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Mechanical and electronic properties of carbon nanobuds: *First-principles* study

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ABSTRACT

Carbon nanobuds (CNBs), a novel carbon nanostructure, can be engineered by attaching C₆₀ (buckyballs) onto the sidewall of a single-walled carbon nanotube (SWCNT). Density functional theory (DFT) calculations are used to investigate the structural, electronic and mechanical properties of armchair (6, 6) and zigzag (10, 0) CNBs. Based on an electronic density of states (DOS) plot, we observed that all CNBs are semiconducting regardless of whether the original SWCNT base is metallic or semiconducting. Our results also indicate that the C–C distances in the C₆₀ molecule and SWCNTs around the attachment region are increased significantly from the original distance. Furthermore, we also observed that the Young's modulus of the CNBs decreased when attaching a fullerene C₆₀ molecule on the surface of zigzag and armchair SWCNTs. In addition, we demonstrate that the Young's modulus of (10, 0) CNB is lower than that of (6, 6) CNB.

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1. Introduction

In the last decade, carbon nanostructures, such as carbon nanotubes (CNTs) and fullerene C₆₀ (buckyballs), have attracted great interest from both fundamental and application perspectives due to their mechanical strength, excellent thermal and electrical conductivities and optical properties [1–4]. Depending on their chirality, CNTs can exhibit either metallic or semiconducting properties [5]. The switch between metal and semiconductor properties can be induced by an external trigger, such as pressure [6,7] or light [8]. Under certain conditions, fullerene C₆₀ is capable of conducting electricity similar to metal atoms.

Over the past decade, research efforts have also been made to synthesize hybrid carbon nanostructures to find new carbon materials with novel properties. The first experimentally constructed hybrid carbon nanostructure was the carbon nanopeapod, in which a chain of C₆₀ molecules was assembled within a carbon nanotube [9]. In 2007, another hybrid carbon nanostructure was fabricated with C₆₀ molecules that covalently attached to the sidewall of single-walled carbon nanotubes (SWCNTs) [10]. This new nanostructure was called a carbon nanobud (CNB).

Previous experimental and theoretical studies have revealed that the electronic properties of CNBs differ from those of fullerenes and

CNTs. For example, CNBs exhibit lower field thresholds and much higher current densities and cold electron field emission efficiencies than pristine SWCNTs [10,11]. The attached C₆₀ molecule on the surface of CNTs results in more space between nanotubes thus, the adhesion between SWCNTs can be weakened and prevent the formation of tight bundles of CNTs. Furthermore, the CNBs can be used as a molecular support to prevent slipping of the matrix in composite materials and to increase the mechanical strength of them.

In composite materials, due to load transfer from the matrix to the filler, information about the mechanical and electronic properties of the filler is very important. Therefore, in this study, we first attached fullerene C₆₀ on the surface of (6, 6) and (10, 0) SWCNTs using different possible configurations and then determined the energetically most favorable position using *first-principles* density functional theory (DFT). In addition, we investigated the mechanical and electronic properties of these CNBs.

2. Computational method

We employed the *first-principles* DFT approaches using numerical atomic orbitals as the basis set to calculate the structure and energy of all of the systems. The unit cells for (10, 0) and (6, 6) nanotubes were tetragonal 30 × 30 × 17.064 Å and 30 × 30 × 17.241 Å with periodic boundary conditions in the z-directions to represent infinite

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tubes, respectively. We used the generalized gradient approximation (GGA) with the Perdew–Burke–Ernzerh of (PBE) functional [12] in density functional theory and the standard norm-conserving Troullier–Martins pseudo-potentials [13]. We used the SIESTA code, which solves the standard Kohn–Sham equations and has been demonstrated to be very efficient for large atomic systems [14–16]. The calculations were performed using a double-z basis composed of numerical atomic orbitals of finite range augmented by polarization functions (DZP) for all of the simulated atoms.

To determine the equilibrium configurations of the systems under study, we relaxed all of the atomic structures of the considered systems by minimization of the total energy using Hellmann–Feynman forces, including Pulay-like corrections. Structural optimizations were performed using the conjugate gradient algorithm until the residual forces were smaller than $0.02 \text{ eV}\text{\AA}^{-1}$. The mesh cutoff, an energy that corresponds to the grid spacing, was selected to be 150 Ry. The k -point was set to $1 \times 1 \times 5$ for all of the chains. In the simulation, a three-dimensional periodic boundary condition was used for the super-cells. A vacuum width of 30 \AA above was constructed, which ensured that the x - and y -axis of the periodic super-cell was sufficiently large that no interaction between nanotubes of adjacent super-cells occurred.

The basis set superposition error (BSSE) was eliminated by adding ghost orbitals to the calculations for the isolated adsorbates. We considered the correction for BSSE using the counterpoise correction (CP) method [17] to further correct the obtained binding energy, E_b , values in all of the systems under study. To estimate the binding energy of the interacting entities, we used the expression

$$E_b = E_{(\text{full}/\text{SWCNT})} - E_{(\text{full}/\text{ghost}/\text{SWCNT})} - E_{(\text{full}/\text{SWCNT}/\text{ghost})} \quad (1)$$

where, $E_{(\text{full}/\text{SWCNT})}$ is the total energy of the SWCNT with the fullerene C_{60} molecule. The 'ghost' term corresponds to additional basis wave functions centered at the position of the SWCNT or the fullerene but without any atomic potential.

3. Results and discussion

Fullerene C_{60} is a molecule composed entirely of 60 sp^2 -hybridized carbon atoms in the form of a hollow sphere with twenty hexagonal and twelve pentagonal rings. The C-C bonds in fullerene can be divided into two types: one type occurs between hexagonal and pentagonal rings, and the other occurs between two hexagonal rings (labeled C_5 - C_6 and C_6 - C_6 in Fig. 1a). Additionally, the C-C bonds in the armchair or zigzag nanotubes are perpendicular (labeled as V) or parallel (labeled as P) and tilted to the tube axis (labeled as T), as

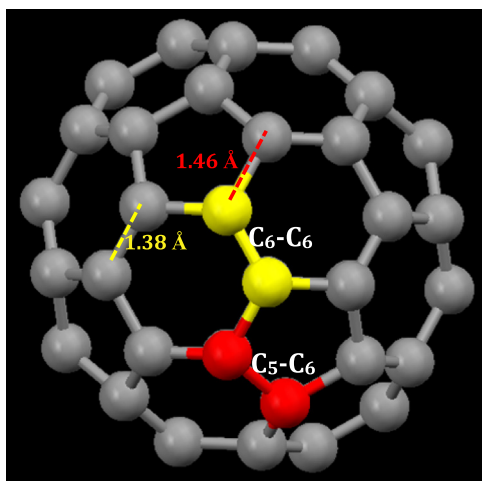


Fig. 1. Optimized structure with two different C-C bonds for fullerene C_{60} .

illustrated in Fig. 2. According to the previous literatures [11], a single C-C covalent bond between C_{60} molecule and the SWCNT is unstable and can spontaneously break. Therefore, at least two C-C covalent bonds are required through the cycloaddition reaction to stabilize the CNBs. It should be noted that the formation of these novel nanostructured materials has been governed by the barriers for cycloadditions between the attached rings of C_{60} and the π -bonds on the CNTs [11]. It was shown by DFT calculations with nudged elastic band (NEB) technique that the energy barrier for the formation is about 2.5 eV for the (5, 5) and (10, 0) CNBs [11]. Meanwhile, after the formation of complex it is expected to be stable at room temperature as shown by the experiment [10] because of rather high energy barrier (about 1 eV) for the CNBs dissociation [11,18].

To fully understand the effect of attaching fullerene on the electronic and mechanical properties of carbon nanotubes, we considered five types of configurations for the armchair (6, 6) and zigzag (10, 0) CNBs, as illustrated in Fig. 3. In the first and second configurations, two carbon atoms in a C-C bond between two hexagonal and pentagonal-hexagonal faces of fullerene are bound to the atoms of a C-C bond perpendicular or parallel to the axis of armchair or zigzag carbon nanotubes. In the third and fourth configurations, both carbons of a C-C bond between two hexagonal and pentagonal-hexagonal faces in fullerene are bound to the atoms of a C-C bond tilted to the tube axis of a (6, 6) or (10, 0) CNTs. Lastly, in the fifth configuration, a C_{60} molecule is connected through six C-C bonds of a hexagonal ring to the zigzag and armchair CNTs.

After the full structural optimizations, we observed that the carbon atoms of the SWCNT near the fullerene C_{60} molecule were pulled outward from the original wall surface due to the covalent bonding with cycloaddition reaction between the fullerene and nanotube; in addition, their bonding was transformed from sp^2 - to sp^3 -hybridization. A comparison of the binding energies, which were obtained using the BSSE corrections for the different configurations, indicates that the most energetically stable state for the armchair (6,6) CNB after adsorption was the fourth configuration, with a binding energy value of -1.82 eV . Additionally, we observed that a C_{60} molecule was attached to the surface of the zigzag (10,0) SWCNT in the first configuration, with a binding energy of -1.68 eV . The obtained results also indicate that the bond length between the fullerene C_{60} molecule and nanotubes (L_{f-n}) for the most stable state is approximately 1.60 \AA , as observed in Fig. 4. Furthermore, as

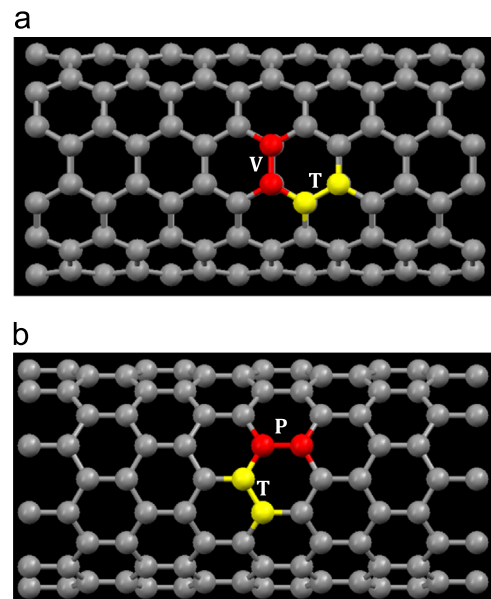


Fig. 2. Optimized structure of (a) a (6,6) SWCNT and (b) a (10,0) SWCNT with two different C-C bonds.

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