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Research paper

Continuous approximation for interaction energy of adamantane encapsulated inside carbon nanotubes

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ABSTRACT

The interaction energy for two adjacent adamantane molecules and that of adamantane molecules encapsulated inside carbon nanotubes are investigated considering only dipole-dipole induced interaction. The Lennard-Jones potential and the continuous approximation are utilised to derive analytical expressions for these interaction energies. The equilibrium distance 3.281 Å between two adamantane molecules is determined. The smallest carbon nanotube radius b_0 that can encapsulate the adamantane molecule and the radius of the tube b_{max} that gives the maximum suction energy, linearly depend on the adamantane radius, are calculated. For larger diameter tubes, the off axis position has been calculated, and equilibrium distance between molecule and tube wall is found to be close to the interlayer spacing in graphene.

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1. Introduction

Conceivably, linear forms of crystalline diamond constitute a new one-dimensional nanomaterial. They are believed to assemble within carbon nanotubes which serve as a template and by taking diamondoids as building blocks. Template synthesis of linear chain nanodiamonds have been considered recently using diamantine polymers [1]. The smallest building block of diamond is adamantane, which is the smallest unit with a diamond lattice. We examine here the interaction energy of adamantane in canbon nanotubes assuming the Lennard-Jones potential and the continuous approximation. Analytical expressions are derived using a highly simplified model, and the derived structural parameters are close to density functional calculations [2].

Adamantane ($C_{10}H_{16}$) is the smallest diamondoid with sp^3 hybridization and hydrogen on its surface [3–5]. It consists of four connected cyclohexane rings, in armchair configuration, and in three dimensions arranges to form a cage, with bond angles the same as those found in diamond. While hydrocarbons with only σ-bonds are relatively chemically inert, adamantane is highly reactive. The four 3-coordinated carbon atoms are particularly reactive while the remaining six 2-coordinated carbon atoms are less reactive. Adamantanes and its derivatives are also used in medical applications, for example; to treat flu [6], avian influenza virus [7,8] and to act as an antiviral agent against HIV [9,10] or as a lubricant stable at elevated temperatures.

In this study, we aim to determine the interaction energy between two adamantane moleclues and that of an adamantane molecule interacting with a carbon nanotube taking only dipole-dipole interaction into account. The equilibrium position of two adamantanes and the encapsulation behaviour of an adamantane molecule are determined. The continuum approach utilised here might also be useful when applied to future one-dimensional nanomaterials or relevant biomedical systems.

In terms of energy calculations, McIntosh et al. [11] use density functional theory and propose that the encapsulation of adamantane molecules inside carbon nanotubes occurs spontaneously. Moreover, they suggest that the (7,7) carbon nanotube ($r = 4.75$ Å) has the ideal radius to contain a single adamantane molecule with optimal suction energy, and the peapod structure [12–14] of the adamantane molecules is found when the radius of the tube is increased. Linear assemblies of adamantanes inside double-wall carbon nanotubes have been studied by Zhang et al. [2] who suggest that the equilibrium distance between two adamantane moleclues is approximately 6.2 Å. Shi et al. [15] report a method for the bulk production of long linear carbon chains in double-walled carbon nanotubes. Further, they find that the equilibrium spacing in

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the carbon chain that is encapsulated in a carbon nanotube is 3.378 Å.

In this paper, we employ applied mathematical modelling to derive analytical expressions for the energy of the system involving adamantane molecules and a carbon nanotube. The Lennard-Jones potential for the non-bonded atoms is assumed to approximate the van der Waals interactions, since it has been confirmed that the dipole-dipole interactions play an important role in systems of adamantanes and carbon nanotubes [2,11,15]. Furthermore, we assume that the continuous approximation, where atoms on the surface of the molecule are assumed to be uniformly distributed over the molecule, can be used to evaluate the total energy of the system. The continuous or continuum approach has been successfully used to determine the energy behaviuor of several nano-scaled systems and, in particular, it has been adopted to determine C_{60} fullerene patterns inside carbon nanotubes, referred as nanopeapods [14] or nobel gases encapsulated in carbon nanotubes [16].

The Lennard-Jones potential function and the continuous approach are presented in the following section and mathematical derivations for spherical and cylindrical shapes are given in Section 3. The results of our findings are presented in Section 4 and finally, a brief summary is given in Section 5.

2. Lennard-Jones potential and continuous approximation

We employ the Lennard-Jones potential and continuous approximation to determine the molecular interatomic energy between two molecules. We assume the 6–12 Lennard-Jones potential given by

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

where ρ denotes the distance between two atoms, $A = 4\epsilon\sigma^6$ and $B = 4\epsilon\sigma^{12}$ are respectively the attractive and repulsive constants, and where ϵ is the energy well depth and σ is the inter-atomic distance when the potential is zero. The minimum of the potential well is located at distance $\rho_0 = (2B/A)^{1/6} = 2^{1/6}\sigma$. Using a continuum approach, atoms at discrete locations on the molecule are assumed to be averaged over its surface, which means that summations over all atoms involved is replaced by surface integrals. The molecular interatomic energy is then obtained by calculating integrals over the surface of each molecule, given by

$$E = \eta_1\eta_2 \int_{S_1}\int_{S_2}\left(-\frac{A}{\rho^6} + \frac{B}{\rho^{12}}\right) dS_2 dS_1, \tag{1}$$

where η_1 and η_2 represent the mean surface density of atoms on each molecule. Further, by writing

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

Eq. (1) can then be written as

$$E = \eta_1\eta_2(-AI_3 + BI_6). \tag{3}$$

To determine the radius of the tube which will maximise the suction energy, we utilize the suction energy concept as proposed in [17]. The suction energy W is defined as the total energy or work gained by the van der Waals interactions acquired by a particular molecule to enter the tube,

$$W = \int_{-\infty}^{\infty} F(Z)dZ = \int_{-\infty}^{\infty} -\frac{\partial E}{\partial Z} dZ, \tag{4}$$

where E is as given in (3) and Z is a distance between two molecules. Note that due to the symmetry of the systems studied here we only need to consider axial forces.

The numerical values of the Lennard-Jones parameters used for nonbonded adamantane sp^3 hybridization and carbon nanotube sp^2 hybridiztion are taken from the work of Rappé et al. [18] where $\epsilon = 0.105$ kcal/mol and $\sigma = 3.851$ Å for both hybridizations. The mean atomic surface density of the carbon nanotube is taken to be 0.3812 $Å^{-2}$ [19], and the adamantane molecule ($C_{10}H_{16}$) is modelled as a sphere. For any given radius a of an adamantane, the mean atomic surface density of carbon atoms on the surface of an adamantane is given by $10/(4\pi a^2)$ $Å^{-2}$.

We note that since the energy well depth of hydrogen is approximately six times less that of carbon, only the carbon atoms are considered and the effect of the hydrogen is ignored. We note that there are two categories of carbon atoms on the adamantane molecule connecting to hydrogen atoms; one category are those which are bonded to only one hydrogen atom, while the other category are those bonded to two hydrogen atoms. Further, the locations of hydrogen are not well defined, since the spherical adamantane molecule has a large curvature. Moreover, hydrogen has already been incorporated in the Lennard-Jones parameter values for sp^3 hybridization.

3. Interaction energy

Here we investigate the energy behaviour of an adamantane molecule inside a single-walled carbon nanotube. Firstly, we determine the equilibrium distance between two adamantane molecules assuming they form a linear array. Secondly, the encapsulation behaviour of an adamantane molecule in a carbon nanotube is studied to determine the tube radius that can encapsulate the molecule.

As mentioned in Section 2, the Lennard-Jones potential is used to determine the interaction energy between two non-bonded atoms. The atoms are uniformly distributed on the surface of the molecule or nanotube and hence an integral expression is utilised using uniform atom densities to determine the total interaction energy between two molecules.

We start by considering a spherical adamantane molecule, consisting of carbon atoms, interacting with a single atom, as described in the following subsection. Subsequently, we assume that the single atom is located either on another spherical adamandane molecule or on the surface of a cylindrical carbon nanotube, and the interaction between two spheres and the interaction between a sphere and a cylinder are determined as described in Sections 3.2 and 3.3, respectively.

Noting that the encapsulation of nano-scaled materials is also dependent on the temperature, other environmental effects and impurities or adsorbed species. The mathematical modelling presented here is an idealised approach which provides reasonably accurate estimates for stable configurations of pristine systems.

3.1. Interaction between sphere and single atom

Here, we determine the interaction energy between a spherical surface and a single atom, a configuration shown in Fig. 1. In the Cartesian coordinate system with origin at the centre of the sphere, the single atom is assumed to be located at $(0, 0, \delta)$, so that the integral I_n defined in (2) becomes

$$I_n = \int_{-\pi}^{\pi}\int_{0}^{\pi} \frac{a^2 \sin\phi}{(a^2 + \delta^2 - 2a\delta\cos\phi)^n} d\phi d\theta,$$

where $\rho^2 = a^2 + \delta^2 - 2a\delta\cos\phi$ and δ is the distance from the single atom to the centre of the sphere. By making the substitution $t = a^2 + \delta^2 - 2a\delta\cos\phi$ and using the fact that I_n is independent of θ, we may deduce

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