# Offset $C_{60}$ fullerene encapsulated inside Goldberg type I fullerenes

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*Abstract*—**The use of nanotechnology in pharmaceutical is an important topic in order to transport drugs to the targeted cells. However, there are a few studies for the mechanics of encapsulated tiny drug molecules into a nano-size capsule. In this paper, we determine the encapsulation of an assumed spherical drug molecule inside a spherical capsule using mathematical model, where both molecules are assumed to be carbon fullerenes with different sizes. Moreover, Lennard-Jones potential function together with the continuous approximation is employed to determine the energy of the system which gives rise to the equilibrium position of the drug molecule in the capsule. Further, an analytical solution is obtained as a function of the molecule radii. This research might be considered as a first step to investigate the encapsulation of drug molecule in a nanocapsule for the medical research.**

***Keywords*—** Drug delivery, Goldberg fullerenes, Lennard-Jones function, Nanotechnology, Mathematical model

## I. Introduction

Carbon nanostructures including fullerenes, carbon nanotubes, and carbon onions have received much attention because of their unique properties, such as their high flexibility, their high thermal conductivity and they are presently the strongest material known [1]. Their special properties have not only led to proposals for many potential nano-devices [2] – [4] but also to the desire to create further new carbon nanostructures and the spherical carbon onions are examples of such structures. The major issue in this regard is the determination of the interspacing layer of $C_{60}$ fullerene encapsulated inside Goldberg type I fullerenes, namely $C_{240}$, $C_{540}$, $C_{960}$ and $C_{1500}$, as a potential application for drug delivery system. In other words, the $C_{60}$ fullerene is assumed as a drug molecule and the Goldberg type I fullerenes are assumed as a nanocapsule.

In this paper rather than undertake such large scale calculations, we employ elementary mechanical principles and classical mathematical modelling to investigate the interaction energies between adjacent shells of fullerenes, which leads to the determination of the equilibrium spacing of such structures. The Lennard–Jones potential and the continuous approach are employed throughout this paper, where the continuous model assumes that the atoms at discrete locations can be approximated by an averaged surface density of atoms which is smeared across the entire surface.

Fullerenes are an extensively studied nanomaterial because of their unique free radical chemistry and antioxidant properties [5]. Moreover, the structure of a $C_{60}$ fullerene is simple, being a spherical surface of radius 3.55 Å and comprising 60 evenly spaced carbon atoms. Further, the ability of a fullerene to induce toxicity may require ultraviolet light and a water environment [6], and they might become dangerous to the environment and biological systems.

Goldberg type I fullerenes of $I_h$ symmetry are suggested by Kroto and McKay [7] as a plausible model for carbon onions. The first five shells of the carbon onion of this type comprise $C_{60}$, $C_{240}$, $C_{540}$, $C_{960}$ and $C_{1500}$, and thus the intershell spacing is approximately 0.34 nm, which is very close to the interlayer spacing in graphite and to the spacing obtained experimentally and theoretically (see for example Kroto and McKay [7]; Banhart et al. [8] and Lu and Yang [9]). Further, the number of carbon atoms on each shell of Goldberg type I is $N = 60n^2$ where $n$ is an integer.

In the following section, we introduce the Lennard–Jones potential for non-bonded atoms. Using the continuous approximation, the analytical expression of the potential energy is determined in Section III. Further, numberical calculations for the preference position of the $C_{60}$ molecule inside four sizes of nanocapsules are presented in Section IV, and finally, summary of the paper is given in Section V.

## II. Lennard-Jones Function

We employ the Lennard-Jones potential function and the continuous approximation to calculate the molecular interatomic energy between a $C_{60}$ fullerene and a single-shell of Goldberg type I fullerene. The 6-12 Lennard-Jones function is given by

$$\Phi = -\frac{A}{\rho^6} + \frac{B}{\rho^{12}}, \tag{1}$$

where $\rho$ denotes the distance between two typical points, and $A$ and $B$ are attractive and repulsive Lennard-Jones constants, respectively. Equation (1) can also be written as

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

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where $\varepsilon$ denotes a well depth and $\sigma$ is the van der Waals diameter, and from which we may deduce that $A = 4\varepsilon\sigma^6$ and $B = 4\varepsilon\sigma^{12}$.

To determine the non-bonded interaction energy between two molecular structures, using the discrete approach we sum the energy for each atom pair, namely

$$E = \sum_i \sum_j \left( -\frac{A}{\rho_{ij}^{\,6}} + \frac{B}{\rho_{ij}^{\,12}} \right),$$

where $\rho_{ij}$ is the distance for atoms $i$ to $j$. Using the continuous approach, where the atoms at discrete locations on the molecule are averaged over a surface, the molecular interatomic energy is obtained by calculating integrals over the surfaces of each molecule, given by

$$E = \eta_1 \eta_2 \int_{S_1} \int_{S_2} \left( -\frac{A}{\rho^6} + \frac{B}{\rho^{12}} \right) dS_1 dS_2 ,$$

where $\eta_1$ and $\eta_2$ represent the mean surface density of atoms on each molecule, and $dS_1$ and $dS_2$ are two surface elements.

The Lennard-Jones parameters used for nonbonding interaction between two fullerenes are taken from the work of Girifalco et al. [10], which are $A$ = 17.4 eV Å$^6$ and $B$ = 29×10$^3$ eV Å$^{12}$.

We assume that fullerene molecules can be modelled as a sphere, and the mean surface density for the spherical molecule can be evaluated by $\eta = N/(4\pi r^2)$ where $N$ is a number of atoms on the molecule which is given by $N = 60n^2$ where $n$ is an integer, and $r$ is the radius of the molecule. The numerical values of the constants used in our model are as given in Table I.

TABLE I
CONSTANTS USED IN THIS MODEL

| Quantity | Values |
|---|---|
| Radius of $C_{60}$ | 3.5481 Å |
| Radius of $C_{240}$ | 7.0728 Å |
| Radius of $C_{540}$ | 10.5528 Å |
| Radius of $C_{960}$ | 14.0342 Å |
| Radius of $C_{1500}$ | 17.5225 Å |
| Mean surface density of $C_{60}$ | 0.3793 Å$^{-2}$ |
| Mean surface density of $C_{240}$ | 0.3818 Å$^{-2}$ |
| Mean surface density of $C_{540}$ | 0.3859 Å$^{-2}$ |
| Mean surface density of $C_{960}$ | 0.3879 Å$^{-2}$ |
| Mean surface density of $C_{1500}$ | 0.3888 Å$^{-2}$ |

Radii of fullerene taken from the work of Dunlap and Zope [11].

## III. MATHEMATICAL DETERMINATION

We aim to determine the equilibrium position of the $C_{60}$ spherical molecule located in the Goldberg type I fullerenes, as shown in Fig. 1, where both molecules are assumed to be sphere. We note that further in the text, the $C_{60}$ molecule might be referred as a drug and the Goldberg type I fullerene will be referred as a capsule. We begin by considering the molecular interaction energy for a point on the capsule and a spherical $C_{60}$ molecule of radius $a$, which is given by

$$E_s = \frac{\pi a \eta_1}{\rho} \left\{ \frac{A}{2} \left[ \frac{1}{(a+\rho)^4} - \frac{1}{(a-\rho)^4} \right] - \frac{B}{5} \left[ \frac{1}{(a+\rho)^{10}} - \frac{1}{(a-\rho)^{10}} \right] \right\}, \quad (2)$$

and the derivation of the above equation can be found in Cox et al. [12]. We note that $\eta_1$ represents the mean atomic surface density of the $C_{60}$ molecule. By placing fractions over common denominators, expanding and reducing to fractions in terms of powers of ($\rho^2$ - $a^2$), it can be shown that

$$\frac{A}{2\rho} \left[ \frac{1}{(a+\rho)^4} - \frac{1}{(a-\rho)^4} \right] = -4aA \left[ \frac{1}{\left(\rho^2 - a^2\right)^3} + \frac{2a^2}{\left(\rho^2 - a^2\right)^4} \right], \quad (3)$$

$$\frac{B}{5\rho} \left[ \frac{1}{(a+\rho)^{10}} - \frac{1}{(a-\rho)^{10}} \right] = -\frac{4aB}{5} \left[ \frac{5}{\left(\rho^2 - a^2\right)^6} + \frac{80a^2}{\left(\rho^2 - a^2\right)^7} + \frac{336a^4}{\left(\rho^2 - a^2\right)^8} + \frac{512a^6}{\left(\rho^2 - a^2\right)^9} + \frac{256a^8}{\left(\rho^2 - a^2\right)^{10}} \right]. \quad (4)$$

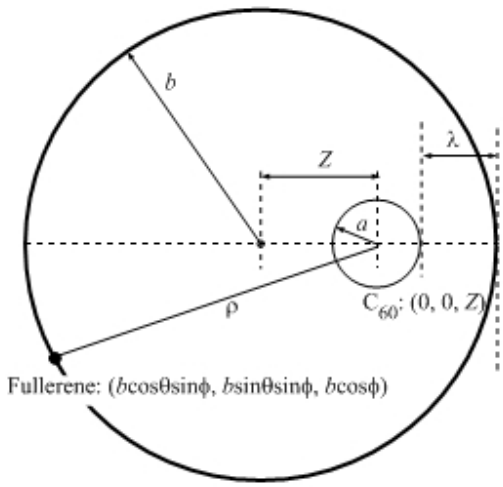


Fig. 1 Model formation for a $C_{60}$ molecule inside a capsule of Goldberg type I fullerene

The total interaction energy between the carbon capsule and the $C_{60}$ molecule is obtained by performing surface integrals for (2) over the other spherical molecule, capsule. Further, we define

$$J_n = \int_S \frac{1}{\left(\rho^2 - a^2\right)^n} dS , \quad (5)$$

where $n$ is a positive integer corresponding to the power of the polynomials appearing in (3) and (4), and $S$ is the surface element of a capsule. The total interaction energy between the

$C_{60}$ molecule and a spherical capsule is given by

$$E = \pi a \eta_1 \left[ -4aA\left(J_3 + 2a^2 J_4\right) + \frac{4aB}{5}\left(5J_6 + 80a^2 J_7 + 336a^4 J_8 + 512a^6 J_9 + 256a^8 J_{10}\right)\right], \quad (6)$$

Next, we consider the interaction energy between two spheres. The distance from the centre of the $C_{60}$ molecule to a surface of the capsule is denoted by $\rho$ and is given by

$$\rho^2 = \left(b\cos\theta\sin\phi\right)^2 + \left(b\sin\theta\sin\phi\right)^2 + \left(b\cos\phi - Z\right)^2 = b^2 - 2bZ\cos\phi + Z^2,$$

where $Z$ is the distance between their centres and $b$ is a radius of a capsule. In Cartesian coordinate system, we may deduce

$$J_n = \eta_2 \int_0^{2\pi}\int_0^{\pi} \frac{b^2 \sin\phi}{\left[b^2 - 2bZ\cos\phi + Z^2 - a^2\right]^n} d\phi d\theta,$$

where $\eta_2$ denotes the mean atomic surface density for the capsule. We make a substitution for $u = \cos\phi$, and we may deduce

$$J_n = 2\pi b^2 \eta_2 \int_{-1}^{1} \frac{1}{\left(b^2 - a^2 + Z^2 - 2bZu\right)^n} du.$$

Straightforwardly, the above integral can be determined which is given by

$$J_n = \frac{\eta_2 \pi b}{(n-1)Z}\left(\frac{1}{\left[(b-Z)^2 - a^2\right]^{n-1}} - \frac{1}{\left[(b+Z)^2 - a^2\right]^{n-1}}\right), \quad (7)$$

Finally, the interaction energy between a $C_{60}$ molecule located inside a spherical capsule can be obtained by substituting $J_n$, which is given by (7), into (6).

## IV. Result

By using the algebraic computer package MAPLE, we show graphically the relation between the potential energy and the distance $Z$ between the centre of the $C_{60}$ molecule and the centre of a capsule, as shown in Fig.2. The preference position of the $C_{60}$ inside the capsule is at the minimum energy location, and since a symmetric property of a sphere, positive and negative values of $Z$ indicate the same position. In the case of $C_{60}@C_{240}$, we observe that the $C_{60}$ molecule is most likely to be located at the centre of the capsule which is $Z = 0$ and it corresponds to $\lambda$ = 3.524 Å which is an interspacing distance between two adjacent carbon spherical layers [7].

Further, the $C_{60}$ molecule moves away from the centre of the capsule as the radius of the capsule increases. The numerical values of $Z$ and $\lambda$ for the capsule of Goldberg type I fullerenes are given in Table II. We observe that the distance $\lambda$ of all cases slightly decrease as the radius of the capsule increases. This is due to two reasons (i) the increasing of a number of carbon atoms for a larger capsule which in turn increasing an attractive force between the two spheres, and (ii) a curvature of the capsule reduced for a larger one. Nevertheless, the spacing $\lambda$ is approximately equilibrium spacing between two layers of carbon onions [7].

In comparison for the four capsules, $C_{240}$, $C_{540}$, $C_{960}$ and $C_{1500}$, the $C_{60}$ molecule is most likely to be encapsulated inside the $C_{240}$ molecule because of the lowest energy level as shown in Fig. 2. However, there is only one $C_{60}$ molecule which can be located inside the $C_{240}$ molecule. For the other three cases, we may encapsulate more than one molecule of $C_{60}$ into such capsules.

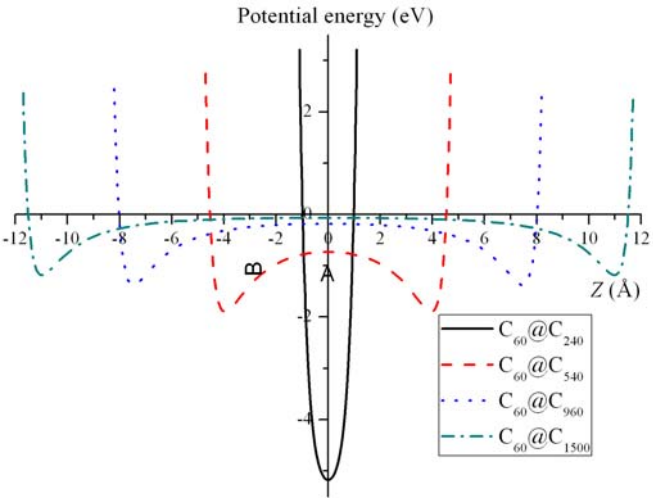


Fig. 2 Interaction energy between $C_{60}$ molecule and the Goldberg type I fullerene, $C_{240}$, $C_{540}$, $C_{960}$ and $C_{1500}$.

TABLE II
EQUILIBRIUM DISTANCES Z AND λ AT THE MINIMUM INTERACTION ENERGY

| Capsule | Z (Å) | λ (Å) |
|---|---|---|
| $C_{240}$ | 0 | 3.5247 |
| $C_{540}$ | 3.9504 | 3.0543 |
| $C_{960}$ | 7.4798 | 3.0063 |
| $C_{1500}$ | 10.9840 | 2.9904 |

## V. Summary

In this paper, we determine the position of the $C_{60}$ molecule inside the Goldberg type I fullerenes, namely $C_{240}$, $C_{540}$, $C_{960}$ and $C_{1500}$. The Lennard-Jones potential function together with the continuous approximation, where we assume that the carbon atoms are uniformly distributed over the surface of the molecule, is employed to determine the preferred position for the molecule of $C_{60}$. The analysis gives rise to the possible location for each capsule size. We find that in the case of $C_{60}@C_{240}$, the $C_{60}$ is most likely to be located at the centre of the $C_{240}$ molecule and gives the lowest energy. Further, the $C_{60}$ molecule moves away from the centre where the radius of the capsule increases. The distances between the wall of $C_{60}$ molecule to the closest wall of the capsules slightly decrease when the capsule radii increase, due to the decreasing of the curvature and the increasing of the number of carbon atoms for a larger capsule. However, these values are comparable where they are approximately 3 Å.

In comparison to other methods used to study nanoscience and nanotechnology, such as first principle calculations, molecular dynamics or Monte Carlo simulations, our applied mathematical modeling approach is not been widely used in this field. The understanding obtained from our model could contribute to considerable insight into the basic concepts of the problem. Our work thus could be viewed as a first experimental step toward designing new nanodevices, such as a nanocapsule to control drug delivery, improve circulatory persistence, and allow the targeting of drugs to specific cells.

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