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ORIGINAL PAPER

Carbon nanotori and nanotubes encapsulating carbon atomic-chains

Kanes Sumetpipat · Richard K. F. Lee · Barry J. Cox · James M. Hill · Duangkamon Baowan

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Abstract In this paper we investigate toroidal carbon nanotubes (carbon nanotori) encapsulating a single symmetrically located carbon atomic-chain. The interaction energy of the carbon chain is found from the Lennard-Jones potential using the continuous approach which assumes that atoms are uniformly distributed over the surface of the torus and the line of the circular chain with constant atomic surface and line densities, respectively. We assume that the chain is centrally located and that the carbon nanotorus is synthesized from a perfect carbon nanotube. We predict that the carbon chain can be encapsulated inside the carbon nanotorus when the cross-sectional radius r of the nanotorus is larger than 3.17 Å. At the minimum energy, a value of the toroidal radius R lies between 3.6 and 3.7 Å corresponding to each value of r. We also investigate the energy of carbon chains inside carbon nanotubes, which are (4,4), (5,5) and (10,0) tubes. We find that they are energetically favourable in (5,5) and (10,0) tubes, but not in a (4,4) tube, because it is geometrically too small, and these results are in agreement with existing studies. The same results for these three carbon nanotubes can also be obtained from the corresponding nanotori when R goes to infinity.

Keywords Nanotori · Carbon atomic-chain · Lennard-Jones potential · Continuous approximation · Encapsulation

K. Sumetpipat · D. Baowan (✉)
Department of Mathematics, Faculty of Science, Mahidol University,
Rama VI Rd., Bangkok 10400, Thailand
e-mail: duangkamon.bao@mahidol.ac.th

R. K. F. Lee · B. J. Cox · J. M. Hill
Nanomechanics Group, School of Mathematical Sciences, The University of Adelaide,
Adelaide, SA 5005, Australia

1 Introduction

Since carbon nanotubes (CNTs) were discovered by Iijima [1] in 1991, experiments for many new potential nanodevices have been investigated. Single-walled carbon nanotube (SWCNT) may be envisaged from a graphene sheet which is rolled up forming a seamless tube [2], and multi-walled carbon nanotubes (MWCNTs) are assumed to be formed as concentric distinct radii SWCNTs [3]. Their mechanical properties are unique such as high strength, low weight, high flexibility and novel electronic properties [4]. Due to these properties, SWCNTs and MWCNTs have been used for many applications [5–7]. For example, CNTs might be used as high frequency nano-oscillators which can generate frequency in the gigahertz range [5,6], so that these nano-oscillators might be used for many novel electrical components.

Cumings and Zettl [5], and Yu et al. [6] study a MWCNT system for which an inner tube oscillates inside an outer one. They show that the frictional force between the inner and the outer tubes is vanishingly small and hardly effects the motion, so that to a first approximation the frictional force might be ignored. Zheng and Jiang [7] examine a similar system using molecular dynamics simulations, and they also suggest a frictionless oscillatory system. Qian et al. [8] and Liu et al. [9] use molecular dynamics simulations to study a C_{60} fullerene inside a CNT, and the results show that the encapsulation and the oscillation of the C_{60} depend on the diameter and the length of the CNT. They show that the frequency of the C_{60} oscillation is in the gigahertz range. Cox et al. [10,11] have derived formulae for the interaction energy and the frequency of the C_{60} and the CNT oscillators, as determined from the Lennard-Jones potential function and the continuum approximation. These results show that the frequency of the C_{60} oscillator is a function of the length and the radius of the CNT which agrees with Qian et al. [8] and Liu et al. [9].

Tomanek and Schluter [12] indicate that carbon atoms can form one dimensional atomic-chain structures providing that the total number of carbon atoms is less than 20. However, Wang et al. [13] experimentally observe that a carbon atomic-chain can be synthesized inside a CNT, and Zhao et al. [14] claim that the carbon atomic-chain inside the CNT is stable even when it has more than 20 atoms. Since carbon atomic-chains can transfer charge [15], such the chain inside the CNT is important for many novel devices.

Carbon nanotori (TCNTs) [16] are formed from SWCNTs that are joined the open ends [17]. Experimentally, the diameter of the ring and the diameter of CNT are found to be larger than 100 and 1 nm, respectively [16]. However using molecular dynamics simulations, Huhtala et al. [18] and Han [19] report that smaller nanotori might exist, such as ring diameter of 22 nm with the CNT diameter below 1.3 nm. Ihara and Itoh [20] predict that the smallest TCNT is a C_{120}. Moreover, continuum elastic shell theory [21] and an empirical mathematical approach [22] have been employed to determine the shape of TCNTs.

Tang [23] reports that carbon chains are possibly encapsulated inside TCNT, and investigates their electronic properties and persistent current. He concludes that the intensity of current depends on the factors of the surrounding environment. Additionally, Lusk et al. [24] study a similar system where the carbon chain is replaced by a metal chain; Fe, Au, and Cu. They use the smallest TCNT, C_{120}, to determine the

binding energy for synthesizing the system and examine the stability of the structure. One of their results is that an Fe-chain can be encapsulated inside a TCNT and it possesses a magnetic moment.

In the present paper, we investigate the energy behaviour of a carbon chain inside a TCNT using the Lennard-Jones potential and the continuum approximation. The radii of CNTs and TCNTs encapsulating a carbon atomic-chains are determined. In Sect. 2, the method for determining the interaction energy is presented. The calculation of the interaction energy for a nanotorus with a symmetrically located carbon atomic chain is determined in Sect. 3. Detailed numerical results and energy profiles are given in Sect. 4. Finally, some brief discussion and a summary are presented in Sect. 5.

2 Method

In this section, the interaction energy between the carbon atomic-chain and the nanotorus is obtained from the 6–12 Lennard-Jones potential and the continuous approximation. For a discrete structure, the non-bonded interaction energy is obtained by the summation of the interaction energy for all non-bonded atomic pairs

$$E = \sum_i \sum_j \Phi(\rho_{ij}),$$

where $\Phi(\rho_{ij})$ is the potential function of atoms i and j with the distance ρ_{ij} apart. In this work, the total potential is found from the continuous approximation which assumes that all atoms are uniformly distributed over the surface of the TCNT and the atomic-chain, and the double summation is replaced by a double integration. The extent of the double integral is the entire surface of the TCNT, S_t, and the entire length of chain, ℓ_m, hence

$$E = \eta_m \eta_t \int_{\ell_m} \int_{S_t} \Phi(\rho)\, \mathrm{d}S_t\, \mathrm{d}\ell_m,$$

where η_m and η_t are the mean atomic line density of atomic-chain and the mean surface atomic density of the carbon atoms in the TCNT, respectively, and ρ denotes the distance between an arbitrary atom on the TCNT and an arbitrary atom on the atomic-chain. The 6–12 Lennard-Jones potential is given by

$$\Phi(\rho) = 4\epsilon \left[-\left(\frac{\sigma}{\rho}\right)^6 + \left(\frac{\sigma}{\rho}\right)^{12} \right],$$

where ϵ is the well depth and σ is the Van der Waals diameter. For different materials, the empirical rule is employed to determine the values of ϵ and σ, given by $\epsilon = (\epsilon_1 \epsilon_2)^{1/2}$ and $\sigma = (\sigma_1 + \sigma_2)/2$, where ϵ_1 and σ_1 are the values for material 1 and ϵ_2 and σ_2 are the corresponding values for material 2. The Lennard-Jones potential function can also be rewritten as

$$\Phi(\rho) = -\frac{A}{\rho^6} + \frac{B}{\rho^{12}},$$

where $A = 4\epsilon\sigma^6$ and $B = 4\epsilon\sigma^{12}$ are termed the attractive and repulsive constants, respectively.

3 Energy for nanotorus interacting with carbon atomic-chain

The full expression for the interaction of the TCNT with the atomic-chain is given by

$$E = \eta_t \eta_m \int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \Phi(\rho) R r (R + r\cos\phi)\, \mathrm{d}\theta\, \mathrm{d}\phi\, \mathrm{d}\theta_1, \tag{1}$$

where R and r are the radius of the nanotorus ring measured from the tube centre and the radius of the tube, respectively, as shown in Fig. 1. The TCNT surface element is parametrically given by

$$(x_t, y_t, z_t) = ((R + r\cos\phi)\cos\theta, (R + r\cos\phi)\sin\theta, r\sin\phi),$$

while a typical element on the carbon chain is given by

$$(x_m, y_m, z_m) = (R\cos\theta_1, R\sin\theta_1, 0).$$

The distance between a typical point on the TCNT surface and a typical point on the atomic-chain is then given by

$$\rho^2 = r^2 + 4R(R + r\cos\phi)\sin^2[(\theta - \theta_1)/2].$$

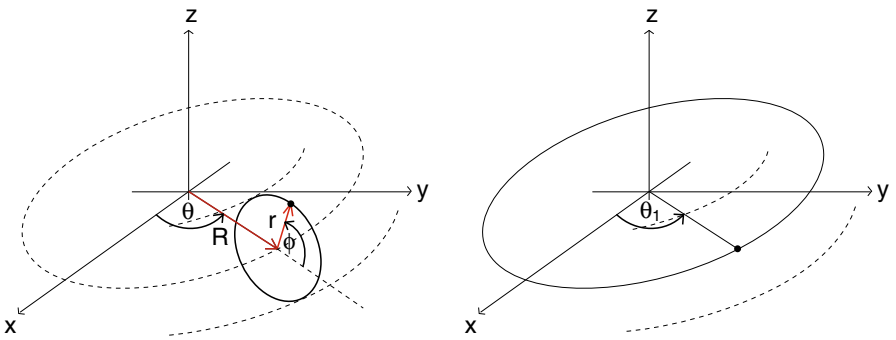

Fig. 1 Coordinates for points on surface of nanotorus (*left*) and on atomic-chain (*right*)

Equation (1) can be rewritten as $E = \eta_t \eta_m(-AD_3 + BD_6)$, where $D_n(n = 3, 6)$ are defined by

$$D_n = \int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \frac{Rr(R + r\cos\phi)}{\rho^{2n}} \mathrm{d}\theta\, \mathrm{d}\phi\, \mathrm{d}\theta_1. \tag{2}$$

The analytical details for determining the final form of this integral are given in Appendix 1, here we have

$$\begin{aligned} D_n &= \frac{4\pi^2}{r^{2n-2}} \sum_{k=0}^{n-1} \binom{n-1}{k}\binom{2k}{k}(-1)^k R^{k+1} Q_k, \\ Q_k &= \frac{2\pi(R + r)^{k+1}}{(2R + r)^{2k+1}} \sum_{i=0}^{k+1} \binom{k+1}{i}\binom{2i}{i}\frac{L_1^i}{2^{2i}} F\left(k + \frac{1}{2}, i + \frac{1}{2}; i + 1; L_2\right), \end{aligned} \tag{3}$$

where $L_1 = -2r/(R + r)$ and $L_2 = 8Rr/(2R + r)^2$. When the ring radius of the nanotorus R is large comparing to r, a section of the giant TCNT can be considered as a CNT because the curvature of the toroidal ring is very small and it can be ignored. As a result, the interaction energy for a CNT with the carbon chain can be examined by assuming that the ring radius R approaches to infinity. From (3), the energy per unit length E^* can be obtained as

$$E^*(\ell, r) = \lim_{R\to\infty} \frac{\ell}{2\pi R} E(R, r) = \lim_{R\to\infty} \frac{n_A}{2\pi R\eta_m} E(R, r), \tag{4}$$

where ℓ is the length of atomic-chain and n_A is the number of atoms in the atomic-chain.

The expression for the interaction energy of an infinitely long CNT with an atomic-chain of length ℓ is given by

$$E'(\ell, r) = \ell\eta_m\eta_t \int_{-\infty}^{\infty}\int_{-\pi}^{\pi} \Phi(\rho) r \mathrm{d}\theta \mathrm{d}z. \tag{5}$$

The coordinates of a typical point on the CNT are given by

$$(x_t, y_t, z_t) = (r\cos\theta, r\sin\theta, z),$$

and the coordinates of an atom located at the origin are $(0, 0, 0)$. Thus, the distance between the atom at the origin and a typical point on the CNT surface is given by $\rho^2 = r^2 + z^2$, where the schematic model is depicted in Fig. 2. Equation (5) becomes $E'(\ell, r) = \ell\eta_m\eta_t(-AJ_3 + BJ_6)$, where the integrals J_n (n=3, 6) are given by

$$J_n = 2\pi \int_{-\infty}^{\infty} \frac{r}{(r^2 + z^2)^n} \mathrm{d}z.$$

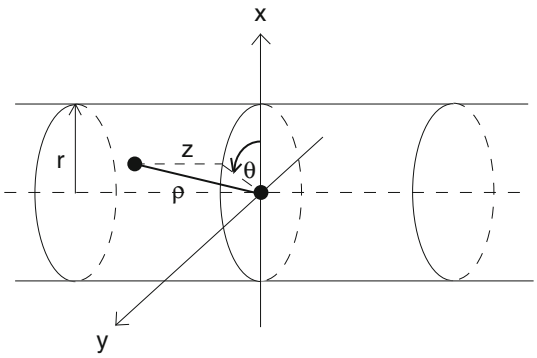

Fig. 2 Coordinates for point on surface of carbon nanotube with atom located at the origin

On making the substitution $z = r \tan x$, we obtain

$$J_n = \frac{2\pi}{r^{2(n-1)}} \int_{-\pi/2}^{\pi/2} \cos^{2(n-1)} x \, \mathrm{d}x = \frac{2\pi}{r^{2(n-1)}} B\left(n - \frac{1}{2}, \frac{1}{2}\right)$$
$$= \frac{2\pi^2}{(2r)^{2(n-1)}} \binom{2(n-1)}{n-1}. \tag{6}$$

4 Results for nanotorus encapsulating carbon chain

In this section, we investigate the equilibrium state of the carbon chain inside the carbon nanotorus. Although the expression for the total interaction energy (3) is complicated, numerical values arising from such expression may be readily evaluated using algebraic packages such as MAPLE and MATLAB. The equilibrium values for the TCNT radius R, the CNT radius r, and the interaction energy per unit length are determined. The parameter values used in this study are given in Table 1.

Figure 3 shows the energy per atom E/η_m for $R = 5$, 7, 12 and 16 Å where the radius r ranges from 3 to 6 Å. We observe that for each value R there is a corresponding

Table 1 Constants used in this model

Attractive constant [25] (eV× Å^6)	$A = 14.8919$
Repulsive constant [25] (eV× Å^{12})	$B = 23005.0954$
Atomic line density of carbon chain of (5, 5) (atom/Å)	$\eta_m = 0.9041$
Atomic line density of carbon chain of (10, 0) (atom/Å)	$\eta_m = 0.8696$
Mean surface density of CNT [10] (atom/Å^2)	$\eta_t = 0.3812$
Radius of (4,4) CNT [26] (Å)	$r = 2.75$
Radius of (5,5) CNT [14] (Å)	$r = 3.387$
Radius of (10,0) CNT [27] (Å)	$r = 3.9$

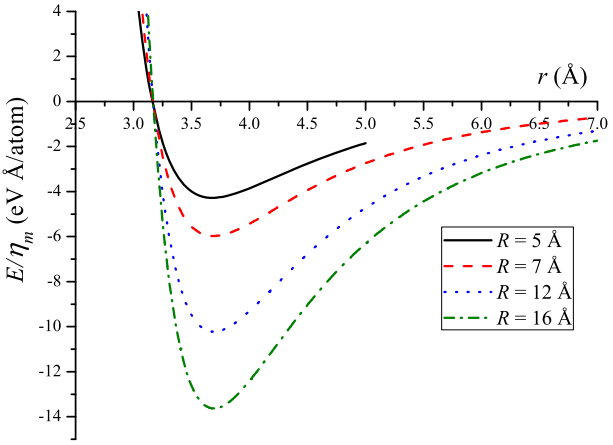

Fig. 3 Energy E/η_m for radii $R = 5$, 7, 12 and 16 Å of nanotori, we comment that $R < r$

value of r in the range 3.6–3.7 Å that minimises the energy, and we comment that for these minimum energy values, the carbon chain is assumed to be centrally located in the TCNT. Further, the energy per atom $E/(2\pi R\eta_m)$ for $R = 5$, 7, 12 and 16 Å is shown in Fig. 4 . In this figure all four curves lie approximately on the same line, showing that the interaction energy is virtually independent of the nanotori radius R. When the radius r is larger than the value of the radius giving the minimum energy r_{min}, the energy tends to zero as r goes to infinity. In this scenario, the carbon chain is more likely to be located offset from the TCNT centre, because the minimum energy location is closer to the tube wall. However, when the radius r is smaller than r_{min} and the interaction energy is negative, the carbon chain is located at the centre inside the TCNT because the minimum energy position is at the centre of the TCNT. For the value of r that gives a positive interaction energy, the encapsulation of the carbon chain inside the TCNT is not likely to occur because the carbon chain will face a large repulsive energy. From Figs. 3 and 4, it is apparent that r should be at least 3.17 Å to give a negative interaction energy, and give rise to a stable configuration.

Figure 5 shows the value of r_{min} at the minimum interaction energy for each value of R. We see that r_{min} increases with increasing R, and r_{min} is approximately 3.69 Å when R is larger than 15 Å. Next we consider the minimum energy per atom $E/(2\pi R\eta_m)$, as shown in Fig. 6. The minimum energy per atom decreases as R increases. We suggest that the results of Figs. 5 and 6 arise from the effect of the interaction energy between the carbon chain and the atoms on the opposite surface of the TCNT. For a large TCNT, the interaction energy from the other side of the torus will not effect to the chain since the van der Waals is a short range interaction, therefore, the values of r_{min} and $E/(2\pi R\eta_m)$ may be assumed to be constants once R is large enough.

Figure 7 shows the energy of an atom inside a large TCNT. When the radius r is larger than 3.69 Å, the minimum energy position is not located at the centre of the TCNT, but it moves to one side of the TCNT because the minimum energy location is closer to the wall of the TCNT. If the radius r is smaller than 3.69 Å and the energy is

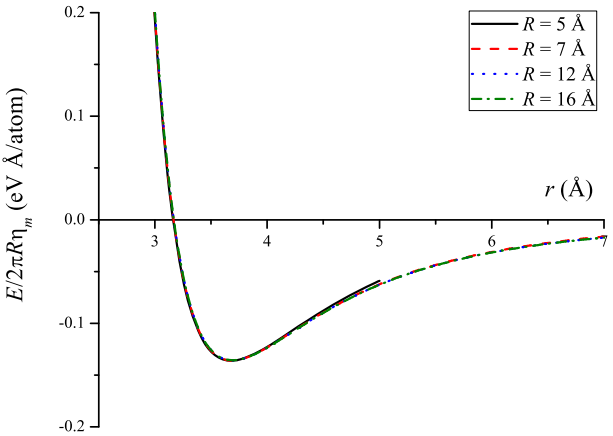

Fig. 4 Energy per atom $E/(2\pi R\eta_m)$ for radii R = 5, 7, 12, and 16 Å of nanotori

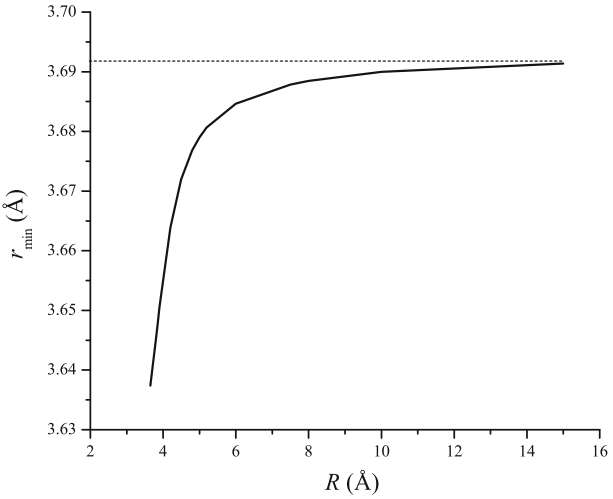

Fig. 5 Relation between r_{min} and R at the minimum energy value

negative, the chain is centrally located in the TCNT as the minimum energy location is at the center of the TCNT. The chain can not be encapsulated in the TCNT once the radius r is less than 3.17 Å since the energy is positive.

We find that $E^*(\ell, r) = E'(\ell, r)$, for the same values of ℓ and r, so the discussion for a CNT with a carbon chain can be considered either from (4) or (6). In (4), we may take R to be infinity so that the curvature of the TCNT is very small and the TCNT can be replaced by the CNT. Alternatively, we can simply calculate the interaction energy of an atomic chain inside the CNT using (6).

In order to make a comparison with the numerical results given in [26] and [27], the (4,4), (5,5), and (10,0) CNTs are examined. The results show that the (5,5) and (10,0) CNTs with centrally located carbon chains are stable and with interaction energies

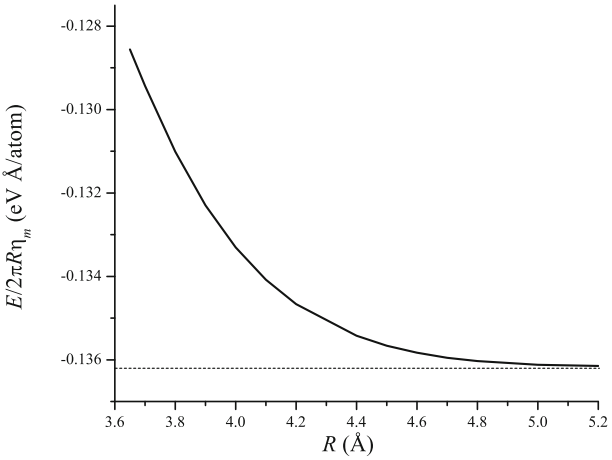

Fig. 6 Value of minimum energy as a function of nanotorus radius R

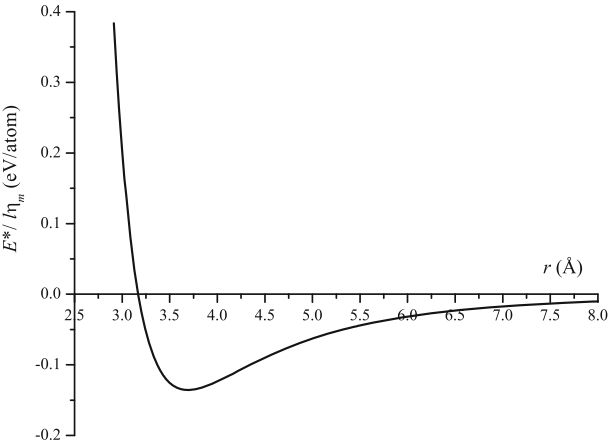

Fig. 7 Interaction energy $E^*/l\eta_m$ as a function of nanotorous radius R where R is assumed to be large and nanotorus can be replace by nanotube

-1.04 and -1.29 eV, respectively. However, the radius r of a (4,4) CNT is too small, and the interaction energy of the system is positive. These results are consistent with the results presented in [26] and [27]. Figure 4 shows that the radius r must be greater than 3.17 Å, otherwise, the interaction energy will be positive and the carbon chain cannot be inside the CNT. The radius r at the minimum energy location of the CNT is around 3.69 Å which is consistent with the study of Hu et al. [28] who predict that the radius of the innermost carbon nanotube with the carbon chain is approximately 3.63 Å. Some calculation details for the cases of (5,5), and (10,0) CNTs are presented in Appendix 2.

5 Discussion and summary

The mechanics of a system comprising a carbon chain inside a TCNT have been studied using the Lennard-Jones potential and the continuum approximation. Formulae for the interaction energies between TCNTs and CNTs with the carbon chain have been derived and they are given by (3) and (6), respectively. We have found that a value of the TCNT radius that gives the minimum energy, r_{min}, is around 3.69 Å. Further, for a TCNT of a ring radius R smaller than 15 Å, r_{min} decreases and ranges from 3.6 to 3.7 Å. The interaction energy increases for R less than 5.2 Å. We predict that the radius r of the TCNT must be larger than 3.17 Å for the chain to be stable inside the TCNT. In the case of conventional (4,4), (5,5), and (10,0) CNTs, we can use either (4) with R tending to infinity or directly from (6) to determine the energy of the system. We predict that the (5,5) and (10,0) CNTs can encapsulate a carbon chain but the (4,4) CNT cannot, and these results are consistent with the results presented in [26] and [27]. Moreover, the radius r_{min} at the minimum energy location of the CNT is approximately 3.69 Å which shows an excellent agreement with the study of Hu et al. [28] who predict that the radius of the innermost carbon nanotube with the carbon chain is approximately 3.63 Å.

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Appendix 1: Interaction of nanotorus with carbon atomic-chain

In this appendix, we simplify the expression (2) for the interaction of the nanotorus with the circular atomic carbon chain,

$$D_n = \int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \frac{Rr(R + r\cos\phi)}{\rho^{2n}} \mathrm{d}\theta\, \mathrm{d}\phi\, \mathrm{d}\theta_1,$$

since ρ depends only on the difference $(\theta - \theta_1)$ we may deduce

$$D_n = 2\pi \int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \frac{Rr(R + r\cos\phi)}{\rho^{2n}} \mathrm{d}\theta\, \mathrm{d}\phi,$$

where $\rho^2 = r^2 + 4R(R + r\cos\phi)\sin^2(\theta/2)$. On defining the integrals I_n as

$$I_n = \int_{-\pi}^{\pi} \frac{1}{\rho^{2n}} \mathrm{d}\theta = \int_{-\pi}^{\pi} \frac{1}{[r^2 + 4R(R + r\cos\phi)\sin^2(\theta/2)]^n} \mathrm{d}\theta$$
$$= 2\int_{0}^{\pi} \frac{1}{[r^2 + 4R(R + r\cos\phi)\sin^2(\theta/2)]^n} \mathrm{d}\theta.$$

Upon making the substitution $t = \sin^2(\theta/2)$, we obtain

$$I_n = \frac{2}{r^{2n}} \int_{0}^{1} \frac{t^{-1/2}(1-t)^{-1/2}}{[1 + 4R(R + r\cos\phi)t/r^2]^n} \mathrm{d}t,$$

which can be written in terms of the hypergeometric function $F(a, b; c; z)$ with $a = n, b = 1/2, c = 1$ and $z = -4R(R + r\cos\phi)/r^2$, so that we have

$$I_n = \frac{2\pi}{r^{2n}} F\left(n, \frac{1}{2}; 1; \frac{-4R(R + r\cos\phi)}{r^2}\right).$$

Then on truncating the hypergeometric series using the transformation $F(a, b; c; z) = (1 - z)^{-b} F(c - a, b; c; z/(z - 1))$, we may deduce

$$I_n = \frac{2\pi(r^2 + 4R(R + r\cos\phi))^{-1/2}}{r^{2n-1}} F\left(1 - n, \frac{1}{2}; 1; \frac{4R(R + r\cos\phi)}{r^2 + 4R(R + r\cos\phi)}\right).$$

Now, the hypergeometric function can be expanded in the series form

$$F(-m, b; c; z) = \sum_{k=0}^{m} \frac{(-m)_k (b)_k}{(c)_k k!} z^k,$$

therefore I_n becomes

$$I_n = \frac{2\pi}{r^{2n-1}} \sum_{k=0}^{n-1} \frac{(1-n)_k (1/2)_k}{(1)_k k!} \frac{(4R)^k (R + r\cos\phi)^k}{[r^2 + 4R(R + r\cos\phi)]^{k+1/2}},$$

this gives

$$D_n = 2\pi \int_{-\pi}^{\pi} I_n R r (R + r\cos\phi)\mathrm{d}\phi = \frac{4\pi^2 R}{r^{2n-2}} \sum_{k=0}^{n-1} \frac{(1-n)_k (1/2)_k}{(1)_k k!} (4R)^k Q_k$$
$$= \frac{4\pi^2}{r^{2n-2}} \sum_{k=0}^{n-1} \binom{n-1}{k} \binom{2k}{k} (-1)^k R^{k+1} Q_k,$$

where

$$Q_k = \int_{-\pi}^{\pi} \frac{(R + r\cos\phi)^{k+1}}{(4R^2 + r^2 + 4Rr\cos\phi)^{k+1/2}} \mathrm{d}\phi = 2\int_{0}^{\pi} \frac{(R + r\cos\phi)^{k+1}}{(4R^2 + r^2 + 4Rr\cos\phi)^{k+1/2}} \mathrm{d}\phi.$$

Next, we use $\cos\phi = 1 - 2\sin^2(\phi/2)$ to give

$$Q_k = 2\int_{0}^{\pi} \frac{(R + r - 2r\sin^2(\phi/2))^{k+1}}{((2R + r)^2 - 8Rr\sin^2(\phi/2))^{k+1/2}} \mathrm{d}\phi,$$

and upon letting $t = \sin^2(\phi/2)$, we obtain

$$Q_k = \frac{2(R + r)^{k+1}}{(2R + r)^{2k+1}} \int_{0}^{1} \frac{t^{-1/2}(1 - t)^{-1/2}(1 + L_1 t)^{k+1}}{(1 - L_2 t)^{k+1/2}} \mathrm{d}t,$$

where

$$L_1 = -2r/(R + r), \qquad L_2 = 8Rr/(2R + r)^2. \tag{7}$$

Next on using the binomial theorem

$$(1 + L_1 t)^{k+1} = \sum_{i=0}^{k+1} \binom{k+1}{i} L_1^i t^i,$$

we obtain

$$Q_k = \frac{2(R + r)^{k+1}}{(2R + r)^{2k+1}} \sum_{i=0}^{k+1} \binom{k+1}{i} L_1^i \int_{0}^{1} \frac{t^{i-1/2}(1 - t)^{-1/2}}{(1 - L_2 t)^{k+1/2}} \mathrm{d}\phi,$$

and the integral may be changed into the hypergeometric form with, $a = k + 1/2$, $b = i + 1/2$, $c = i + 1$ and $z = L_2$

$$\begin{aligned} Q_k &= \frac{2(R + r)^{k+1}}{(2R + r)^{2k+1}} \sum_{i=0}^{k+1} \binom{k+1}{i} L_1^i \frac{\Gamma(i + 1/2)\Gamma(1/2)}{\Gamma(i + 1)} F\left(k + \frac{1}{2}, i + \frac{1}{2}; i + 1; L_2\right) \\ &= \frac{2\pi(R + r)^{k+1}}{(2R + r)^{2k+1}} \sum_{i=0}^{k+1} \binom{k+1}{i} \binom{2i}{i} \frac{L_1^i}{2^{2i}} F\left(k + \frac{1}{2}, i + \frac{1}{2}; i + 1; L_2\right). \end{aligned}$$

So that in summary we have the formulae

$$E = \eta_t \eta_m(-AD_3 + BD_6),$$
$$D_n = \frac{4\pi^2}{r^{2n-2}} \sum_{k=0}^{n-1} \binom{n-1}{k} \binom{2k}{k} (-1)^k R^{k+1} Q_k,$$
$$Q_k = \frac{2\pi(R+r)^{k+1}}{(2R+r)^{2k+1}} \sum_{i=0}^{k+1} \binom{k+1}{i} \binom{2i}{i} \frac{L_1^i}{2^{2i}} F\left(k+\frac{1}{2}, i+\frac{1}{2}; i+1; L_2\right),$$

where L_1 and L_2 are defined by (7).

Appendix 2: Interaction energy for carbon chain inside nanotube

In this appendix, we show the calculation of the interaction energy for (5,5) and (10,0) CNTs. Firstly, we assume that carbon chain consisting of ten atoms is located inside the (5,5) CNT, where the CNT has the radius of 3.387 Å and the value of the C-C bond length is taken from [14] where it is 1.229 Å, so that

$$\ell = 9 \times 1.229 = 11.061, \quad \eta_m = 10/11.061 = 0.9041.$$

Therefore, we consider

$$E^*(11.061, 3.387) = \lim_{R\to\infty} \frac{11.061}{2\pi R} E(R, 3.387).$$

For the second case, we consider a carbon chain consisting of ten atoms located inside the (10,0) CNT. The CNT has the radius of 3.9 Å and the length of chain is taken from [27] which is 11.5 Å, then we have

$$\ell = 11.5, \quad \eta_m = 10/11.5 = 0.8696.$$

Hence, the interaction energy can be obtained as

$$E^*(11.5, 3.9) = \lim_{R\to\infty} \frac{11.5}{2\pi R} E(R, 3.9).$$

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