



Density functional theory study on configurations and electronic properties of periodic nanoridges



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ABSTRACT

Periodic nanoridges (PNRs), a new kind of hybrid nanostructures which consists of graphene monolayer and zigzag single-wall carbon nanotube (SWCNT), were engineered in this work. With density functional theory methods, two stable hybrid carbon nanostructures coming from two different types of absorption between SWCNT and graphene were obtained. Based on calculations of electron density distribution and binding energy, the first structure (PNR-1) is revealed to be more thermodynamically favorable, compared with the second one (PNR-2). Electronic band structures analyses suggest that both PNR-1 and PNR-2 are narrow-band-gap semiconducting with a direct band gap, which indicates promising applications for photocatalyst.

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1. Introduction

The sp^2 systems of carbon-related materials, such as fullerenes, carbon nanotubes (CNTs), and graphene monolayer, have attracted lots of attentions, owing to their extraordinary physical and chemical properties and their potential applications in nanoelectronics, sensors and gas storage [1–8]. A fullerene is composed of carbon atoms which form a spherical or elliptical cage. In a graphene monolayer, all the sp^2 carbon atoms are in the same plane, giving rise to a honeycomb structure [8]. Graphene monolayer is considered to be semimetal with an exact zero gap. Graphene nanoribbons can be regarded as elongated strips of graphene monolayer with a finite width in a certain direction [9–11]. By rolling a graphene monolayer into a hollow cylinder, a single-walled carbon nanotube (SWCNT) is formed and its structure is specified by a chiral vector

$$C_h = na_1 + ma_2 \equiv (n, m), (n, m \text{ are integers}, 0 \leq |m| \leq n).$$

As for SWCNTs, the electronic properties depend sensitively on the chiral vector C_h . When $n - m = 3q$ (where q is an integer), carbon nanotubes are metallic. In the case of $n - m \neq 3q$, tubes are semiconducting with an energy gap of the order of ~ 0.5 eV [12–14].

Research efforts have been made to fabricate hybrid carbon nanostructures with novel properties which have not been found in traditional sp^2 systems of carbon-related materials. To date, two types of hybrid carbon nanostructures have been reported.

One hybrid carbon nanostructure is carbon nanopeapod in which a chain of C_{60} buckyballs are assembled in a SWCNT [15–17]. The other hybrid carbon nanostructure is the so-called carbon nanobuds where C_{60} buckyballs are covalently attached to the sidewall of a SWCNT [18]. With density functional theory method, Wu and Zeng designed theoretically a kind of hybrid carbon nanostructure named as periodic graphene nanobuds that C_{60} buckyballs are covalently bonded to graphene monolayer or that fragmented C_{60} buckyballs are fused onto graphene monolayer [19].

In this paper, we report a new kind of computer-aided hybrid carbon nanostructures consisting of graphene monolayer and (8, 0) zigzag SWCNT, namely periodic nanoridges (PNRs), which retain a narrow-band-gap semiconducting behavior. Physical and chemical properties of the PNRs have been investigated by the first-principles methods.

2. Computational methods

Spin-polarized density functional theory calculations with Grimme dispersion correction (DFT-D) [20] to describe non-covalent interaction between graphene monolayer and SWCNT were performed with using ultrasoft pseudopotential in Cambridge Sequential Total Energy Package (CASTEP) within the Materials Studio 5.5 Package [21,22]. The exchange-correlation of electron was treated with the generalized gradient approximation (GGA) [23], as implemented by Perdew–Burke–Ernzerhof (PBE) form [24]. The basis set, as defined by the energy cutoff value, is an important parameter that determines the accuracy of a CASTEP calculation. In the present work, the energy cutoff was set to be 240.0 eV, including a sufficient number of wave functions to get

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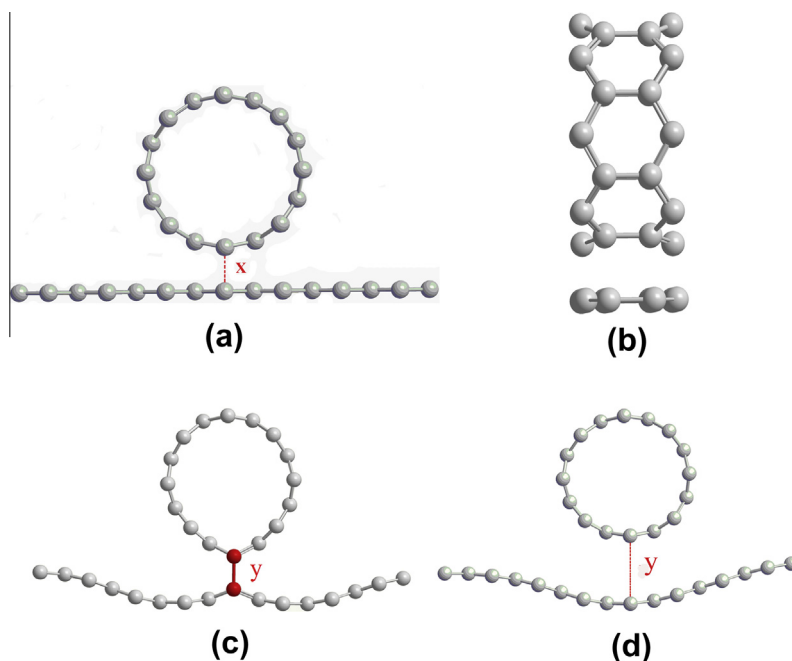


Fig. 1. Original model (a front view, b side view) and stabilized hybrid structures (c PNR-1, d PNR-2). X and Y are the distances between the bottom of the carbon nanotube and the graphene monolayer in original model and stabilized structures, respectively.

precise information about electronic structure of PNRs and the Brillion zone was sampled by $5 \times 5 \times 2$ k-points using the Monkhorst–Pack scheme [25]. The vacuum layer in the supercell was set to be 15 Å, large enough to avoid the interlayer interaction. After geometric optimization, a tetragonal supercell with dimension $19.2 \times 4.2 \times 24.0 \text{ \AA}^3$ was adopted.

3. Results and discussion

In the PNRs, the axes of nanobube are parallel to the graphene plane (Fig. 1a and b). After geometry optimization on the original models was carried out with the PBE method, two types of PNRs were located (Fig. 1c and d). In the first type (PNR-1), chemical bonds are formed between SWCNT and graphene with corresponding C–C bond of 1.64 Å. However, the other type, PNR-2, is stabilized by the physical adsorption between two periodic structures. The shortest C–C distance between SWCNT and graphene is about 3.53 Å, similar with the interlayer distance in graphite [26]. It is speculated that the configuration of stabilized hybrid structure is closely related to the original distance between the bottom of the nanotube and the graphene monolayer. When the distance is below a threshold, PNR-1 is formed. On the contrary, when the distance is upon the threshold, PNR-2 is formed. The threshold, which

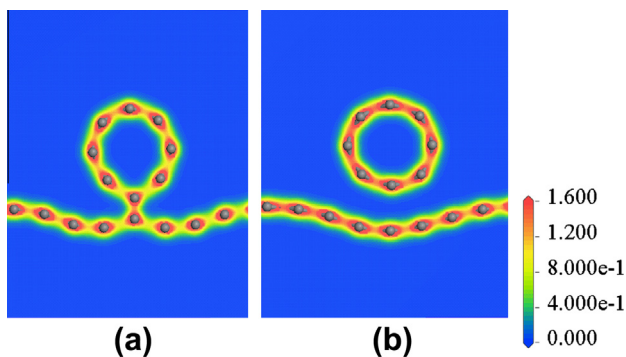


Fig. 2. Electron density of two types of hybrid structures: (a) PNR-1 and (b) PNR-2.

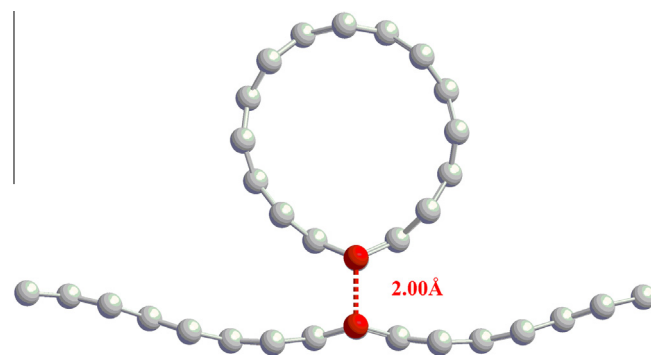


Fig. 3. Transition State (TS) on the potential energy surface. The distance between the bottom of the SWCNT and graphene monolayer is 2.00 Å.

is similar to the nearest distance between nanotubes and graphene at the transition state between PNR-1 and PNR-2 (discussed below), is about 1.90 Å.

Fig. 1 original model (a front view, b side view) and stabilized hybrid structures (c PNR-1, d PNR-2). X and Y are the distances between the bottom of the carbon nanotube and the graphene monolayer in original model and stabilized structures, respectively.

In order to have a deeper insight into the electronic structure of PNR-1 and PNR-2, electron density map of PNR-1 and PNR-2 are presented in Fig. 2. For PNR-1, significant electron density is distributed between SWCNT and graphene, which indicates that chemical bonds are formed between SWCNT and graphene. In contrast to PNR-1, no significant overlap of electron density has been found between SWCNT and graphene in PNR-2, suggesting that SWCNT is physically adsorbed on graphene.

In order to assess the stability of PNR-1 and PNR-2, the binding energies (E_b) were calculated based on the following formula:

$$E_b = E_{\text{PNR}} - E_{\text{graphene}} - E_{\text{tube}}$$

where E_{PNR} , E_{graphene} and E_{tube} are the total energy per supercell of hybrid structure, graphene and SWCNT, respectively. The binding energies of PNR-1 and PNR-2 are predicted at the PBE level of theory

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