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ORIGINAL PAPER

Encapsulation behaviours of nanoparticles entering two-section carbon nanotubes

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Abstract Carbon nanotubes are special nanostructures due to their unique mechanical and electronic properties. One of the proposed applications is a container for drug delivery. In this paper, we consider two-section carbon nanotubes for their uses as nanocapsules to encapsulate a single atom and a C_{60} fullerene. The Lennard-Jones function and the continuous approach are employed to determine the molecular interactions. Moreover, the explicit forms of their interaction energies are determined. The suction energies are utilised to determine the encapsulated conditions of both nanoparticles, where they depend on the radii of the particle and the nanocapsule. This theoretical study can be thought of as the first step to design the nanocapsule for the drug delivery devices.

Keywords Two-section carbon nanotube · Lennard-Jones potential function · Suction energy · Encapsulation behaviour

1 Introduction

The discovery of carbon nanotubes by Iijima [1] has created enormous impact in many scientific areas. Because of their unique mechanical and electronic properties [2] such as high strength, low weight, thermal stability, and flexibility in changing volume for providing a higher payload capacity [3], carbon nanotubes have attracted considerable

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attention for applications in nanobiotechnology. For example, carbon nanotubes may be used as drug and gene containers for applications in pharmaceuticals and cosmetics [4]. Researchers believe that drugs contained in the nanotubes can be directed to the target cell [5] and then taken up by the cell nucleus [6]. This is the concept of magic bullet proposed by Paul Ehlrich [7].

Since nanocapsules are high-pressure vessels, adsorbents and safe-keepings which are described in [8]. Vakhrushev et al. [8] designed a nanocapsule which comprises a combination of three nanotubes : (20, 20), (10, 10) and (8, 8) for methane container. They constructed a fill-and-lock system by the aid of a locking particle. Following the work by Vakhrushev et al. [8], we firstly design a nanocapsule by combining two sizes of carbon nanotubes and refer to it as a two-section carbon nanotube. We note that the mathematical derivation for the three or more sections of carbon nanotubes can be determined using the same approach described later in the text.

In this research, we use the concept of suction energy proposed by Cox et al. [9] to determine whether an atom and a C_{60} fullerene will be encapsulated into a two-section nanocapsule by the van der Waals forces alone. The van der Waals interaction can be obtained by three formulae, a discrete atom-atom model, a continuous model, and a hybrid discrete-continuous approach. Hilder et al. [10] calculated the interaction energies between an atom and a carbon nanotube using the three approaches and found that they give similar results. They also stated that the most suitable approach for symmetrical structures is a continuous approximation. The interaction energies of many C_{60}-nanotube systems have been studied using a continuous approximation [11–14]. In this research, we use the continuous approximation to determine the interaction energies between a two-section carbon nanotube and nanoparticles. Further, the Lennard-Jones function is employed as a potential function for the systems of non-polar interactions considered here.

Cox et al. [9] studied the mechanics of atom and fullerene in single-walled carbon nanotubes by considering the acceptance conditions and suction energies. In the atomic case, they concluded that the carbon nanotube will accept an atom when the tube radius is greater than 3.276 Å, and the maximum suction energy occurs when the tube radius is 3.739 Å. For the interaction between a C_{60} fullerene and a carbon nanotube, they found that when the tube radius is greater than 6.338 Å, the tube will accept a C_{60} fullerene and the maximum suction energy occurs when the tube radius is 6.783 Å. Baowan et al. [15] considered the suction behaviours of TiO_2-nanoparticles into single-walled carbon nanotubes using the Lennard-Jones potential. They found that the radius difference between a TiO_2-nanoparticle and the carbon nanotube is a condition for the uptake capacities. Further, Hilder et al. [16] considered the interaction between a carbon nanotube and a cisplatin, a platinum based anticancer drug. Their results showed that the nanotube will accept the drug molecule when the tube radius is at least 4.785 Å, and the maximum suction energy occurs when the tube radius is 5.27 Å.

In this paper, we aim to study the mechanics of a two-section carbon nanotube which has different radii and infinite lenght. First, we use an elementary mechanics and applied mathematical modelling to find the interaction energies between two-section carbon nanotubes and the encapsulated particles, which are a single atom and a C_{60} fullerene. The concept of the suction energy is used to examine the encapsulation behaviours of the particles in the nanocapsule. In the following section, the

continuous model and the energy function are described. Sections 3 and 4 detail mathematical derivations for a single atom and a C_{60} encapsulated into a two-section carbon nanotube, respectively. Finally, conclusions are given in Sect. 5.

2 Continuous approach and energy function

The non-bonded interaction energy can be obtained by three formulations, that are a discrete atom-atom formulation, a continuous approach, and a hybrid discrete-continuous model. The discrete formulation is given by

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

where $\upsilon(\rho_{ij})$ is the potential function for atoms i and j such that ρ_{ij} defines a distance between each atom pair. When atoms are assumed to be uniformly distributed over the molecule, we can determine the interaction energy using a continuous approximation,

$$E = \eta_1 \eta_2 \iint \upsilon(\rho)\, \mathrm{d}\Sigma_1\, \mathrm{d}\Sigma_2,$$

where η_1 and η_2 denote the surface densities of atoms on the two molecules, and ρ represents the distance between two typical surface elements $\mathrm{d}\Sigma_1$ and $\mathrm{d}\Sigma_2$ of the interacting molecules. The third formula is a hybrid discrete-continuous model which is given by

$$E = \eta_1 \sum_i \int \upsilon(\rho_i)\, \mathrm{d}\Sigma_1,$$

where η_1 denotes the surface density of atoms on one molecule, and the integration is taking over the entire surface of the molecule. These three formulations give similar results in terms of the interaction energy between two molecules [10]. In this research, we use a continuous approach to determine the interaction energy between two molecules since it is suitable for symmetric nanostructures [10].

Here, we use the classical Lennard-Jones inverse power model to determine the potential energy. The Lennard-Jones function is given by

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

where $A = 17.4\ \mathrm{eV\,\AA^6}$ and $B = 29 \times 10^3\ \mathrm{eV\,\AA^{12}}$ denote the attractive and the repulsive constants, respectively.

The suction energy is a total work done by van der Waals interaction [9]. Here the interaction force (F) is considered along the z-axis, that is, $F_z = -\frac{\partial E}{\partial z}$ where E is the total interaction energy. Therefore, the suction energy can be obtained by integrating

$F_z(Z)$ from $-\infty$ to ∞ which is the sum of the kinetic energy when a molecule moves along the z-axis. We also note that the molecule is accepted inside the carbon nanotube when the suction energy is positive.

The values of the mean surface densities of a fullerene and a carbon nanotube (graphene sheet) are employed as $0.3789\,\text{Å}^{-2}$ and $0.3812\,\text{Å}^{-2}$, respectively, which are taken from the work by Cox et al. [9]. Further, the radius of a C_{60} fullerene is taken to be 3.55 Å.

3 Mathematical derivation for a single atom

The interaction energy between an atom and a single-walled carbon nanotube in a cylindrical coordinate system with a fixed cylindrical radius a is given by

$$E = \eta_g \int_0^{2\pi}\int_0^{\infty} \left(-\frac{A}{\rho^6} + \frac{B}{\rho^{12}}\right) a \, \mathrm{d}z \, \mathrm{d}\theta,$$

where η_g is the mean surface density of atoms on a carbon nanotube, ρ denotes the distance between a single atom and a typical atom of the surface of the tube. The schematic model is shown in Fig. 1.

In an axially symmetric cylindrical polar coordinate system (r, z), we assume that a single atom is located at $(0, Z)$, and a carbon nanotube is centered on the positive z-axis. The Cartesian coordinates of a typical atom on the tube surface is denoted by $(a_1 \cos\theta, a_1 \sin\theta, z)$; where $z \in [0, z_1]$ in the first part, and $(a_2 \cos\theta, a_2 \sin\theta, z + z_1)$ where $z \in [0, \infty)$ in the second part of the tube.

From Fig. 1, ρ_1 and ρ_2 are the distances between a single carbon atom and the typical atom of the first and the second parts of a carbon nanotube, respectively. Therefore, we may deduce

$$\rho_1^2 = (a_1 \cos\theta)^2 + (a_1 \sin\theta)^2 + (z - Z)^2 = a_1^2 + (z - Z)^2, \;\; z \in [0, z_1],$$
$$\rho_2^2 = (a_2 \cos\theta)^2 + (a_2 \sin\theta)^2 + (z + z_1 - Z)^2 = a_2^2 + (z + z_1 - Z)^2, \;\; z \in [0, \infty),$$

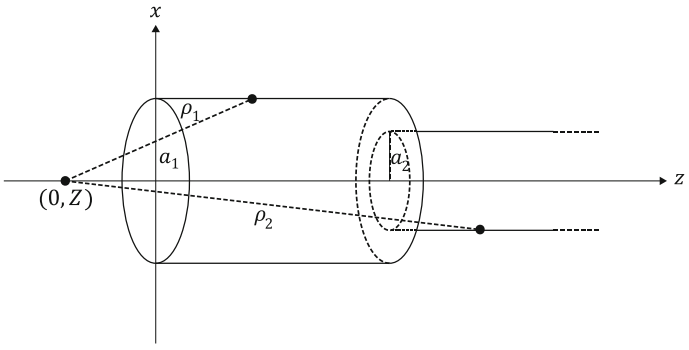

Fig. 1 Schematic model of single atom entering into carbon nanotube of two sections with different radii

where a_1 and a_2 are the radii of the first and the second parts of the tube, respectively, and z_1 is the lenght of the first part.

Thus we have

$$E = 2\pi a_1 \eta_g \int_0^{z_1} \left(-\frac{A}{\rho_1^6} + \frac{B}{\rho_1^{12}} \right) \mathrm{d}z + 2\pi a_2 \eta_g \int_0^{\infty} \left(-\frac{A}{\rho_2^6} + \frac{B}{\rho_2^{12}} \right) \mathrm{d}z.$$

Noting that ρ_1 and ρ_2 are independent of θ, then the integration with respect to θ can be straightforwardly obtained as 2π.

For convenience, we define

$$I_n = \int_0^{z_1} \frac{1}{\rho_1^{2n}} \mathrm{d}z,$$

and

$$J_n = \int_0^{\infty} \frac{1}{\rho_2^{2n}} \mathrm{d}z.$$

Firstly, we consider

$$I_n = \int_0^{z_1} \frac{1}{\left[a_1^2 + (z - Z)^2\right]^n} \mathrm{d}z.$$

On substituting $z = Z + a_1 t$, we get

$$\begin{aligned} I_n &= a_1^{(1-2n)} \int_{-t_1}^{t_2} \frac{1}{(t^2+1)^n} \mathrm{d}t \\ &= a_1^{(1-2n)} \left[\int_0^{t_2} \frac{1}{(t^2+1)^n} \mathrm{d}t + \int_0^{t_1} \frac{1}{(t^2+1)^n} \mathrm{d}t \right], \end{aligned}$$

where $t_1 = Z/a_1$ and $t_2 = (z_1 - Z)/a_1$. Then we substitute $x = t(1+t^2)^{-\frac{1}{2}}$, which gives $t = x(1-x^2)^{-\frac{1}{2}}$ and $\mathrm{d}t = (1-x^2)^{-\frac{3}{2}}\mathrm{d}x$ to obtain

$$I_n = a_1^{1-2n} \left[\int_0^{x_2} (1-x^2)^{-\frac{3}{2}+n} \mathrm{d}x + \int_0^{x_1} (1-x^2)^{-\frac{3}{2}+n} \mathrm{d}x \right],$$

where $x_1 = \frac{Z}{a_1}\left[1+\left(\frac{Z}{a_1}\right)^2\right]^{-\frac{1}{2}}$ and $x_2 = \left(\frac{z_1-Z}{a_1}\right)\left[1+\left(\frac{z_1-Z}{a_1}\right)^2\right]^{-\frac{1}{2}}$. We substitute $u = x/x_2$ and $u = x/x_1$ in the first and the second terms of the above equation, respectively, and let $t = u^2$. From a relation $B(\beta, \gamma-\beta)F(\alpha, \beta; \gamma; z) = \int_0^1 x^{\beta-1}(1-x)^{\gamma-\beta-1}(1-xz)^{-\alpha}\,\mathrm{d}x$, we have

$$I_n = a_1^{1-2n}\left[\frac{z_1-Z}{(a_1^2+(z_1-Z)^2)^{\frac{1}{2}}}F\left(\frac{3}{2}-n, \frac{1}{2}; \frac{3}{2}; \frac{(z_1-Z)^2}{a_1^2+(z_1-Z)^2}\right) + \frac{Z}{(a_1^2+Z^2)^{\frac{1}{2}}}F\left(\frac{3}{2}-n, \frac{1}{2}; \frac{3}{2}; \frac{Z^2}{a_1^2+Z^2}\right)\right], \tag{1}$$

where $F(\alpha, \beta; \gamma; z)$ is a hypergeometric function and $B(\beta, \gamma-\beta)$ denotes a Beta function.

Next we consider J_n,

$$J_n = \int_0^\infty \frac{1}{\left[a_2^2+(z+z_1-Z)^2\right]^n}\,\mathrm{d}z.$$

We make a substitution $z = (Z-z_1)+a_2t$ to obtain

$$J_n = a_2^{(1-2n)}\int_{-t_3}^{\infty}\frac{1}{(t^2+1)^n}\,\mathrm{d}t = \lim_{R\to\infty}\left\{a_2^{(1-2n)}\left[\int_0^{t_3}\frac{1}{(t^2+1)^n}\,\mathrm{d}t + \int_0^R\frac{1}{(t^2+1)^n}\,\mathrm{d}t\right]\right\},$$

where $t_3 = -(z_1-Z)/a_2$. Similar to I_n, we make a substitution $x = t(1+t^2)^{-\frac{1}{2}}$, and we may deduce

$$J_n = \lim_{R\to\infty}\left\{a_2^{1-2n}\left[\int_0^{x_3}(1-x^2)^{n-\frac{3}{2}}\,\mathrm{d}x + \int_0^{x_4}(1-x^2)^{n-\frac{3}{2}}\,\mathrm{d}x\right]\right\}, \tag{2}$$

where $x_3 = (Z-z_1)/\left[a_2^2+(Z-z_1)^2\right]^{\frac{1}{2}}$ and $x_4 = R/(1+R^2)^{\frac{1}{2}}$. For the first term of the above equation, we substitute $u = x/x_3$, and we define

$$J_{n_1} = \int_0^{x_3}(1-x^2)^{n-\frac{3}{2}}\,\mathrm{d}x = x_3\int_0^1(1-x_3^2u^2)^{n-\frac{3}{2}}\,\mathrm{d}u.$$

On letting $t = u^2$, J_{n_1} becomes

$$J_{n_1} = \frac{x_3}{2} \int_0^1 t^{-\frac{1}{2}} (1 - x_3^2 t)^{n-\frac{3}{2}} \, \mathrm{d}t.$$

Again, we use a relation $B(\beta, \gamma - \beta) F(\alpha, \beta; \gamma; z) = \int_0^1 x^{\beta-1}(1-x)^{\gamma-\beta-1}(1 - xz)^{-\alpha} \, \mathrm{d}x$ to write J_{n_1} in terms of the hypergeometric function, which can be given by

$$J_{n_1} = \frac{Z - z_1}{[a_2^2 + (Z - z_1)^2]^{\frac{1}{2}}} F\left(\frac{3}{2} - n, \frac{1}{2}; \frac{3}{2}; \frac{(Z - z_1)^2}{a_2^2 + (Z - z_1)^2}\right).$$

Similarly, using the same derivation to the second term of (2) and taking the limit of R to infinity, we may deduce

$$J_{n_2} = \int_0^{x_4} (1 - x^2)^{n-\frac{3}{2}} \, \mathrm{d}x = \frac{R}{(1 + R^2)^{\frac{1}{2}}} F\left(\frac{3}{2} - n, \frac{1}{2}; \frac{3}{2}; \frac{R^2}{1 + R^2}\right).$$

Finally, J_n is given by

$$J_n = a_2^{1-2n} \left[\frac{Z - z_1}{(a_2^2 + (Z - z_1)^2)^{\frac{1}{2}}} F\left(\frac{3}{2} - n, \frac{1}{2}; \frac{3}{2}; \frac{(Z - z_1)^2}{a_2^2 + (Z - z_1)^2}\right) + F\left(\frac{3}{2} - n, \frac{1}{2}; \frac{3}{2}; 1\right) \right]. \tag{3}$$

Therefore, the interaction energy between a single atom and the entire carbon nanotube is

$$E = 2\pi a_1 \eta_g (-AI_3 + BI_6) + 2\pi a_2 \eta_g (-AJ_3 + BJ_6),$$

where I_n and J_n are given by (1) and (3), respectively.

We aim to determine the condition for a two-section carbon nanotube which allows an atom to enter into the first part. From the suction energy of an atom depicted in Fig. 2, the suction energy is positive when the radius of the nanotube is greater than or equal to 3.210 Å. This value is in a good agreement made by Cox et al. [9]. The result shows that a single atom will be encapsulated into the first part of the nanocapsule when $a_1 \geq 3.210$ Å. The interaction energy between an atom and the nanocapsule when $a_1 = a_2 = 3.210$ Å is shown in Fig. 3a.

Now we consider the condition of a two-section carbon nanotube which allows an atom to be encapsulated into the second part. Let $S_1(a)$ be the suction energy of a carbon nanotube of radius a. Firstly, we consider $3.210\,\text{Å} \leq a_1 < 3.739\,\text{Å}$. From Fig. 2, the atom will be accepted by the second part when $a_1 \leq a_2 \leq a_0$ where the suction energy for the tube of radius a_0 is approximately equal to the suction energy for the tube of radius a_1, $S_1(a_0) \approx S_1(a_1)$. For example, let $a_1 = 3.278$ Å, the atom can pass through the second part when $3.278\,\text{Å} \leq a_2 \leq 5.534$ Å, see Fig. 2. The energy profiles of this case are illustrated in Fig. 3b. For any given the value of a_1, we can determine the value of a_2 for which the atom can be encapsulated into a

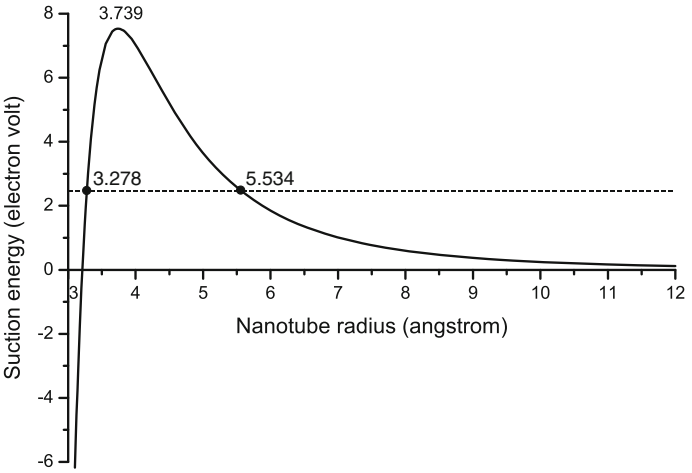

Fig. 2 Suction energy for single atom entering into carbon nanotube

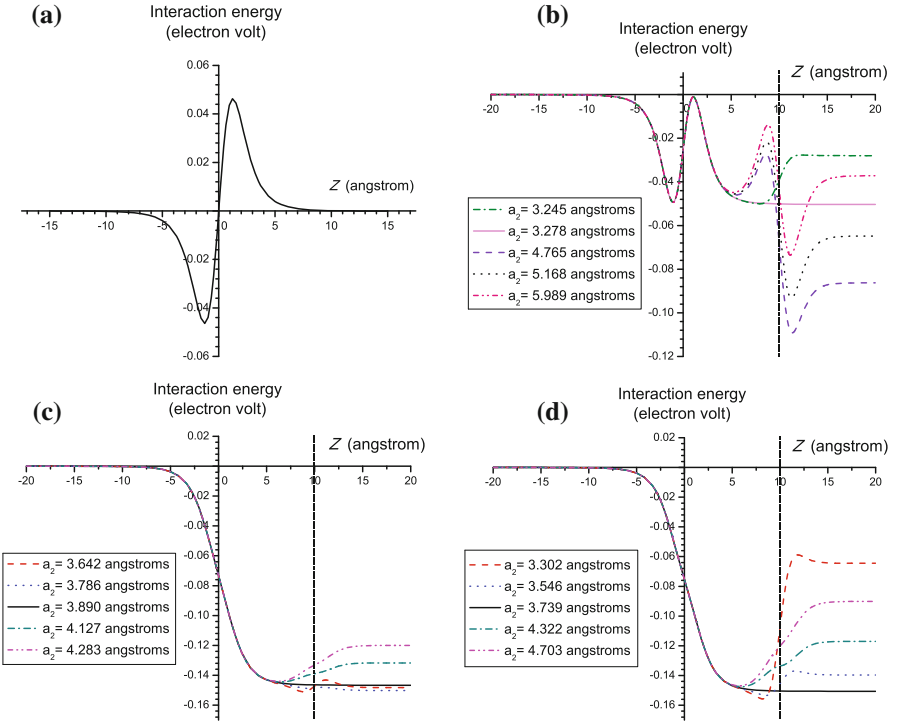

Fig. 3 The interaction energies between single atom and two-section carbon nanotube when **a** $a_1 = a_2 = 3.210\,\text{Å}$, **b** $a_1 = 3.278\,\text{Å}$, **c** $a_1 = 3.890\,\text{Å}$, and **d** $a_1 = 3.739\,\text{Å}$

two-section carbon nanotube. For example, if $a_1 = 3.345\,\text{Å}$, then the atom can go inside the second part when $3.345\,\text{Å} \leq a_2 \leq 4.771\,\text{Å}$, and if $a_1 = 3.545\,\text{Å}$, we need $3.545\,\text{Å} \leq a_2 \leq 4.016\,\text{Å}$.

Secondly, we consider the case when $a_1 > 3.739$ Å which is greater than the radius that gives the maximum suction energy. From Fig. 2, the atom will pass through the second part when $a_0^{'} \leq a_2 \leq a_1$ where $S_1(a_0^{'}) \approx S_1(a_1)$. For example, if $a_1 = 3.890$ Å, then the atom can enter into the second part when $3.617\,\text{Å} \leq a_2 \leq 3.890$ Å as shown in Fig. 3c. Moreover, if $a_1 = 4.592$ Å, a single atom can go inside the second part when $3.373\,\text{Å} \leq a_2 \leq 4.592\,\text{Å}$, and if $a_1 = 5.568$ Å, we require $3.276\,\text{Å} \leq a_2 \leq 5.568$ Å.

Finally, when $a_1 = 3.739$ Å which is the radius of the carbon nanotube that gives the maximum suction energy, we find that the atom cannot pass through the second part for any value of a_2 except for $a_2 = 3.739$ Å. The energy profiles of this case are shown in Fig. 3d. We comment that the lenght of the first part z_1 has only a minor effect to the encapsulation behaviour, it changes only the amplitude of energy level.

4 Mathematical derivation for a C_{60} fullerene

Now we consider the system of a spherical molecule, a C_{60} fullerene, and a carbon nanotube with two sections of different radii which is shown in Fig. 4. The total interaction energy of this system can be given by

$$E = \eta_g \eta_f \int_{\Sigma_2} \int_{\Sigma_1} \left(-\frac{A}{p^6} + \frac{B}{p^{12}} \right) \mathrm{d}\Sigma_1 \, \mathrm{d}\Sigma_2,$$

where η_f is the mean surface density for a fullerene, $\mathrm{d}\Sigma_1$ and $\mathrm{d}\Sigma_2$ are typical surface elements of the spherical molecule of radius b and a carbon nanotube, respectively. Note that $p^2 = b^2 + \tilde{\rho}^2 - 2b\tilde{\rho}\cos\phi$, where $\tilde{\rho}$ denotes the distance between a centre of the fullerene and a typical atom of the tube (see Fig. 11 in Cox et al. [9]). Here, we determine the interaction energy from the first part (E_1) and the second part (E_2) of the nanocapsule separately, and the total energy of the system can be obtained as $E = E_1 + E_2$.

Following the work by Cox et al. [9], the interaction energy between a point and a sphere of radius b is given by

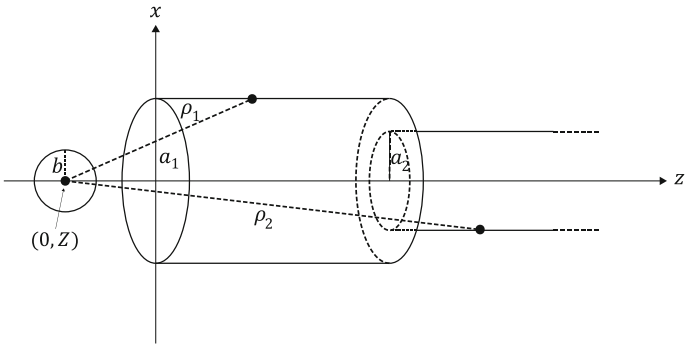

Fig. 4 Schematic model of sphere entering into carbon nanotube of two sections with different radii

$$P(\tilde{\rho}) = -4n_f\pi b^2 A\left(\frac{1}{(\tilde{\rho}^2-b^2)^3}+\frac{2b^2}{(\tilde{\rho}^2-b^2)^4}\right) + \frac{4}{5}n_f\pi b^2 B\left(\frac{5}{(\tilde{\rho}^2-b^2)^6}+\frac{80b^2}{(\tilde{\rho}^2-b^2)^7}+\frac{336b^4}{(\tilde{\rho}^2-b^2)^8}+\frac{512b^6}{(\tilde{\rho}^2-b^2)^9}+\frac{256b^8}{(\tilde{\rho}^2-b^2)^{10}}\right).$$

Now we consider the first part of the tube, where $\tilde{\rho}^2 = \rho_1^2 = a_1^2 + (z-Z)^2$. Assuming $\lambda_1 = [a_1^2 - b^2 + (z-Z)^2]/b^2$ so that

$$P(\rho_1) = -\frac{4n_f\pi}{\lambda_1^3 b^4}\left[A\left(1+\frac{2}{\lambda_1}\right) - \frac{B}{5\lambda_1^3 b^6}\left(5+\frac{80}{\lambda_1}+\frac{336}{\lambda_1^2}+\frac{512}{\lambda_1^3}+\frac{256}{\lambda_1^4}\right)\right].$$

The interaction energy for the first part of a carbon nanotube E_1 is given by

$$E_1 = a_1 n_g \int_{-\pi}^{\pi}\int_0^{z_1} P(\rho_1)\,\mathrm{d}z\,\mathrm{d}\theta = 2\pi a_1 n_g \int_0^{z_1} P(\rho_1)\,\mathrm{d}z.$$

Now we consider $\int_0^{z_1}\frac{1}{\lambda_1^n}\,\mathrm{d}z$ and by letting $z - Z = \sqrt{a_1^2-b^2}\tan\alpha$, we have

$$\int_0^{z_1}\frac{1}{\lambda_1^n}\,\mathrm{d}z = \int_{\alpha_0}^{\alpha_1}\frac{b^{2n}}{(a_1^2-b^2)^n\sec^{2n}\alpha}\sqrt{a_1^2-b^2}\sec^2\alpha\,\mathrm{d}\alpha = b^{2n}(a_1^2-b^2)^{\frac{1}{2}-n}\int_{\alpha_0}^{\alpha_1}\cos^{2n-2}\alpha\,\mathrm{d}\alpha,$$

where $\alpha_0 = \arctan\left(\frac{-Z}{\sqrt{a_1^2-b^2}}\right)$ and $\alpha_1 = \arctan\left(\frac{z_1-Z}{\sqrt{a_1^2-b^2}}\right)$. If we write $K_n = b^{2n}(a_1^2-b^2)^{\frac{1}{2}-n}\int_{\alpha_0}^{\alpha_1}\cos^{2n-2}\alpha\,\mathrm{d}\alpha$, then E_1 becomes

$$E_1 = -\frac{8\pi^2 a_1 n_g n_f}{b^4}\left[A\,(K_3+2K_4) - \frac{B}{5b^6}\,(5K_6+80K_7+336K_8 + 512K_9+256K_{10})\right].$$

Next we consider the second part of a carbon nanotube, where $\tilde{\rho}^2 = \rho_2^2 = a_2^2 + (z+z_1-Z)^2$, and we assume that $\lambda_2 = [a_2^2 - b^2 + (z+z_1-Z)^2]/b^2$. Similar to the first part, we get

$$P(\rho_2) = -\frac{4n_f\pi}{\lambda_2^3 b^4}\left[A\left(1+\frac{2}{\lambda_2}\right) - \frac{B}{5\lambda_2^3 b^6}\left(5+\frac{80}{\lambda_2}+\frac{336}{\lambda_2^2}+\frac{512}{\lambda_2^3}+\frac{256}{\lambda_2^4}\right)\right].$$

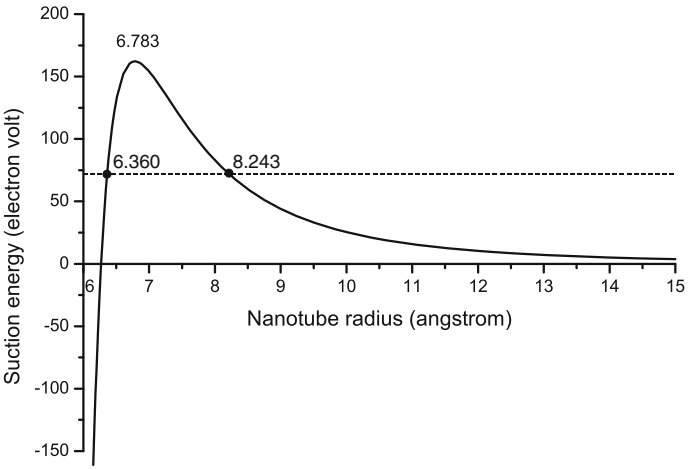

Fig. 5 Suction energy for C_{60} fullerene entering into carbon nanotube

The interaction energy for the second part of the tube E_2 is given by

$$E_2 = a_2 n_g \int_{-\pi}^{\pi} \int_{0}^{\infty} P(\rho_2)\, \mathrm{d}z\, \mathrm{d}\theta = 2\pi a_2 n_g \int_{0}^{\infty} P(\rho_2)\, \mathrm{d}z.$$

Again, by letting $z + z_1 - Z = \sqrt{a_2^2 - b^2}\tan\beta$, we have

$$\int_0^{\infty} \frac{1}{\lambda_2^n}\, \mathrm{d}z = \int_{\beta_0}^{\frac{\pi}{2}} \frac{b^{2n}}{(a_2^2 - b^2)^n \sec^{2n}\beta} \sqrt{a_2^2 - b^2}\sec^2\beta\, \mathrm{d}\beta$$

$$= b^{2n}(a_2^2 - b^2)^{\frac{1}{2}-n} \int_{\beta_0}^{\frac{\pi}{2}} \cos^{2n-2}\beta\, \mathrm{d}\beta,$$

where $\beta_0 = \arctan\left(\frac{z_1 - Z}{\sqrt{a_2^2 - b^2}}\right)$. We define $L_n = b^{2n}(a_2^2 - b^2)^{\frac{1}{2}-n} \int_{\beta_0}^{\frac{\pi}{2}} \cos^{2n-2}\beta\, \mathrm{d}\beta$, so that the interaction energy for the second part of the tube can be written as

$$E_2 = -\frac{8\pi^2 a_2 n_g n_f}{b^4}\left[A\,(L_3 + 2L_4) - \frac{B}{5b^6}\,(5L_6 + 80L_7 + 336L_8 + 512L_9 + 256L_{10})\right].$$

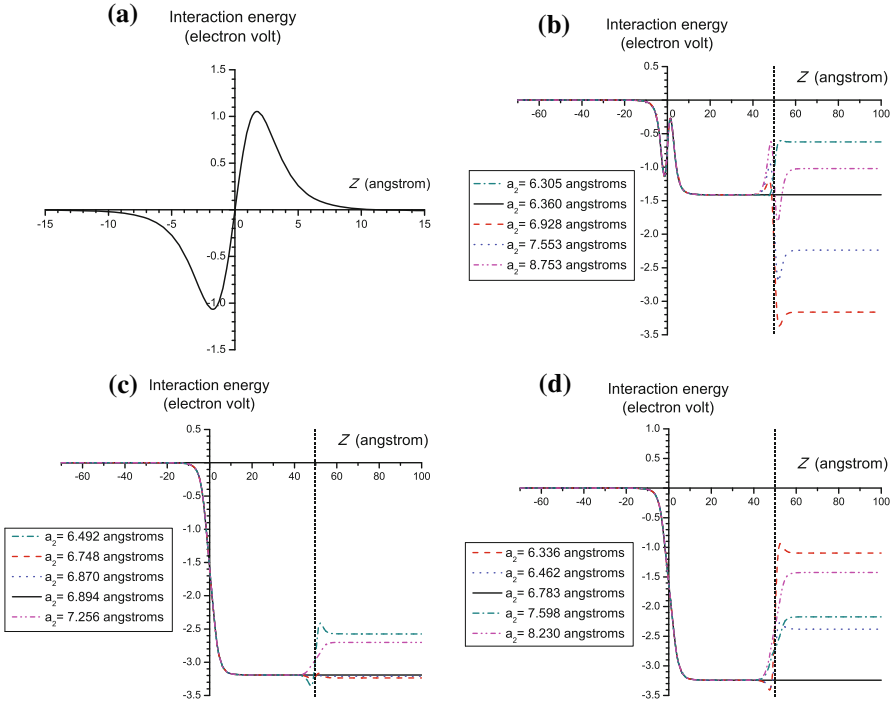

Fig. 6 The interaction energies between C_{60} fullerene and two-section carbon nanotube when **a** $a_1 = a_2 = 6.271$ Å, **b** $a_1 = 6.360$ Å, **c** $a_1 = 6.894$ Å, and **d** $a_1 = 6.783$ Å

Therefore the total interaction energy between a sphere and the entire carbon nanotube is obtained by $E = E_1 + E_2$, where

$$\int \cos^{2p}\varphi \, \mathrm{d}\varphi = \frac{1}{2^{2p}}\left[\binom{2p}{p}\varphi + \sum_{l=0}^{p-1}\binom{2p}{l}\frac{\sin(2(p-l)\varphi)}{p-l}\right].$$

First, we aim to find the condition of a two-section carbon nanotube which allows a spherical C_{60} fullerene to be encapsulated into the first part. From Fig. 5, the suction energy of a C_{60} fullerene is positive when the radius of the nanotube is not less than 6.271 Å, which is in a comparison made by Cox et al. [9]. Therefore, we can conclude that the fullerene can be encapsulated into the first part of the nanocapsule when $a_1 \geq 6.271$ Å. The interaction energy between the fullerene and the nanocapsule for $a_1 = a_2 = 6.271$ Å is illustrated in Fig. 6a. We note that the radius of a C_{60} fullerene is taken to be 3.55 Å.

Now we consider the condition for a two-section carbon nanotube to allow the fullerene to pass through the second part. Let $S_2(a)$ be the suction energy of a carbon nanotube of radius a. From Fig. 5, if $6.271\,\text{Å} \leq a_1 < 6.783\,\text{Å}$, then the sphere can enter the second part when $a_1 \leq a_2 \leq a_0$ where $S_2(a_0) \approx S_2(a_1)$. For example, if $a_1 = 6.360$ Å, the fullerene can pass through the second part when $6.360\,\text{Å} \leq a_2 \leq 8.243\,\text{Å}$, see the horizontal line in Fig. 5. The energy behaviours are shown

Table 1 Some values of a_1 and a_2 considered here for the nanoparticles encapsulated into two-section carbon nanotube

Particle	Radius of the first part, a_1 (Å)	Radius of the second part, a_2 (Å)
Atom	I. $3.210\,\text{Å} \le a_1 < 3.739\,\text{Å}$	$a_1 \le a_2 \le a_0$, $S_1(a_0) \approx S_1(a_1)$
	$a_1 = 3.278\,\text{Å}$	$3.278\,\text{Å} \le a_2 \le 5.534\,\text{Å}$
	$a_1 = 3.345\,\text{Å}$	$3.345\,\text{Å} \le a_2 \le 4.771\,\text{Å}$
	$a_1 = 3.545\,\text{Å}$	$3.545\,\text{Å} \le a_2 \le 4.016\,\text{Å}$.
	II. $a_1 > 3.739\,\text{Å}$	$a_0^{'} \le a_2 \le a_1$, $S_1(a_0^{'}) \approx S_1(a_1)$
	$a_1 = 3.890\,\text{Å}$	$3.617\,\text{Å} \le a_2 \le 3.890\,\text{Å}$
	$a_1 = 4.592\,\text{Å}$	$3.373\,\text{Å} \le a_2 \le 4.592\,\text{Å}$
	$a_1 = 5.568\,\text{Å}$	$3.276\,\text{Å} \le a_2 \le 5.568\,\text{Å}$
	III. $a_1 = 3.739\,\text{Å}$	$a_2 = 3.739\,\text{Å}$
C_{60} fullerene	I. $6.271\,\text{Å} \le a_1 < 6.783\,\text{Å}$	$a_1 \le a_2 \le a_0$, $S_2(a_0) \approx S_2(a_1)$
	$a_1 = 6.360\,\text{Å}$	$6.360\,\text{Å} \le a_2 \le 8.243\,\text{Å}$
	$a_1 = 6.403\,\text{Å}$	$6.403\,\text{Å} \le a_2 \le 7.807\,\text{Å}$
	$a_1 = 6.652\,\text{Å}$	$6.652\,\text{Å} \le a_2 \le 6.949\,\text{Å}$.
	II. $a_1 > 6.783\,\text{Å}$	$a_0^{'} \le a_2 \le a_1$, $S_2(a_0^{'}) \approx S_2(a_1)$
	$a_1 = 6.894\,\text{Å}$	$6.689\,\text{Å} \le a_2 \le 6.894\,\text{Å}$
	$a_1 = 7.464\,\text{Å}$	$6.461\,\text{Å} \le a_2 \le 7.464\,\text{Å}$
	$a_1 = 8.589\,\text{Å}$	$6.339\,\text{Å} \le a_2 \le 8.589\,\text{Å}$
	III. $a_1 = 6.783\,\text{Å}$	$a_2 = 6.783\,\text{Å}$

in Fig. 6b. Moreover, if $a_1 = 6.403\,\text{Å}$, then the fullerene can enter into the second part when $6.403\,\text{Å} \le a_2 \le 7.807\,\text{Å}$, and if $a_1 = 6.652\,\text{Å}$, then we require $6.652\,\text{Å} \le a_2 \le 6.949\,\text{Å}$.

Once $a_1 > 6.783\,\text{Å}$ which is greater than the radius that gives the maximum suction energy, the fullerene is accepted into the second part when $a_0^{'} \le a_2 \le a_1$ where $S_2(a_0^{'}) \approx S_2(a_1)$. For example, if $a_1 = 6.894\,\text{Å}$, then the fullerene can pass through the second part when $6.689\,\text{Å} \le a_2 \le 6.894\,\text{Å}$ as illustrated in Fig. 6c. Moreover, if $a_1 = 7.464\,\text{Å}$, the fullerene can enter into the second part when $6.461\,\text{Å} \le a_2 \le 7.464\,\text{Å}$, and if $a_1 = 8.589\,\text{Å}$, then we need $6.339\,\text{Å} \le a_2 \le 8.589\,\text{Å}$.

However, if $a_1 = 6.783\,\text{Å}$ which gives the maximum suction energy, the fullerene can enter into the second part only when $a_2 = 6.783\,\text{Å}$. The interaction behaviour of this case is shown in Fig. 6d. We also comment here that the lenght z_1 effects only to the energy level of the system, the encapsulation behaviour remains the same. Table 1 shows some examples of the radii of the first part (a_1) and the radii of the second part (a_2) where the particles can be encapsulated into the two-section carbon nanotubes.

5 Summary

In this research, we design a nanocapsule by combining two different radii of carbon nanotubes and then consider the mechanics of the encapsulated particles. First, we

determine the explicit formulae for the interaction energies between the two-section carbon nanotubes and the encapsulated particles which are a single atom and a C_{60} fullerene by using a continuous approach and the well-known Lennard-Jones potential function. The closed forms of the interaction energies for the atom and the C_{60} fullerene are obtained.

Further, we find the suction energies of the encapsulated particles to determine the encapsulation behaviours. In terms of a single atom, our results show that the atom can enter into the first part when the suction energy is positive, that is, when $a_1 \geq 3.210$ Å. The condition for the atom to enter into the second part is considered in three cases. First, when $3.210\,\text{Å} \leq a_1 < 3.739$ Å, the atom can enter into the second part when $a_1 \leq a_2 \leq a_0$ where the suction energy for the tube radius a_0 is approximately equal to the suction energy for the tube radius a_1, $S_1(a_0) \approx S_1(a_1)$ where $S_1(a)$ denotes the suction energy between an atom and a carbon nanotube of radius a. The second case is that $a_1 > 3.739$ Å, the atom can be encapsulated into the tube when $a_0^{'} \leq a_2 \leq a_1$ where $S_1(a_0^{'}) \approx S_1(a_1)$. Finally, when $a_1 = 3.739$ Å which is the radius of the carbon nanotube that gives the maximum suction energy, there is only one value of a_2 that allows the atom to pass through the second part which is $a_2 = a_1$.

For a C_{60} fullerene, it can enter into the first part when $a_1 \geq 6.271$ Å. The condition for the fullerene entering into the second part is also considered in three cases. When $6.271\,\text{Å} \leq a_1 < 6.783$ Å, the fullerene can be encapsulated into the second part when $a_1 \leq a_2 \leq a_0$ where $S_2(a_0) \approx S_2(a_1)$ and $S_2(a)$ is the suction energy between the fullerene and a carbon nanotube of radius a. If $a_1 > 6.783$ Å, the fullerene can go inside the second part when $a_0^{'} \leq a_2 \leq a_1$ where $S_2(a_0^{'}) \approx S_2(a_1)$. For $a_1 = 6.783$ Å which gives the maximum suction energy of fullerene, the fullerene can go inside the second part when $a_2 = a_1$. The values of the tube radii a_1 and a_2 studied in this paper for which an atom and a C_{60} fullerene can be encapsulated inside are completely given in Table 1.

From our results, we obtain a basic theoretical knowledge but useful. The understanding obtained from our model could contribute considerable insight into the basic concepts of the encapsulation behaviour. Our work thus could be viewed as the first step toward designing new nanodevices where the nanocapsule may be used as a drug container which can be utilised in pharmaceuticals and cosmetics.

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