Strain energy and Young's modulus of single-wall carbon nanotubes calculated from electronic energy-band theory

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The strain energies in straight and bent single-walled carbon nanotubes (SWNT's) are calculated by taking account of the total energy of all the occupied band electrons. The obtained results are in good agreement with previous theoretical studies and experimental observations. Young's modulus and the effective wall thickness of SWNT's are obtained from the bending strain energies of SWNT's with various cross-sectional radii. The repulsion potential between ions contributes the main part of Young's modulus of SWNT's. The wall thickness of the SWNT comes completely from the overlap of electronic orbits and is approximately of the extension of the π orbit of carbon atom. Both Young's modulus and the wall thickness are independent of the radius and the helicity of SWNT, and insensitive to the fitting parameters. The results show that continuum elasticity theory can serve well to describe the mechanical properties of SWNT's.

Since their discovery in 1991,[1] carbon nanotubes (CNT's) have invoked considerable interest[2] in the last decade. There are many works on both theoretical[3–5] and experimental[6] studies about the electronic structure of CNT's, and many exciting and novel properties have been discovered. For example, it was found that the insulating, semimetallic, or metallic behavior depends upon the radius and the helicity of CNT's.[3] With respect to thermal and the mechanical properties, the tubes are significantly stiffer than any material presently known.[7] To understand these many intriguing properties, many groups have calculated the strain energy[8–13] and Young's modulus[14–16] of single-wall carbon nanotubes (SWNT's). Among these calculations, many depend on the choice of an empirical potential between the carbon atoms, such as the Tersoff-Brenner potential.[17] Lenosky *et al.*[11] employed an empirical model with three parameters reducible to a continuous model with two elastic moduli.[13] They showed that the continuum elasticity model serves well to describe the deformation of multiwall carbon nanotubes (MWNT's). Recent theoretical studies[14–16] on Young's moduli of SWNT's show some discrepancies coming from the adoption of different empirical potentials and different relations in the continuum elasticity theory (CET), in particular, the different values of the effective wall thickness of the SWNT. How to calculate the Young's modulus of SWNT is still an open question.

Here we present a simple method for the computation of the strain energy of straight SWNT's directly from the electronic band structure without introducing any empirical potential. This method had also been extended to calculate the strain energy of bent tubes. It is found that the wall thickness of SWNT's can be calculated simply from the band electrons and Young's modulus by consideration of both the repulsion energy between ions and the bond-length dependencies of the electronic energy. Our results show that CET can well describe the bending of SWNT's and that both Young's modulus and the effective wall thickness are independent of the radius and the helicity of the tubes, and insensitive to the fitting parameters. We obtained Young's modulus of

SWNT's about 5 TPa, 5 times larger than the value of MWNT or graphite bulk samples, and the effective wall thickness about 0.7 Å , the size of carbon atom.

Generally, the total energy of the carbon system is given by the sum:[18,19]

$$E_{total} = E_{el} + E_{rep}, \qquad (1)$$

where E_{el} is the sum of the energy of band electrons of the occupied states and E_{rep} is given by a repulsive pair potential depending only on the distance between two carbon atoms. They are given by

$$E_{el} = \sum_{occ} E_k \qquad (2)$$

and

$$E_{rep} = \sum_i \sum_{j>i} \phi(r_{ij}), \qquad (3)$$

respectively. Since $\phi(r)$ is a short-range potential,[18] only interaction between neighbor atoms needs to be considered. On account of the relaxation effect,[3–5] the bond length of a SWNT is slightly larger than that of graphite ($r_0 = 1.42$ Å). However, even in C_{60}, for which the relaxation effect is significant on account of its small radius, calculations show that the energy contribution of the bond relaxation can still be safely ignored.[11] The total energy can now be rewritten as

$$E_{total} = \frac{1}{2} \sum \mathcal{E}_0 (\delta r_{ij})^2 + E_{ang}, \qquad (4)$$

where the first term on the right-hand side of E_{total} is the sum of the repulsion energy between ions and the electronic energy contribution of the bond length change with δr_{ij} as the change of the distance between the ith and the jth atoms in a SWNT from that in graphene. The second term is the electronic energy contribution of the angular change of the

bond, when rolling from graphene to SWNT. The positions of the atoms of straight SWNT's are located on the cylindrical surface of the tube when the relaxation effect of the bonds is neglected. δr_{ij} is proportional to ρ^{-2}, where ρ is the cross-sectional radius of the SWNT, and the first term of Eq. (4) can be ignored, since it is of ρ^{-4} order. Therefore, the strain energy of straight SWNT's comes from the curvature-induced electronic energy change and can be obtained by taking account of the electronic energy of all the occupied bands.

In order to calculate the electronic energy bands of SWNT's, we use a simple nearest-neighbor tight-binding (TB) model. This model contains nine TB parameters of graphite: four hopping, including $V_{ss\sigma} = -6.679$, $V_{sp\sigma} = -5.580$, $V_{pp\sigma} = 5.037$, $V_{pp\pi} = -3.033$ in units of eV; four overlapping integration, including $S_{ss\sigma} = 0.212$, $S_{sp\sigma} = 0.102$, $S_{pp\sigma} = -0.146$, $S_{pp\pi} = 0.129$; and an energy difference between the $2s$ orbit and the $2p$ orbit of the carbon atoms $\Delta\mathcal{E} = (\mathcal{E}_{2s} - \mathcal{E}_{2p}) = -8.868$ eV.[4] The model has been used widely for the calculation of the electronic properties of both graphenes and SWNT's. In general, these TB parameters depend upon the bond length as follows:[18]

$$V_{\lambda\lambda'\mu}(r) = V_{\lambda\lambda'\mu}(r_0)\exp[-\gamma(r-r_0)]. \tag{5}$$

However, in case of straight SWNT's, the ρ^{-2} order dependence of the strain energy will not be affected even if we ignore simultaneously these dependencies and the repulsion energy.

With the notation used by White et al.,[5] each SWNT is indexed by a pair of integers (n_1, n_2) corresponding to the lattice vector $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2$ on the graphene, where $\vec{a}_1$ and $\vec{a}_2$ are the unit cell vectors of the graphene. The tube structure is obtained by a rotation operation $\mathcal{C}_N$ and a screw operation $\mathcal{S}(h,\alpha)$. The operation $\mathcal{C}_N$ is a rotation of $2\pi/N$ about the axis, where N is the largest common factor of n_1 and n_2. The $\mathcal{S}(h,\alpha)$ operation is a rotation of an angle α about the axis of SWNT in conjunction with a translation of h units along the axis, which both h and α depending on the tube parameters.[5] Let $[m,l]$ denote a primitive unit cell in the tube generated by mapping the $[0,0]$ cell to the surface of the cylinder first and then translating and rotating this cell by l applications of the rotational operator $\mathcal{C}_N$ followed by m applications of $\mathcal{S}(h,\alpha)$. Because $\mathcal{S}(h,\alpha)$ and $\mathcal{C}_N$ commute with each other, we can generalize the Bloch sums and obtain the Hamiltonian matrix:

$$\mathcal{H}_{ij}^{AA}(k,n) = \mathcal{H}_{ij}^{BB}(k,n) = \mathcal{E}_i\delta_{ij},$$

$$\mathcal{H}_{ji}^{BA}(k,n) = [\mathcal{H}_{ij}^{AB}(k,n)]^*, \tag{6}$$

$$\mathcal{H}_{ij}^{AB}(k,n) = \sum_r \exp\left[\frac{2ni\pi}{N}\Delta l(r) + ik\Delta m(r)\right]\mathcal{V}_{ij}^{AB}(r),$$

where $[\Delta m(r), \Delta l(r)]$ ($r=1,2,3$) are the cell indices of the primitive unit cells located by the three nearest-neighbor atoms B of atom A in the tube, and A and B are two independent carbon atoms in a primitive unit cell of a SWNT. Let $n=0,1,\ldots,N-1$ represent the N sub-Brillouin zones, and k be a one-dimensional wave vector. $\mathcal{E}_1 = \mathcal{E}_{2s}$, $\mathcal{E}_i = \mathcal{E}_{2p}$ for i
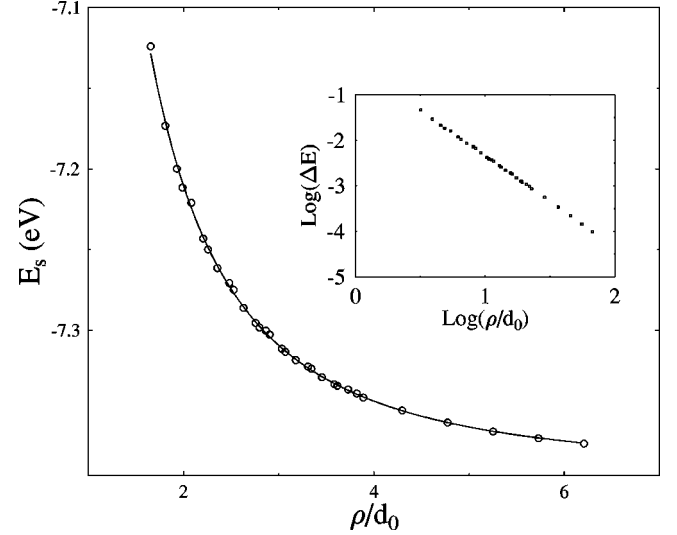

FIG. 1. The strain energy per atom versus the radius of (n,m) tubes, where $n=6-13$ and $m=0$, 1, 2, or n. The solid line corresponds to a least square fit to the $\mathcal{C}/\rho^2$ behaviors. $\mathcal{C} = 0.71 r_0^2 \approx 1.44$ eV Å²/ atom. $\mathcal{C}$ is independent of the helicity of tubes. The $\rho^{-\beta}$ behaviors is clearly shown in the inset ($\beta \approx 2.03$). Here r_0 is 1.42 Å and the cohesive energy of graphite is -7.39 eV.

$=2,3,4$. Taking the $2p$ wave function as a vector and $2s$ wave function as a scalar, one can easily obtain

$$\mathcal{V}_{p_i,p_j}^{AB}(r) = (\hat{e}_{A_i} \cdot \hat{e}_{B_j(r)})V_{pp\pi}$$

$$- (\hat{e}_{A_i} \cdot \hat{u}_r)(\hat{e}_{B_j(r)} \cdot \hat{u}_r)(V_{pp\pi} - V_{pp\sigma}),$$

$$\mathcal{V}_{s,p_i}^{AB}(r) = [\hat{e}_{B_i(r)} \cdot \hat{u}_r]V_{sp\sigma}, \tag{7}$$

$$\mathcal{V}_{p_i,s}^{AB}(r) = -(\hat{e}_{A_i} \cdot \hat{u}_r)V_{sp\sigma},$$

$$\mathcal{V}_{s,s}^{AB}(r) = V_{ss\sigma},$$

where $\hat{u}_r$ ($r=1,2,3$) is the unit vector from the atom A to its three neighboring atoms B. $\hat{e}_{A_i}$ and $\hat{e}_{B_j}(r)$ are the unit vectors of the $2p_i$ wave function of atom A and the unit vector of the $2p_j$ wave function of atom B, respectively. The overlapping integration matrix $\mathcal{S}(k,n)$ has the same form as the Hamiltonian matrix, with four overlapping integration parameters to replace the four hopping integration parameters, and with units to replace the energy of the $2s$ and $2p$ wave functions $\mathcal{E}_{2s}$ and $\mathcal{E}_{2p}$. Thus we obtain an 8×8 Hamiltonian matrix $\mathcal{H}(k,n)$ and an overlapping integration matrix $\mathcal{S}(k,n)$. By solving the secular equation $\mathcal{H}(k,n)\mathcal{C}_i(k,n) = E_i\mathcal{S}(k,n)\mathcal{C}_i(k,n)$, we can calculate the electronic energy band E_i of SWNT's.

Taking account of the total energy of all the occupied band electrons in SWNT's relative to that in graphene, we have calculated the strain energy E_s of the straight SWNT's. With the possible bond-length dependence of the TB parameters being neglected, and with the real bond length of SWNT as $|\vec{u}_r|$, where $\vec{u}_r$ represents vectors between the nearest-neighbor atoms in the tube,[20] we have calculated the direction cosines $\hat{e}_i \cdot \hat{u}_r$ of Eq. (7). Figure 1 shows that E_s

depends only on the radius ρ of the tubes. The characteristic behavior $E_s = \mathcal{C}/\rho^2$ is found with $\mathcal{C} \approx 1.44$ eV Å²/ atom, in good agreement with previous calculated value 1.34 (Ref. 12) or 1.53 eV Å² / atom (Ref. 13), and excellently close to the value of 1.57 extracted from the measured phonon spectrum of graphite.[21]

Recently, "curved SWNT's" and "toruslike SWNT's" have been found.[22] They still have the sp^2 bond structure, but they are predicted to have pentagon-heptagon defects.[11] In curved SWNT's, the bond length is nearly the same as that in graphite sheet, since the distortion that is created by the bending nature of the curved tube is topologically relaxed by the inclusion of fivefold and sevenfold rings. However, the application of an external force moment at the two ends of the tube gives a different deformation. The hexagonal structure of the tube will not change until it reaches a critical bending curvature.[23] The tube undergoes only a simple compression on the inner side and a stretching on the outer side. In the following discussion, the term "curved SWNT" refers to the SWNT grown with pentagon-heptagon defects, and the term "bent SWNT" refers to a SWNT that bends with outer-stretching and inner-compressing deformations under external force moments applied to the two ends of the tube. Using an empirical model employed by Lenosky et al.,[11] Ou-Yang et al.[13] have developed a macroscopic continuous elastic model to calculate the curved SWNT. In their work, the strain energy of the curved SWNT comes from the angular change of the bonds or the curvature of the tubes. However, in the case of bent SWNT, the bond-length effect will contribute the main part of the strain energy. In what follows, we will treat only the latter case.

The bent SWNT surface can be described by[13]

$$\vec{Y}(s,\phi) = \vec{r}(s) + \rho[\vec{N}(s)\cos\phi + \vec{b}(s)\sin\phi], \qquad (8)$$

where $\vec{r}(s)$ is the position vector of the axis and $0 < s \leqslant l$ is the arc-length parameter along the bent SWNT axis; $0 < \phi \leqslant 2\pi$. $\vec{N}(s)$ and $\vec{b}(s)$ are unit normal and unit binormal vector of $\vec{r}(s)$, respectively. The position of each carbon atom is described by two parameters, s and ϕ. The two operations $\mathcal{C}_N$ and $\mathcal{S}(h,\alpha)$ can still be used to determine the positions of atoms in the SWNT. Therefore, a translation of h units along the axis of the SWNT means an addition of h to s, and a rotation of α about the axis means an addition of α to ϕ. However, because the rotational symmetry about the axis of the bent SWNT is broken, $\mathcal{C}_N$ and $\mathcal{S}(h,\alpha)$ are not symmetry operations. It is necessary to generalize the Bloch sums in the crystal unit cell containing $\mathcal{M} \times N$ primitive unit cells of SWNT. Here $\mathcal{M}$ is the length of the cell along the axis direction (the unit is h). $\mathcal{M} = 2(n_1^2 + n_2^2 + n_1 n_2)/N^2$ for $n_1 - n_2$ not a multiple of $3N$, and $\mathcal{M} = 2(n_1^2 + n_2^2 + n_1 n_2)/(3N^2)$ for $n_1 - n_2$ a multiple of $3N$.[24] We calculate only SWNT's with constant radius of curvature R. It is not in principle difficult to extend the present treatment to general bent SWNT's. In the bent SWNT, $\mathcal{V}_{ij}^{AB}(r)$ depends on the position of atom A and will be written as $\mathcal{V}_{ij}^{AB}(l,m;r)$, where $[m,l]$ are indices of the primitive unit cell of the atom A. When the SWNT is bent to a different direction $\vec{N}(s)$, $\mathcal{V}_{ij}^{AB}(r)$ will be different, but the Hamiltonian matrix elements are almost independent of the bending direction. We
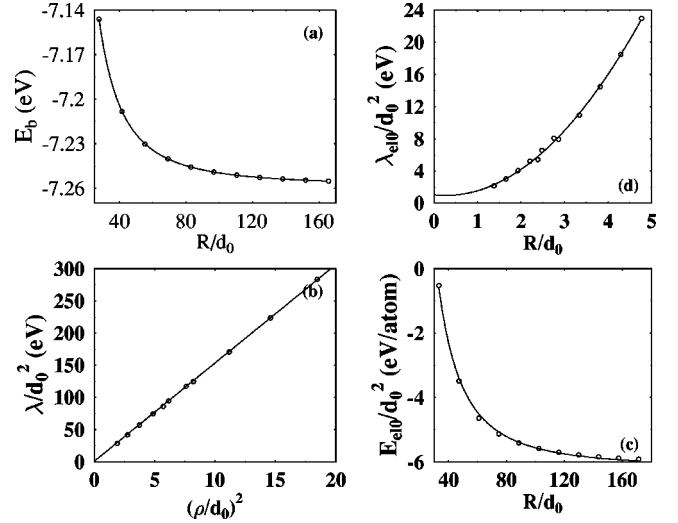

FIG. 2. (a) Strain energy per atom versus the bending radius R in a (5,5) tube. The solid line is a fit to the $E_s + \lambda/R^2$, where E_s is the cohesive energy of straight (5,5) tube. $\lambda = 86.1 \times 1.42^2$ eV Å²/ atom. (b) The value of λ of some $(n,0)$ and (n,n) tubes. The solid line is a fit to $a^* + b^* \rho^2, b^* \approx 15.27$ eV. (c) E_{el0} versus the bending radius R in the (5,5) tube. The solid line is a fit to $E_0 + \lambda_{el0}/R^2$. The zero point of E_{el0} has moved. (d) The value of λ_{el0} of these tubes. The solid line is a fit to $a_0 + a_1\rho + a_2\rho^2$, and the $a_0 \approx 1.05$.

have found that the anisotropy effect is very small. Similar to the case of the straight SWNT's, it is easy to obtain the $(8\mathcal{M}N) \times (8\mathcal{M}N)$ matrices of the Hamiltonian and the overlapping integration.

Since the change of bond length δr in bent SWNT's is proportional to ρ/R, the energy contribution of the bond stretching and bond compressing will be of the order of $1/R^2$. It is necessary to calculate both the electronic energy E_{el} and the repulsion energy E_{rep} between the ions. In order to fit the force constant of graphite,[25] we take $\gamma = 1.024$ Å^{-1}, $\phi' = \partial\phi/\partial r = -13.63\gamma$ eV/Å and $\phi'' = 60.4$ eV/ Å². With these parameters, we arrive correctly at the second derivative of the stretching energy E_c of SWNT's, $D = \partial^2 E_c/\partial\epsilon^2 = 58.5$ eV, and at the Poisson ratio, $\sigma = 0.24$, where ϵ is the relative compression along the axis of the SWNT.

Figure 2(a) shows the strain energy E_b per atom of the (5,5) SWNT as a function of the bending radius R. The data follow quite well with the expected behavior $E_b = E_s + \lambda/R^2$. A least-square fit to the data yields a value of $\lambda \approx 173$ eV Å²/ atom. Previous studies on curved SWNT's give a simple formula:[13]

$$E_b = \frac{\mathcal{C}R}{\rho^2\sqrt{R^2 - \rho^2}} \approx \frac{\mathcal{C}}{\rho^2} + \frac{\mathcal{C}}{2R^2}. \qquad (9)$$

In comparing with our results, we find that the value of λ for curved SWNT's is equal to $\mathcal{C}/2$, only 0.7 eV Å²/ atom. It implies that the strain energy of pentagon-heptagon defects is far less than the strain energy of the stretching and compressing of the bond length. The experimental fact that the deformations of bent SWNT's are the change of bond length rather than the pentagon-heptagon defect reveals that there is

a high potential barrier between the two deformations to prevent the change of the hexagonal structure under the addition of a moment of external force at the two ends of the SWNT.

By CET, we can calculate Young's modulus Y of a SWNT from three different strain energies. They are the rolling energy E_s, the compressing or stretching energy E_c, and the bending strain energy ΔE_b. The three energies are given by

$$E_s = \frac{\mathcal{C}}{\rho^2}, \tag{10}$$

$$E_c = \frac{1}{2} D \epsilon^2, \tag{11}$$

$$\Delta E_b = \frac{\lambda}{R^2}, \tag{12}$$

where ϵ is the relative stretch or compression along the axis of SWNT's, and D is the second derivative of E_c. The three quantities $\mathcal{C}$, D, and λ are given by

$$\mathcal{C} = \frac{\Omega}{24(1-\sigma^2)} Y b^3, \tag{13}$$

$$D = \Omega Y b, \tag{14}$$

$$\lambda = \frac{\Omega}{4} Y b (\rho^2 + b^2/4), \tag{15}$$

respectively. Where $\Omega = 2.62$ Å^2/atom is the occupied area per carbon atom in SWNT's, b is the effective wall thickness of the SWNT. Previous calculations[8,14–16] indicate that the value of D of SWNT's is about 58 eV/atom, the same as that of graphites. However, since the wall thickness is not well defined in a single-layered structure, various values of b are used in the studies, and thus the obtained Y are quite different. Lu[15] and Hernández et al.[16] took the interwall distance of graphite (3.4 Å) as the thickness, and obtained the average Young's modulus of a SWNT as about 1 TPa, in consistency with the corresponding measurement in multiwall nanotubes[27] and bulk graphite samples. But the average value of Y cannot describe all the deformations of SWNT's, such as the rolling of graphene and the bending of SWNT's, though it can describe the stretching and compressing deformation along the axis direction of SWNT's. Yakobson et al.[14] have given $Y = 5.5$ TPa and $b = 0.66$ Å by using the rolling energy formula of the graphite sheet [Eq. (14)] and the stretching energy formula of graphene or SWNT's [Eq. (13)] simultaneously. The obtained value of b is about the π orbital extension of carbon atom, which corresponds to the general fact that elasticity results from the overlapping of electron cloud between atoms. However, since Eq. (13) describes the rolling of single-layered graphene, the results given by Yakobson et al. seem to correspond to the graphite sheet rather than the SWNT. Young's modulus and the ef-

fective wall thickness of SWNT's and their dependence of the tube radius and helicity still remain unknown.

With Eq. (15), from the calculation of the bending strain energy of SWNT's with various radius, one may simultaneously find Y and b of SWNT's. Figure 2(b) shows the relationship between λ and the radius of the tube in the form $\lambda = b^* \rho^2 + a^*$. In comparison with Eq. (15), it implies that both Y and b are independent of the radius and helicity of SWNT's. The value of $b^* = 15.3$ eV/atom is consistent with the value $D/4 = 14.7$ eV/atom. However, it is difficult to obtain the exact value of a^*, because the first term of λ is much greater than the second term a^* and introduces high errors in the fitting of a^*. Careful analysis of the strain energy of bent SWNT's tells us only that the electronic energy from the angular change of the bond can contribute to the ρ^0 order of the bending strain energy of SWNT. The other terms, including the repulsion energy between ions and the electronic energy from the nonzero γ effects [Eq. (5)], depend on δr, and hence on the radius of the tube ρ. For the wall thickness, is is unnecessary to consider the bond-length dependence of TB parameters and the repulsion energy. One needs only to calculate the $\gamma = 0$ bond angular contribution E_{el0} of the electronic energy. When $\gamma = 0$, the $(1/R)$th order perturbation of Hamiltonian is zero, and $E_{el0} = \lambda_{el0}/R^2$. The ρ^0 order term of λ comes completely from the λ_{el0} and the residual part of λ affects only the value of ρ^2 order. The exact value of a^* can be obtained by calculating E_{el0}. Figure 2(c) shows the expected relationship $E_{el0} = \lambda_{el0}/R^2$. Figure 2(d) gives values of λ_{el0} for some SWNT's. It leads to $a^* = 1.05 r_0^2$ eV Å^2/ atom by fitting it to $a^* + a_1 \rho + a_2 \rho^2$ (Ref. 26). The wall thickness of the tube is supposed to be identical to that of graphite; then from Eqs. (13) and (15), one gets $a^* = \frac{3}{2}(1 - \sigma^2)\mathcal{C} \approx 1.0 r_0^2$ eV Å^2/atom. Therefore, b is about 0.74 Å, and Y is about 5.1 TPa. This shows that both Y and b are independent of the radius and helicity of the tube, and Young's modulus of the SWNT is 5 times greater than the average value of MWNT. The obtained value of b is independent of the fitting parameters γ and ϕ'', and Y is also insensitive to these parameters.

In summary, our calculation shows the following results: the strain energy of the straight SWNT come mainly from the occupied band electrons and the obtained Young's modulus of the SWNT is independent of the radius and the helicity and is much larger than the modulus of the bulk sample. The effective thickness of SWNT is about the size of the carbon atom, far less than the distance between the layers of the graphite. These results show that CET can well describe the deformation of the bent tubes.

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