

Effective masses of charge carriers in selected symmorphic and nonsymmorphic carbon nanotubes

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We performed *ab initio*, self-consistent calculations for the electronic structure of selected semiconducting carbon nanotubes in the symmorphic and nonsymmorphic groups. We employed a real space approach in the linear combination of atomic orbital formalism. We utilized a nonlocal density-functional potential in the generalized gradient approximation. We present the electronic structure and effective masses of charge carriers in symmorphic nanotubes that include (10,0), (13,0), (17,0), and (22,0), and the nonsymmorphic tubes (8,4) and (10,5). For nonsymmorphic carbon nanotubes (8,4) and (10,5), the top of the highest occupied valence band and the bottom of the lowest unoccupied conduction band are not at the Γ point, but at about $\pm 0.1(1,0,0)\pi/L$, where the tubule axis is defined as the (1,0,0) direction. The band gaps in the nonsymmorphic (8,4) and (10,5) can be direct for transitions at $+0.1(1,0,0)\pi/L$ or $-0.1(1,0,0)\pi/L$, and can also be indirect for transitions from $+0.1(1,0,0)\pi/L$ to $-0.1(1,0,0)\pi/L$, or vice versa.

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I. INTRODUCTION

Single-walled carbon nanotubes (SWCNT's) are potentially ideal materials for building electronic devices at nanometer scales.¹⁻³ Understanding their electronic properties is essential for large scale applications. However, such materials are usually too small for many conventional measurements. Predictive calculations with certain reliability are indispensable to obtain their physical properties.

In the last several years, tight-binding calculations have been extensively used to study the electronic structure of carbon nanotubes.⁴ Tight-binding approximations based on the symmetry of the honeycomb lattice of graphite predicted that SWCNT's could be semiconducting or metallic depending on their index (n, m). Although the tight-binding approximation is a useful tool to estimate the basic electronic structure of SWCNT's, the curvature-related effects and the hybridization of different electron states of graphite could lead to the electronic properties of SWCNT's that are substantially different from that of the tight-binding calculations. Zigzag ($n, 0$) (where n is a multiple of 3) SWCNT's which were predicted to be metallic from tight-binding calculations were found to have small energy gaps at their Fermi level.⁵⁻⁸

Ab initio quantum calculations, which do not have these deficiencies, can be used to obtain the electronic properties of individual SWCNT's. Prior *ab initio* density-functional calculations were mostly applied to the studies of the electronic structure of symmorphic SWCNT's.⁹⁻¹⁶ Nonsymmorphic SWCNT's, which are encountered more often in experiments than the symmorphic ones such as zigzag and armchair SWCNT's, need attention. Nonsymmorphic SWCNT's generally involve a large number of atoms in their unit cells. For example, nonsymmorphic tubes (8,4) and (10,5) have 112 and 140 atoms in their unit cells, respectively. The large number of atoms in the unit cells presents some technical challenges for *ab initio* calculations. Reich *et al.* recently reported the electronic band structure of some

chiral nanotubes in nonsymmorphic group.¹⁷ They used the local-density approximation (LDA) and nonlocal normconserving pseudopotentials. In their calculation, the valence electrons were described by localized pseudoatomic orbitals with a double ζ singly polarized basis set.

The calculation or prediction of the effective masses of charge carriers in SWCNT's requires a reliable result of the dispersions of the electron energy bands. Although, the electron energy bands from the tight-binding approximation can be adjusted to agree approximately with the results of the *ab initio* calculations. Such adjustment of the tight-binding parameters cannot lead to a prediction of the effective masses of charge carriers in SWCNT's. In this work, we report the all electron and full potential *ab initio* calculations of the effective masses of charge carriers and other related properties of some symmorphic and nonsymmorphic SWCNT's. We utilized *ab initio*, nonlocal density-functional calculations in the generalized gradient approximation (GGA).¹⁸ We used the formalism of the linear combination of atomic orbitals (LCAO) in real space. We describe our method in Sec. II. Section III presents our results for selected symmorphic and nonsymmorphic nanotubes, in that order. We utilized the calculated results of the electronic energy bands to predict the effective masses of charge carriers (electrons and holes) in selected semiconducting carbon nanotubes. A brief conclusion is provided in Sec. IV.

II. METHOD

Our calculations of the electronic structure of SWCNT's are based on the density-functional theory of Hohenberg-Kohn and Kohn-Sham.^{19,20} The Schrodinger-like equations (also known as the Kohn-Sham equations) of many electron system¹⁹⁻²¹ are

$$\left\{ -\frac{\hbar^2}{2m} \nabla^2 - \sum_{lm} \frac{e^2 Z_m}{|\vec{r} - \vec{r}_m - \vec{R}_l|} + e^2 \int \frac{\rho(\vec{r}')}{|\vec{r} - \vec{r}'|} dv' + V_{xc} \right\} \Psi_{ki}^- = E_{ki}^- \Psi_{ki}^-, \quad (1)$$

where E_{ki}^- and Ψ_{ki}^- are the eigenenergy and eigenfunction of the i th electronic state at the k point in the Brillouin zone; \vec{r}_m and Z_m are the position and the nuclear charge of the m th ion; \vec{R}_l is a translational vector; V_{xc} is the exchange-correlation potential of the many-electron system. We employed nonlocal density-functional calculations for the exchange-correlation energies and potentials in the generalized gradient approximation that was developed by Perdew and Wang.¹⁸ In the Kohn-Sham equations, the electron density $\rho(\vec{r})$ depends on the wave functions Ψ_{ki}^- of the occupied electron states, i.e.,

$$\rho(\vec{r}) = \sum_{ki} f_{ki}^- |\Psi_{ki}^-|^2, \quad (2)$$

where f_{ki}^- is the Fermi distribution function.

In the LCAO method,²²⁻²⁷ we expand the electronic eigenfunction Ψ_{ki}^- of the many-atom system as a linear combination of the atomic wave functions. We calculated the atomic wave function using a separate computer program that employed *ab initio* density-functional computations. We further expanded the atomic wave functions as a linear combination of Gaussian orbitals in real space. In the calculation of the atomic orbitals of carbon, we included 13 Gaussian orbitals. We employed a set of even-tempered Gaussian exponentials with a minimum of 0.124 and a maximum of 0.1365×10^5 in atomic unit, in the calculation for the carbon atom. The electron densities were also expressed as a linear combination of Gaussian functions in real space. The computation for the exchange-correlation potentials was done in real space using a mesh of points around each atom. The numbers of mesh points per atomic site varied from 3150 to 3250, depending on the local structure of the atom. We solved the Kohn-Sham equations by a self-consistent iteration procedure. The self-consistent potentials converged to a difference around 10^{-5} after an average of about 40 iterations.

III. RESULTS

A. Symmorphic zigzag carbon nanotubes

We calculated the electronic structure of selected symmorphic SWCNT's that included semiconducting zigzag tubes (10,0), (13,0), (17,0), and (22,0). The diameters of these symmorphic SWCNT's are 7.83, 10.18, 13.31, and 17.23 Å, respectively. There are a relatively large number of atoms in the nanotube unit cells. SWCNT's (10,0), (13,0), (17,0), and (22,0) have 40, 52, 68, and 80 carbon atoms in their unit cells, respectively. Their unit cell lengths in the direction of the nanotube axis are the same at 4.26 Å.

We first tested the convergency of the electronic structure calculations with respect to the size of the basis sets of atomic orbitals.²⁸ As a demonstration, we present the following calculated results for SWCNT (10,0). We first carried out

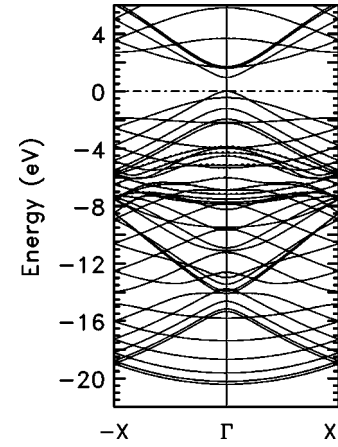


FIG. 1. The comparison of the calculated electron energy bands of SWCNT (10,0) from calculations III and IV. Calculation III utilized the atomic orbitals of C(1s2s3s 2p3p). Calculation IV included an additional orbital of C(4s). The solid lines represent the results of Calculation III; the dashed lines show the results from Calculation IV.

completely self-consistent calculation for SWCNT (10,0) using a minimal LCAO basis set that included atomic orbitals of C(1s 2s 2p). We then repeated the self-consistent calculation using an augmented basis set that also includes the atomic orbital of C(3s⁰). In the self-consistent calculations, we took C(1s) as a core state. We then plotted the resulting energy bands from these two distinct self-consistent calculations. We observed that the occupied and unoccupied bands from the two calculations differ considerably.

The next step was to repeat our procedure, for a third time, with a new basis set that also included C(3p⁰) orbital. The results of the third calculation and of the second calculation are compared. The calculated electron energy bands of the two differ slightly. We then repeated the procedure for a fourth time to include C(4s⁰) in the calculation. The results of the fourth calculation (dashed lines) and of the third calculation (solid lines) are shown in Fig. 1. The calculated electron energy bands from the third calculation do not have a noticeable difference from that of the fourth calculation. The average difference between the occupied energy bands from the two calculations in Fig. 1 is at the order of 1 mRy. The third calculation (the solid lines of Fig. 1) which includes the atomic orbitals of C(1s 2s 3s 2p 3p) leads to sufficiently converged electron energy bands of SWCNT (10,0) with respect to the size of the basis set. We chose the top of the highest occupied band at the Γ point as the zero of the energy.

From the results in Fig. 1, we conclude that SWCNT (10,0) has a direct band gap of 0.95 eV at the Γ point. The highest occupied valence band and the lowest unoccupied conduction band of symmorphic zigzag SWCNT (10,0) are doubly degenerate near the Γ point. We did not include the relativistic effect in these calculations. Our calculated band-gap energy of 0.95 eV for SWCNT (10,0) is very close to the ones obtained by other *ab initio* calculations using the density-functional calculations and to experimental measurements. Mazzoni and Chacham²⁸ obtained a band gap of

0.92 eV for zig-zap SWCNT (10,0), utilizing the SIESTA program that implemented density-functional theory, within the generalized gradient approximation, for the exchange-correlation potential and norm-conserving pseudopotentials. Our calculated band gap also agrees well with the first-principles LDA calculations performed by Mintmire, Robertson, and White.²⁹ We also performed LDA calculations for the electronic structure of SWCNT (10,0) and found a direct band gap at the Γ point that is smaller than that from our GGA calculations by about 0.003 eV. Odom *et al.* performed the measurements using the scanning tunneling microscopy for various carbon nanotubes and presented the band-gap energies in a range of 0.9–0.96 eV for tube diameters around 7.8 Å.³⁰ The tube diameter of SWCNT (10,0) is 7.83 Å.

We utilized the results of the third calculation to compute the total energies of SWCNT (10,0) at the relaxed structures of various C-C bond lengths. The stable structure of SWCNT (10,0) was determined from the minimization of the total energies. Two of the three C-C bond lengths in SWCNT (10,0) are the same at 1.416 Å and one of them is 1.420 Å. These calculated bond lengths agree well with the C-C bond length of 1.42 Å (Ref. 31) in graphite and with the commonly observed C-C bond length in carbon nanotubes. We also compared the GGA results with those of our LDA calculations. Our LDA calculations found relatively smaller C-C bond lengths in SWCNT (10,0). Two of the C-C bond lengths are 1.39 Å and one is 1.40 Å.

From these test calculations as discussed above and the comparisons of the calculated results of various methods and that with the results of experimental measurements, we can conclude that the electronic energy bands of SWCNT (10,0) as presented in Fig. 1 are reasonably reliable. We can further use the calculated electronic structure to obtain other physical quantities. The effective mass of charge carriers in semiconductors is an important physical quantity that is used in analysis of the electron transport properties, particularly in the effective-mass approximation.^{32–35} In these previous analyses, the effective masses of charge carriers in carbon nanotubes were used as adjustable parameters. In this work, we utilized the results of the *ab initio* calculations to obtain the effective masses of charge carriers in SWCNT's. The calculated effective mass of charge carriers near the top of the valence band, which are referred to as holes, is $0.1m_0$, where m_0 is the free electron mass. The effective mass of charge carriers (electrons) near the bottom of the conduction band is also $0.1m_0$, which nearly is the same as that of the effective mass of holes. This property is different from that of many other semiconductors in which the effective masses (or band masses) of holes are usually larger than that of electrons. The closeness of the effective masses of holes to those of the electrons in SWCNT (10,0) is attributed to its electron energy bands. The dispersions of the highest occupied valence band (HOVB) and of the lowest unoccupied conduction band (LUCB) in SWCNT (10,0) are nearly symmetric around the Γ point. One can see this feature from Fig. 1. Other valence and conduction bands away from the Fermi level (E_F) do not have this symmetry property.

We used the same computational techniques to calculate the electronic structure of other SWCNT's that have relatively larger diameters and involve many more atoms in their

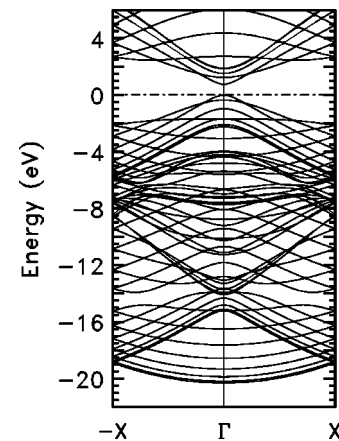


FIG. 2. The calculated electron energy bands of SWCNT (13,0).

unit cells. They include SWCNT's (13,0), (17,0), and (22,0) which have 52, 68, and 88 atoms in their unit cells, respectively. We present the calculated electron energy bands of these SWCNT's in Figs. 2–4. These symmetric zigzag SWCNT's are direct band-gap semiconductors. The band-gap energies of SWCNT (13,0), (17,0), and (22,0) are 0.75, 0.54, and 0.44 eV, respectively. The HOVB and LUCB of these zigzag SWCNT's are doubly degenerate near the Γ point, as was the case of (10,0). Even though these SWCNT's have different diameters, the widths of their valence bands below E_F are approximately the same. This width is 20.4 eV. By valence bands, in this context, we mean the occupied bands as shown in the figures of the band structures.

We also calculated the effective masses of charge carriers in SWCNT's (13,0), (17,0), and (22,0). The calculated results are presented in Table I. $E_v^{(1)}$ in Table I refers to the first valence band near the Fermi level (E_F), whereas $E_c^{(1)}$ refers to the first conduction bands from E_F . In Table I, E_m is the energy (in eV) of the top of the valence band or of the bottom of the conduction band. The energy of the top of the first valence band $E_v^{(1)}$ is chosen to be zero in Table I. “Deg” refers to the degeneracy of the bands. As in the case of

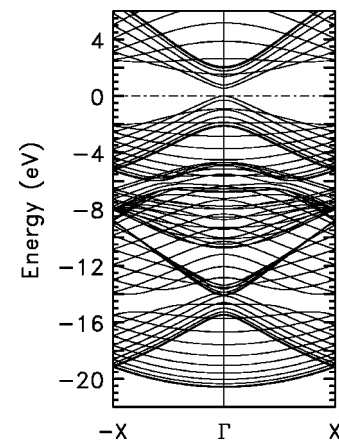


FIG. 3. The calculated electron energy bands of SWCNT (17,0).

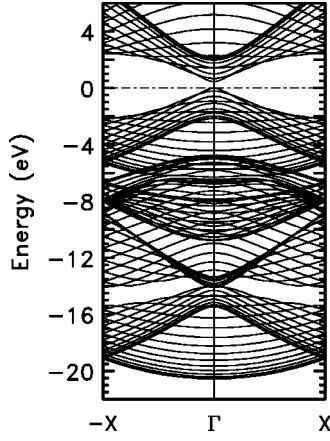


FIG. 4. The calculated electron energy bands of SWCNT (22,0).

SWCNT (10,0), the effective masses of electrons around the bottom of the conduction bands in these SWCNT's are nearly the same as that of holes around the top of the valence bands. In SWCNT (13,0), the first conduction band above E_F is symmetric to the first valence band below E_F as presented in Fig. 2. The second conduction band above E_F is nearly symmetric to the second valence band below E_F , but the separation of the first two conduction bands is slightly larger than that of the first two valence bands by about 0.05 eV at the Γ point. In SWCNT's (17,0) and (22,0), the first two conduction bands above E_F are symmetric to the first two valence bands below E_F as presented in Figs. 3 and 4. Other electron bands away from E_F do not have the symmetry property.

TABLE I. The calculated effective masses (m^*) of charge carriers in various 1D SWCNT's.

Band	E_m (eV)	Deg	m^* (m_0)
SWCNT	(10,0)		
$E_v^{(1)}$	0.0	2	0.10
$E_c^{(1)}$	0.95	2	0.10
SWCNT	(13,0)		
$E_v^{(1)}$	0.0	2	0.09
$E_c^{(1)}$	0.75	2	0.09
SWCNT	(17,0)		
$E_v^{(1)}$	0.0	2	0.11
$E_c^{(1)}$	0.54	2	0.11
SWCNT	(22,0)		
$E_v^{(1)}$	0.0	2	0.057
$E_c^{(1)}$	0.44	2	0.056
SWCNT	(8,4)		
$E_v^{(1,2)}$	0.0	1	0.13
$E_c^{(1,2)}$	0.96	1	0.13
SWCNT	(10,5)		
$E_v^{(1,2)}$	0.0	1	0.11
$E_c^{(1,2)}$	0.74	1	0.11

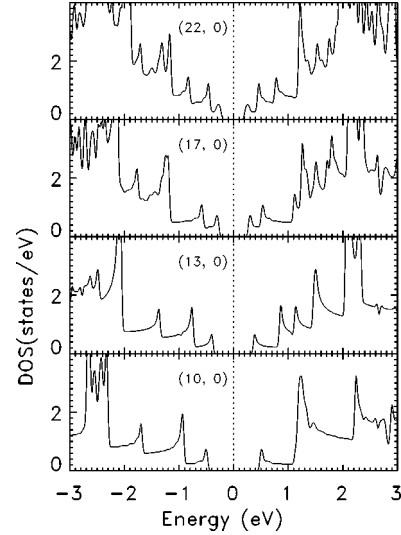


FIG. 5. The calculated electron density of states of SWCNT's (10,0), (13,0), (17,0), and (22,0).

We calculated the electron densities of states (DOS) of the one-dimensional (1D) nanotubes using the following formulas:³⁶

$$D(E) = \frac{1}{N} \sum_{ki} \delta(E - E_{ki}), \quad (3)$$

where E_{ki} is the energy of the i th electron band at the \vec{k} point in the irreducible Brillouin zone; N is the total number of \vec{k} points. In our calculations of DOS, the δ function in Eq. (3) was replaced with a Gaussian function,

$$\delta(E) \approx \frac{1}{\Delta\sqrt{\pi}} \exp\left[-\left(\frac{E}{\Delta}\right)^2\right] \quad (4)$$

We used $\Delta = 2$ mRy (or 0.027 eV) in these calculations. We calculated the DOS over an energy range of 30 eV and used 3000 points. We utilized the *ab initio* computations to obtain the electronic energy levels at 40 k points in the irreducible Brillouin zone of 1D SWCNT's. Additionally, we implemented a linear interpolation method to calculate the electron energy levels at other ten k points between any two k points of the *ab initio* results. We then included a total of about 400 k points in the irreducible Brillouin zone of 1D SWCNT's for the calculations of the DOS. The calculated results of the DOS of zigzag SWCNT's are presented in Fig. 5. The zero of the energy in Fig. 5 is set at the middle of the band gaps. The calculated densities of states in Fig. 5 show Van Hove singularities (the peaks) at the extremal points of energy bands. Figure 5 shows that the location and the relative height of the first peak below the Fermi level are nearly symmetric to that of the first peak above the Fermi level in the zigzag SWCNT's. These results are consistent with the data in Table I where the effective masses of holes in these SWCNT's are nearly the same as those of the corresponding electrons.

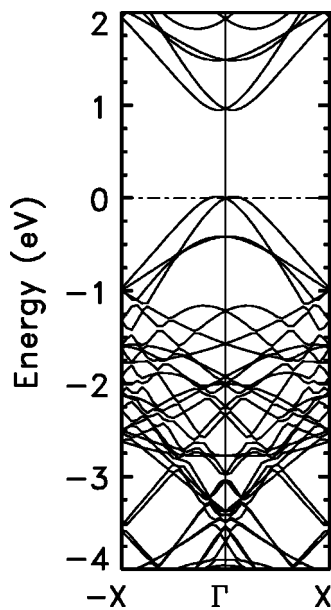


FIG. 6. The calculated electron energy bands of SWCNT (8,4).

B. Nonsymmorphic carbon nanotubes (8,4) and (10,5)

We calculated the electronic structure of nonsymmorphic SWCNT's (8,4) and (10,5), utilizing the nonlocal density-functional calculations in the generalized gradient approximation. The length of the unit cells of these two SWCNT's along the tubule axis is 11.27 Å. The diameters of these nanotubes are 8.29 Å for (8,4) and 10.36 Å for (10,5). There are 112 and 140 carbon atoms in the unit cells of SWCNT's (8,4) and (10,5), respectively.

The calculated electron energy bands of nonsymmorphic SWCNT's (8,4) and (10,5), are presented in Figs. 6 and 7. Unlike the energy bands of symmmorphic zigzag SWCNT's,

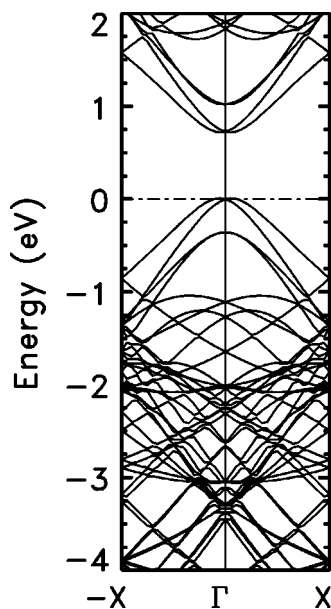


FIG. 7. The calculated electron energy bands of SWCNT (10,5).

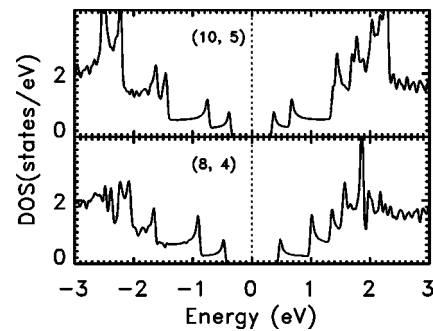


FIG. 8. The calculated electron density of states of SWCNT (8,4) and (10,5).

the top of the HOVB and the bottom of the LUCB of nonsymmorphic (8,4) and (10,5) are not at the Γ point, but at about $\pm 0.1(1,0,0)\pi/L$. Both bands are nondegenerate. We may view the HOVB and LUCB of (8,4) and (10,5) as if the doubly degenerate bands near the Fermi level of symmmorphic zigzag SWCNT split off from the Γ point symmetrically and form the two nondegenerate bands of nonsymmorphic SWCNT's (8,4) and (10,5). Nonsymmorphic SWCNT's (8,4) and (10,5) have band-gap energies of 0.96 and 0.74 eV, respectively. The band gaps in nonsymmorphic SWCNT's (8,4) and (10,5) can be direct for transitions at $+0.1(1,0,0)\pi/L$ or $-0.1(1,0,0)\pi/L$. The band gaps in SWCNT's (8,4) and (10,5) can also be indirect for transitions from $+0.1(1,0,0)\pi/L$ to $-0.1(1,0,0)\pi/L$, or vice versa. The energies of the direct and indirect band gaps are the same. These are the first cases of semiconductors that present such a peculiar property, to our knowledge.

Optical measurements of the low-energy excitations in SWCNT's (8,4) and (10,5) should reveal the direct band gaps as well as the indirect band gaps. However, the indirect absorption process has to be assisted through the absorption or excitations of phonons or others quasiparticles. The probability of indirect transitions will generally be lower than that of direct excitations. Since the phonon excitations are generally temperature dependent, the indirect transitions in SWCNT's (8,4) and (10,5) will present a temperature dependent behavior.

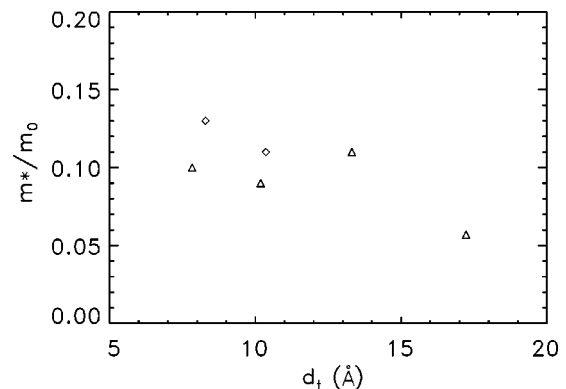


FIG. 9. The effective masses m^* of charge carriers of the semiconducting carbon nanotubes as a function of the tube diameters d_t , where m_0 is the free electron mass.

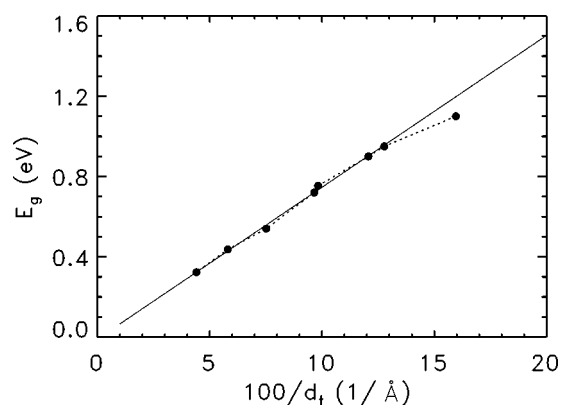


FIG. 10. The calculated band-gap energy E_g of semiconducting SWCNT's as a function of $100/d_t$, where d_t (in Å) is the diameter of SWCNT.

We also calculated the electron density of states of (8,4) and (10,5) that are presented in Fig. 8. The zero of the energy in Fig. 8 is set at the middle of the band gaps. The calculated densities of states in Fig. 8 show Van Hove singularities at the extremal points of energy bands. As in the case of zigzag SWCNT's, the locations and the relative heights of the first peaks below and above the Fermi level are nearly symmetric in these nonsymmorphic SWCNT's. So the effective masses of holes will be similar to that of the electrons in (8,4) and (10,5). The calculated effective masses of charge carriers (including electrons and holes) in (8,4) and (10,5) are 0.13 and $0.11m_0$, respectively, and are listed in Table I.

We summarize the effective masses of charge carriers of the semiconducting carbon nanotubes as a function of the tube diameters in Fig. 9. The open triangles in Fig. 9 represent the data for the symmmorphic SWCNT's (10,0), (13,0), (17,0), and (22,0); the open diamonds represent the results for nonsymmorphic SWCNT's (8,4) and (10,5). Although the data points do not fall on a simple line, the general trend is that the effective masses of charge carriers decrease as the tube diameters increase. At comparable tube diameters, the effective masses of charge carriers of nonsymmorphic SWCNT's are slightly larger than those of symmmorphic ones.

Finally, we present the calculated band-gap energies, E_g , of the semiconducting carbon nanotubes as a function of $100/d_t$ in Fig. 10. The data include symmmorphic zigzag SWCNT's and nonsymmorphic SWCNT's (8,4) and (10,5). For the SWCNT's with relatively large diameters, the band-

gap energy is a linear function of $100/d_t$. This result is consistent with the findings of tight-binding calculations by Mintmire, Robertson, and White.²⁹ Utilizing the Huckel tight-binding calculations, they obtained the relation, $E_g = \gamma_0 a_{c-c}/d_t$, where a_{c-c} is the nearest-neighbor C-C distance on a graphite sheet, and γ_0 is a tight-binding parameter. However, the band-gap energies of the SWCNT's whose diameters are smaller than 7.5 Å, do not follow the above relation. The deviation from the tight-binding calculations is primarily due to the curvature effect of carbon nanotubes.

IV. CONCLUSION

We successfully performed *ab initio* calculations for the electronic structure of selected symmmorphic and nonsymmorphic carbon nanotubes. These carbon nanotubes are semiconductors. The large numbers of atoms in the unit cells of nonsymmorphic carbon nanotubes (8,4) and (10,5) lead to significant computational efforts. We employed a real space approach in the LCAO formalism. We presented the effective masses of charge carriers in these carbon nanotubes. The calculated electronic structures indicate that the symmmorphic zigzag SWCNT's (10,0), (13,0), (17,0), and (22,0) are direct band-gap semiconductors. For nonsymmorphic SWCNT's (8,4) and (10,5), the top of the highest occupied valence band and the bottom of the lowest unoccupied conduction band are not at the Γ point, but at about $\pm 0.1(1,0,0)\pi/L$. The band gaps in nonsymmorphic SWCNT (8,4) and (10,5) can be direct for transitions at $+0.1(1,0,0)\pi/L$ or $-0.1(1,0,0)\pi/L$, and can also be indirect for transitions from $+0.1(1,0,0)\pi/L$ to $-0.1(1,0,0)\pi/L$ or vice versa. The effective masses of holes are nearly the same as those of the electrons in these SWCNT's.

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