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ORIGINAL PAPER

# Mathematical modelling for equilibrium configurations of concentric gold nanoparticles

**Duangkamon Baowan · Kittisak Chayantrakom · Pairote Satiracoo · Barry J. Cox**

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**Abstract** Nanotechnology is a promising research area, and it is believed that the unique properties of molecules at the nano-scale will benefit mankind especially in the medical exploration. Here we utilize an applied mathematical modelling to investigate spherical and cylindrical concentric structures of gold nanoparticles, with the aim of maximising the free space for which to improve amount of drug or gene to bind on the nanoparticle surfaces and deliver to the target cells. The energy between two gold molecules is modelled by the 6–12 Lennard-Jones potential function, and the total potential between two layers for such particles is calculated using the continuous approximation. On minimising the energy function, the radii for five layers for the concentric sphere and likewise for the cylinder are presented. Further, the equilibrium spacing between any two layers is predicted to lie in the range 2.94–2.96 Å, for both concentric structures. There are at present no experimental or simulation results for comparison with the theoretical equilibrium configurations for concentric gold nanoparticles predicted by this study.

**Keywords** Gold nanoparticles · Lennard-Jones potential · Mathematical modelling

D. Baowan (✉) · K. Chayantrakom · P. Satiracoo
Department of Mathematics, Faculty of Science, Mahidol University, Bangkok 10400, Thailand
e-mail: scdbw@mahidol.ac.th

D. Baowan · K. Chayantrakom · P. Satiracoo
Centre of Excellence in Mathematics, CHE, Si Ayutthaya Rd., Bangkok 10400, Thailand

B. J. Cox
Nanomechanics Group, School of Mathematical Sciences, The University of Adelaide, Adelaide, SA 5005, Australia

## 1 Introduction

The structure and property designs of nanoparticles have stimulated the growth of nanotechnology, where the principle feature is the size and shape of the nanostructures. Mornet et al. [1] investigate a magnetic design of nanoparticles in order to enhance the magnetic resonance imaging which can be used in therapeutic research [1]. Further, Stella et al. [2] study polyethylene glycol coated biodegradable nanoparticles in order to design a protein that can bind on the surface of tumoral cells. In this paper, we investigate the structure of concentric gold nanoparticles with the purpose of maximising the free space between the layers of such nanoparticles, and thereby increasing the number of drug or gene to bind on the concentric surfaces.

Gold nanoparticles have been comprehensively studied in biological and medical areas, where the extensive literature reviews [3–9] can be found. Moreover, it has been experiments shown that mammalian cells can uptake gold nanoparticles [10]. As a result, gold nanoparticles might be utilized as a nanocapsule to deliver drugs or genes to target cells in the body. In terms of structural study of the gold nanoparticles, Pu et al. [11] employ molecular dynamics simulations to stretch gold nanowires in solvents, and they conclude that the packing density of a gold surface is smaller than that in the system comprising the benzenedithiol solvent and the gold particles. A molecular dynamics study for the diffusion of a gold nanocluster on graphite has been performed by Lewis et al. [12] where they find that the diffusion of the gold cluster takes place at a comparable rate to that for a single atom. Further, the structure of gold nanoparticles inside carbon nanotubes is determined by Arcidiacono et al. [13] who observe a strong layered structure at low temperature. Bilalbegovic [14] also determines temperature dependence of structural properties for infinitely long gold nanowires using molecular dynamics simulation and the embedded-atom potential, and he find the coaxial cylindrical shells nanowires.

In order to enhance the amount of drug and gene delivered to the target cells, we propose two concentric structures for the gold nanoparticles which are spherical and cylindrical configurations. The 6–12 Lennard-Jones potential function, which has been used in the system containing the gold nanoparticles as presented in the works of Lewis et al. [12] and Arcidiacono et al. [13], and a continuous approximation, where the atoms are assumed to be uniformly distributed over the surface of a molecule, are utilized to determine the energy of the system. Further on minimising the energy function, the inter-spacing between any two adjacent layers is determined which gives rise to a free space inside the concentric structure to deposit more biomolecules than is possible with a single layer of gold nanoparticles. We comment that there are many choices of force fields that may be used to study the system comprising gold nanoparticles such as many-body embedded atom method [12], Tersoff potential [13] and glue potential [13], or using sophisticated quantum mechanical calculations [11]. In this paper, we utilise the 6–12 Lennard-Jones potential to determine the interaction energy of the system of gold nanoparticles with the aim to derive an analytical expressions for such systems.

In the following section, the 6–12 Lennard-Jones potential function together with the continuous approach is presented. The mathematical determinations for the spherical and the cylindrical concentric gold nanoparticles are detailed in Sects. 3 and 4,

respectively. Moreover, the numerical calculations for a radius of each concentric layer are calculated, and an equilibrium spacing between the layers are investigated. Finally, a summary is presented in Sect. 5.

## 2 Lennard-Jones function and continuous approximation

We employ the Lennard-Jones potential function and the continuous approximation to calculate the molecular interatomic energy for a system of gold nanoparticles. 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

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

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

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

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

where $\eta_1$ and $\eta_2$ represent the mean surface density of atoms on each molecule. Further, we may define the integral $I_n$ in the form of

$$I_n = \int_{S_1}\int_{S_2} \rho^{-2n} dS_2 dS_1, \quad n = 3, 6,$$

and therefore, $E = \eta_1\eta_2(-AI_3 + BI_6)$.

The Lennard-Jones parameters for gold nanoparticles are taken from the work of Pu et al. [11], who use $\epsilon = 0.039\,\text{kcal mol}^{-1}$ and $\sigma = 2.934\,\text{Å}$ corresponding to $A = 7.2465\,\text{eV} \times \text{Å}^6$ and $B = 4,622.6273\,\text{eV} \times \text{Å}^{12}$. From the fact that gold adopts a face-centred cubic (fcc) crystal structure, the triangular arrangement is employed to determine a mean surface density of gold nanoparticles. Assuming that each atom of gold is coordinated with six other atoms, the area of a unit cell is given by $A^\star = \sqrt{3}d^2/2\,\text{Å}^2$ where $d$ denotes the equilibrium spacing which can be obtained as $d = 2^{1/6}\sigma = 3.2933\,\text{Å}$. Consequently, the mean surface density $\eta$ of the gold layers is taken to be $1/A^\star = 0.1065\,\text{Å}^{-2}$.

## 3 Concentric spherical structure

Here we assume that gold nanoparticles can arrange themselves to form a concentric spherical shape which can be referred as an onion structure. Firstly, we consider the molecular interaction energy for a point and a sphere as depicted in Fig. 1a. With reference to a Cartesian coordinates system $(x, y, z)$, a centre of a sphere $S_1$ is assumed to be located at the origin, and a typical point on its surface has coordinates $(a_1 \cos\theta \sin\phi, a_1 \sin\theta \sin\phi, a_1 \cos\phi)$, where $a_1$ denotes the radius of the sphere $S_1$. With reference to the same coordinates system, an atom has coordinates $(0, 0, \delta)$, where $\delta$ denotes a distance from the centre of the sphere $S_1$. We comment that later in the calculation, this atom is assumed to be located on a spherical surface $S_2$ of radius $a_2$, in order to determine the molecular energy between two concentric spheres. The spacing between two spherical surfaces is simply given by $\xi = a_2 - a_1$. The integral $I_n$ becomes

$$I_n = a_1^2 \int_0^{\pi} \int_{-\pi}^{\pi} \frac{\sin\phi}{\left[a_1^2 \sin^2\phi + (a_1 \cos\phi - \delta)^2\right]^n} \, d\theta \, d\phi.$$

Since the integrand is independent of $\theta$, we may deduce

$$\begin{aligned} I_n &= 2\pi a_1^2 \int_0^{\pi} \frac{\sin\phi}{\left[\delta^2 + a_1^2 - 2\delta a_1 \cos\phi\right]^n} \, d\phi, \\ &= 2\pi a_1^2 \int_0^{\pi} \frac{2\sin(\phi/2)\cos(\phi/2)}{\left[(\delta - a_1)^2 + 4\delta a_1 \sin^2(\phi/2)\right]^n} \, d\phi, \end{aligned}$$

by using of the trigonometric identities $1 - \cos\phi = 2\sin^2(\phi/2)$ and $\sin\phi = 2\sin(\phi/2)\cos(\phi/2)$. We now make the substitution $t = \sin^2(\phi/2)$ and take out a factor of $2(\delta - a_1)^{-2n}$, thus the integral becomes

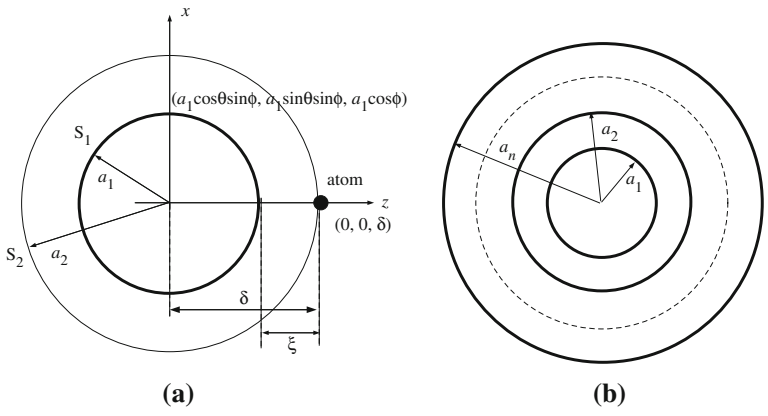


**Fig. 1** Model formations for **a** two layers, and **b** $n$-layers of concentric spherical gold nanoparticles

$$I_n = \frac{4\pi a_1^2}{(\delta - a_1)^{2n}} \int_0^1 \left(1 + \frac{4\delta a_1}{(\delta - a_1)^2} t\right)^{-n} dt.$$

This integral is in the form of the hypergeometric function $F(a, b; c; z)$, and therefore,

$$I_n = \frac{4\pi a_1^2}{(\delta - a_1)^{2n}} F\left(n, 1; 2; -\frac{4\delta a_1}{(\delta - a_1)^2}\right).$$

At this point we note that in the argument of the hypergeometric function $c = 2b$, consequently we may use a quadratic transformation [15],

$$F(a, b; 2b; z) = (1 - z)^{-a/2} F\left(a, 2b - a; b + 1/2; -\frac{\left(1 - \sqrt{1 - z}\right)^2}{4\sqrt{1 - z}}\right),$$

which gives

$$I_n = \frac{4\pi a_1^2}{\left(\delta^2 - a_1^2\right)^n} F\left(n, 2 - n; 3/2; -\frac{a_1^2}{\delta^2 - a_1^2}\right),$$

and because $F(a, b; c; z) = F(b, a; c; z)$ this may be transformed into a Chebyshev polynomial of the second kind

$$U_n(x) = (n + 1) F(-n, n + 2; 3/2; (1 - x)/2),$$

which leads to the expression

$$I_n = \frac{4\pi a_1^2}{(n - 1)\left(\delta^2 - a_1^2\right)^n} U_{n-2}\left(\frac{\delta^2 + a_1^2}{\delta^2 - a_1^2}\right).$$

Therefore, the total interaction energy for a point and a sphere is given by

$$E_s = 4\pi a_1^2 \eta \left[-\frac{A}{2\left(\delta^2 - a_1^2\right)^3} U_1\left(\frac{\delta^2 + a_1^2}{\delta^2 - a_1^2}\right) + \frac{B}{5\left(\delta^2 - a_1^2\right)^6} U_4\left(\frac{\delta^2 + a_1^2}{\delta^2 - a_1^2}\right)\right], \tag{2}$$

where $\eta$ is the atomic surface density of the gold layer and has a value of $0.1065\,\text{Å}^{-2}$, as calculated in Sect. 2.

Here we consider the two concentric spheres $S_1$ and $S_2$ with radii of $a_1$ and $a_2$, respectively, and with centred at the origin, as shown in Fig. 1. Then we employ the formula for the interaction of a point and a sphere $E_s$, given in (2), and replace $\delta$ by the distance from the centre of $S_1$ to the typical surface element on $S_2$, which in this

case is simply $\delta = a_2$. This expression is then integrated over the surface of $S_2$, which gives

$$E_{ss} = 4\pi a_1^2 \eta^2 \left[ -\frac{A}{2\left(a_2^2 - a_1^2\right)^3} U_1 \left( \frac{a_2^2 + a_1^2}{a_2^2 - a_1^2} \right) + \frac{B}{5\left(a_2^2 - a_1^2\right)^6} U_4 \left( \frac{a_2^2 + a_1^2}{a_2^2 - a_1^2} \right) \right] \times \int_0^{\pi} \int_{-\pi}^{\pi} a_2^2 \sin\phi \, d\theta \, d\phi.$$

This may be integrated immediately to give

$$E_{ss}(a_1, a_2) = 16\pi^2 a_1^2 a_2^2 \eta^2 \left[ -\frac{A}{2\left(a_2^2 - a_1^2\right)^3} U_1 \left( \frac{a_2^2 + a_1^2}{a_2^2 - a_1^2} \right) + \frac{B}{5\left(a_2^2 - a_1^1\right)^6} U_4 \left( \frac{a_2^2 + a_1^2}{a_2^2 - a_1^2} \right) \right]. \tag{3}$$

Since the Lennard-Jones potential is significant only over a short range, the total molecular energy for the $n$ layers of concentric spherical gold nanoparticles may be determined by considering only the nearest neighbour layers. In order to calculate the preferred inter-shell spacing, the radius of the inner most sphere is assumed to be fixed, and the radius of the 2nd-layer can be determined by minimising $E_{ss}$. By iteratively using the radius of the $(n-1)$th shell as the inner radius, the radius of the $n$th-layer can be obtained. Further, the inter-spacing between adjacent layers is calculated by $\xi = a_i - a_{i-1}$, for $i = 1, 2, 3, \ldots, n$.

### 3.1 Numerical calculations for concentric spheres

The numerical calculations for the concentric spheres are given in this section. We begin by considering the spheres comprising two layers. Figure 2 shows the relation between the potential energy and the radius $a_2$ of the outer layer for particular values of the inner spherical radii $a_1$. The equilibrium spacing between two layers occurs at the minimum energy level which we obtain $\xi = a_2 - a_1 \approx 2.95$ Å. This value is comparable with the finding of Archdiacono et al. [13] where the gold nanoparticles can form layers with the inter-spacing around 2.5 Å. Moreover, we find that the inter-spacing between the two layers slightly decreases as the radius of the sphere increases. This is due to the curvature effect, where a smaller sphere has higher curvature than a larger one. Table 1 presents the numerical values for $a_2$ at the minimum energy, $a_2^{\min}$, and the equilibrium spacing $\xi$ for five fixed inner spherical radii $a_1$.

For the $n$ layers of a concentric sphere, we assume that the 1st layer, or the core, has a radius of 5 Å. The radius of the 2nd layer can be determined by minimising the total interaction energy $E_{ss}$ given in (3). On recurring this process, the radii of the five layers of the concentric spherical gold nanoparticles can be determined, and they

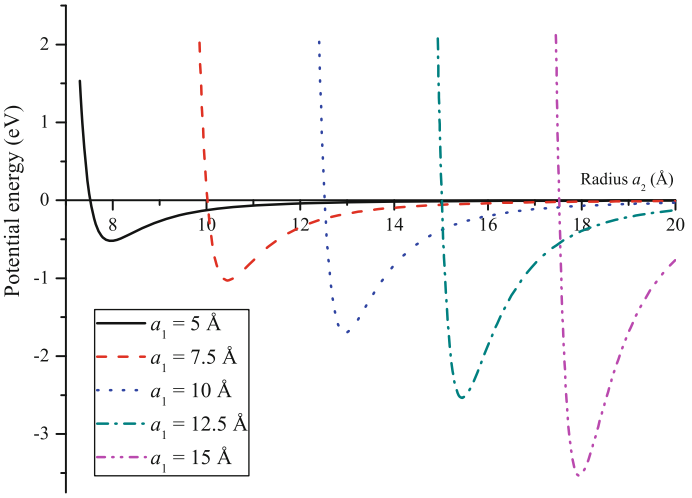


**Fig. 2** Energy profiles for two layers of concentric spheres with given values of $a_1$

**Table 1** Numerical calculations for radii $a_1$ and $a_2^{\min}$ of two layers of concentric sphere and equilibrium spacing $\xi$.

| $a_1$ (Å) | 5.0 | 7.5 | 10.0 | 12.5 | 15.0 |
|---|---|---|---|---|---|
| $a_2^{\min}$ (Å) | 7.9636 | 10.4559 | 12.9515 | 15.4485 | 17.9464 |
| $\xi$ (Å) | 2.9636 | 2.9559 | 2.9515 | 2.9485 | 2.9464 |

**Table 2** Radii of the five layers of concentric spherical gold nanoparticles

| $n$th layer | 1st | 2nd | 3rd | 4th | 5th |
|---|---|---|---|---|---|
| Radius (Å) | 5.0000 | 7.9636 | 10.9185 | 13.8688 | 16.8161 |

are given in Table 2. We note that the major contribution for the molecular interaction energy arises from the nearest layers, and we obtain 0.1% smaller spacing when considering the interaction energy for the three adjacent layers.

## 4 Concentric cylindrical structure

In this section, gold nanoparticles are assumed to form a concentric cylinder, which might be termed as a Russian doll structure. With reference to a Cartesian coordinates system $(x, y, z)$, a cylinder $C_1$ of radius $b_1$ is assumed to be axially located on the $z$-axis, and a typical point on its surface has coordinates $(b_1 \cos\theta_1, b_1 \sin\theta_1, z_1)$. Further, we assume that the cylinder $C_1$ is infinite in length. With reference to the same coordinates system, an atom which is assumed to be an arbitrary point on the cylinder $C_2$ has coordinates $(\delta, 0, 0)$, where $\delta$ denotes the perpendicular distance from

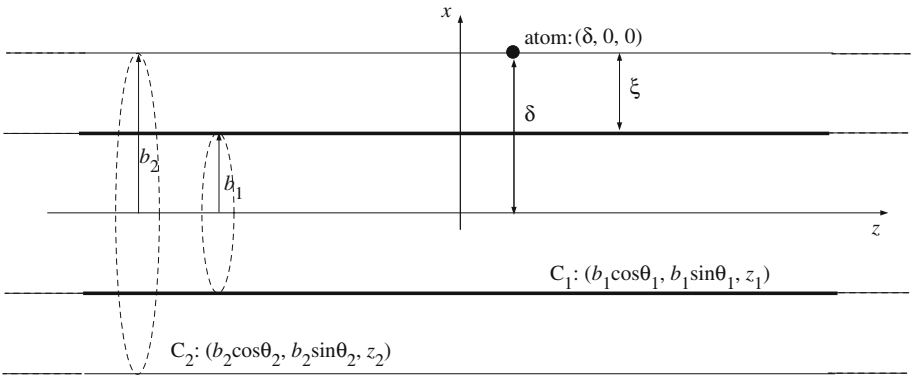


**Fig. 3** Model formations for concentric cylindrical gold nanoparticles

the $z$-axis as shown in Fig. 3. An expression for the distance $\rho$, from an arbitrary area element on the surface of the cylinder $C_1$ to the atom, is given by

$$\rho^2 = (\delta - b_1)^2 + 4\delta b_1 \sin^2(\theta_1 / 2) + z_1^2.$$

The cylindrical surface integral $I_n$ can be evaluated as follows

$$I_n = b_1 \int_{-\infty}^{\infty} \int_{-\pi}^{\pi} \frac{1}{\left[(\delta - b_1)^2 + 4\delta b_1 \sin^2(\theta_1/2) + z_1^2\right]^n} \, d\theta_1 \, dz_1.$$

We begin by defining $\lambda^2 = (\delta - b_1)^2 + 4\delta b_1 \sin^2(\theta_1 / 2)$, and then we make the substitution $z_1 = \lambda \tan \psi$, which gives

$$I_n = b_1 \int_{-\pi/2}^{\pi/2} \cos^{2n-2} \psi \, d\psi \int_{-\pi}^{\pi} \frac{1}{\lambda^{2n-1}} \, d\theta_1 = b_1 \mathrm{B}(n - 1/2, 1/2) \int_{-\pi}^{\pi} \frac{1}{\lambda^{2n-1}} \, d\theta_1,$$

where $B(x, y)$ is the beta function. Now on making the further substitution $t = \sin^2(\theta_1/2)$, it yields

$$I_n = \frac{2b_1}{(\delta - b_1)^{2n-1}} \mathrm{B}(n - 1/2, 1/2) \int_0^1 t^{-1/2}(1 - t)^{-1/2}(1 - \mu t)^{1/2-n} \, dt,$$

where $\mu = -4b_1\delta/(\delta - b_1)^2$, and we may deduce

$$I_n = \frac{2\pi b_1}{(\delta - b_1)^{2n-1}} \mathrm{B}(n - 1/2, 1/2) F\left(n - 1/2, 1/2; 1; -\frac{4\delta b_1}{(\delta - b_1)^2}\right).$$

Upon employing the quadratic transformation for the hypergeometric function [15] it yields

$$I_n = \frac{2\pi b_1}{\delta^{2n-1}} \mathrm{B}(n-1/2, 1/2) F\left(n-1/2, n-1/2; 1; \frac{b_1^2}{\delta^2}\right).$$

We write the hypergeometric function as a series and simplify the beta function as simple factorial terms, we find that $I_n$ is given by

$$I_n = \frac{4\pi^2 b_1}{(2\delta)^{2n-1}(2n-2)!} \sum_{m=0}^{\infty} \left(\frac{(2n+2m-2)!\, b_1^m}{(n+m-1)!\, m!\, (4\delta)^m}\right)^2,$$

and therefore, the total energy $E_c$ for an infinite cylinder and an exterior atom is given by

$$E_c = \frac{\pi^2 b_1 \eta}{192}\left[-\frac{A}{\delta^5}\sum_{m=0}^{\infty}\left(\frac{(2m+4)!\, b_1^m}{(m+2)!\, m!\, (4\delta)^m}\right)^2 + \frac{B}{9676800\,\delta^{11}}\sum_{m=0}^{\infty}\left(\frac{(2m+10)!\, b_1^m}{(m+5)!\, m!\, (4\delta)^m}\right)^2\right], \tag{4}$$

where $\eta$ is the mean surface density of the cylinder $\mathrm{C}_1$, as calculated in Sect. 2.

The molecular interaction energy between two infinite cylinders diverges, therefore, in this case, we may calculate an interaction energy per unit length, and a result of minimising such energy gives rise to an equilibrium structure. Then we employ the formula for the interaction of a point and an infinite cylinder $E_c$, given in (4), and replace $\delta$ with the distance from the centre of $\mathrm{C}_1$ to the typical surface element on $\mathrm{C}_2$, which is $\delta = b_2$. This expression is then integrated over the surface of $\mathrm{C}_2$, which gives

$$E_{cc} = \frac{\pi^2 b_1 \eta^2}{192}\left[-\frac{A}{b_2^5}\sum_{m=0}^{\infty}\left(\frac{(2m+4)!\, b_1^m}{(m+2)!\, m!\, (4b_2)^m}\right)^2 + \frac{B}{9676800\, b_2^{11}}\sum_{m=0}^{\infty}\left(\frac{(2m+10)!\, b_1^m}{(m+5)!\, m!\, (4b_2)^m}\right)^2\right]\int_{-\pi}^{\pi} b_2 d\theta_2.$$

This integral may be immediately evaluated to give

$$E_{cc} = \frac{\pi^3 b_1 \eta^2}{96}\left[-\frac{A}{b_2^4}\sum_{m=0}^{\infty}\left(\frac{(2m+4)!\, b_1^m}{(m+2)!\, m!\, (4b_2)^m}\right)^2 + \frac{B}{9676800\, b_2^{10}}\sum_{m=0}^{\infty}\left(\frac{(2m+10)!\, b_1^m}{(m+5)!\, m!\, (4b_2)^m}\right)^2\right]. \tag{5}$$

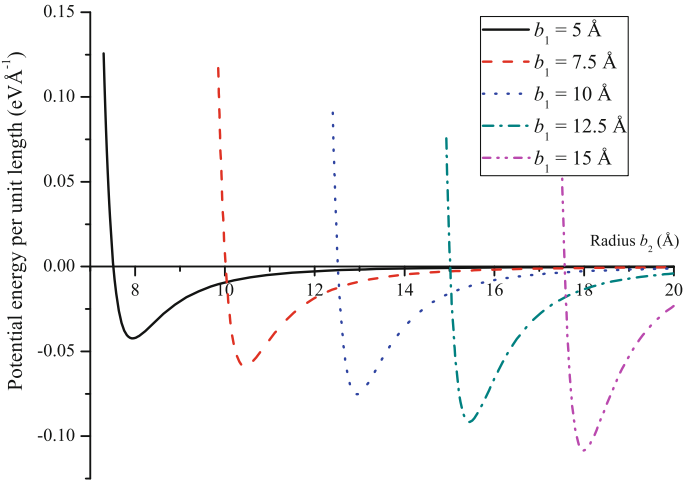


**Fig. 4** Energy profiles for two layers of concentric cylinders with given values of $a_1$

As in the case of spherical particles, the $n$ layers of concentric cylindrical gold nanoparticles can be determined by the iterative process as described earlier. We aim to minimise $E_{cc}$, as given in (5), where the radius of the core is fixed, and at the minimum energy level we obtain a radius of the next layer which also gives rise to an equilibrium spacing $\xi$ between the two adjacent layers.

### 4.1 Numerical calculation for concentric cylinders

Assuming that concentric cylinder consisting of gold nanoparticles comprises two layers, we graphically show the relation between the potential energy per unit length and the radius $b_2$ of the outer cylinder for five given values of the inner radii $b_1$, as shown in Fig. 4. The equilibrium spacing between the two layers is determined at the minimum energy position, and it is given by $\xi = b_2^{\min} - b_1$.Table 3 presents the outer cylindrical radius at the minimum energy level $b_2^{\min}$ and the resultant equilibrium spacing $\xi$ corresponding to the five values of the inner cylindrical radii $b_1$. This coaxial cylindrical shells structure is also reported by Bilalbegovic [14] using molecular dynamics study but the inter-spacing value has not been described. Further, we find that the equilibrium spacing is approximately 2.94 Å for the five cases, and it decreases as the inner cylindrical radius increases. Likewise, this result comes from the fact that the cylinder with a large radius can be approximated as a flat plane which has less curvature effect. We note that by using the same Lennard-Jones potential function and the parameters given in Sect. 2, the equilibrium spacing between two flat planes is obtained as 2.934 Å.

In terms of the $n$ concentric cylindrical layers, we employ the recurring process to obtain the radius of the $(n+1)$th layer. Here we demonstrate an example for five layers of a concentric cylinder, where the radius of the inner most core is assumed to be 5 Å. The five numerical values of the five radii are given in Table 4. We find that

**Table 3** Numerical calculations for radii $b_1$ and $b_2^{\min}$ of two layers of concentric cylinder and equilibrium spacing $\xi$

| $b_1$ (Å) | 5.0 | 7.5 | 10.0 | 12.5 | 15.0 |
|---|---|---|---|---|---|
| $b_2^{\min}$ (Å) | 7.9454 | 10.4434 | 12.9418 | 15.4406 | 17.9398 |
| $\xi$ (Å) | 2.9454 | 2.9434 | 2.9418 | 2.9406 | 2.9398 |

**Table 4** Radii of the five layers of concentric cylindrical gold nanoparticles

| $n$th layer | 1st | 2nd | 3rd | 4th | 5th |
|---|---|---|---|---|---|
| Radius (Å) | 5.0000 | 7.9454 | 10.8885 | 13.8298 | 16.7700 |

the five radii of the concentric spherical and cylindrical structures are comparable, therefore, both of them might be used as nanocapsules that may increase the number of biomolecules to be loaded inside.

## 5 Summary

In medical research, the control of size and shape of nanoparticles has been widely studied in order to enhance the drug or gene capacity of a nanocapsule, and then send the capsule to the targeting cells. A commonly used material for nanoparticles is gold, however, the cost of experimental research using gold nanoparticles is quite high. In this paper, we propose the use of a mathematical model to determine the structural property of the concentric gold nanoparticles. Moreover, an analytical expressions for the interaction energy of such system are determined. The 6–12 Lennard-Jones potential function and the continuous approach are employed to determine the equilibrium spacing between two concentric layers of the spherical and the cylindrical configurations. The equilibrium spacing for the spherical and cylindrical concentric structures are in the range of 2.94–2.96 Å. These results are in good agreement with molecular dynamics simulations made by Arcidiacono et al. [13] for the concentric sphere and by Bilalbegovic [14] for the concentric cylinder. Furthermore, on fixing the radius of the inner most layer, the radii of the four outer layers are determined by minimising the energy function. On using an iterative process, the equilibrium spacing and the radii of the $n$ layers of the concentric structures can be obtained. The concentric structures are believed to create more free space between the layers, therefore, it might be one useful technique to increase a number of drug molecules or gene strands to pack on the nanoparticles. We comment that such theoretical structures have yet to be confirmed either experimentally or by molecular dynamics simulations.

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