the two carbon nanotubes, which one nanotube is metallic with $n = 0$ and $m = 6$ and the other is semiconductive with $n = 0$ and $m = 5$. As shown in this figure, the band gap for the metallic nanotube is almost zero, and for the semiconductive nanotube is a nonzero value.

For a chiral carbon nanotube with $n = 4$ and $m = 2$, with the similar way as described for the two zigzag nanotubes in Figure 7, k_x and k_y will be obtained as

$$\begin{aligned} k_x^{(4,2)} &= \frac{9s}{14\sqrt{3}} \frac{\pi}{a} - \frac{k}{2\sqrt{7}}, \\ k_y^{(4,2)} &= \frac{s}{14} \frac{\pi}{a} + \frac{3\sqrt{3}}{2\sqrt{7}} k. \end{aligned} \quad (28)$$

In Figure 8, the energy dispersion variations versus k has been plotted for a chiral carbon nanotube with $n = 4$ and $m = 2$, which is neither metallic nor semiconductive.

4. Conclusions

In this paper we have studied the basic structure of graphene and its resulted element carbon nanotube. Using

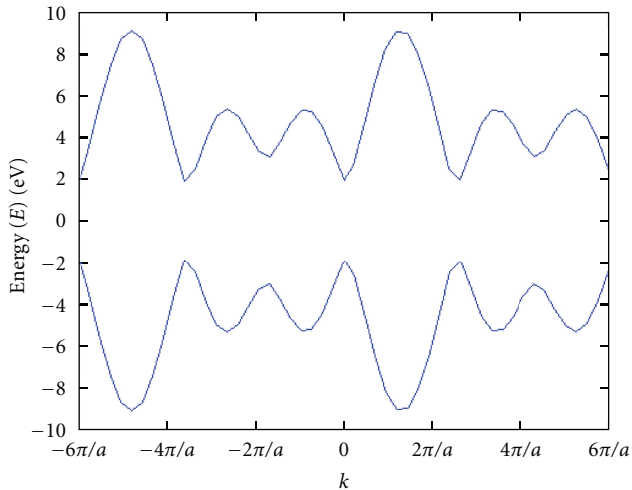


FIGURE 8: The energy dispersion variations of a chiral carbon nanotube, with $m = 2$ and $n = 4$.

the tight binding approximation theory, we have analyzed the variations of energy band gap for SWCNTs (single-walled carbon nanotubes). According to the chiral indices, the related expressions for energy dispersion variations of these elements have been analyzed and also plotted using MATLAB [12] for zigzag and chiral nanotubes.

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