Solid State Communications 229 (2016) 43–48

Contents lists available at ScienceDirect

Solid State Communications

journal homepage: www.elsevier.com/locate/ssc

Charge distribution of Lithium-doped graphane/graphene hybrid system: Role of nearly-free electronic states

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ARTICLE INFO

Article history:
Received 17 July 2015
Received in revised form
13 November 2015
Accepted 28 December 2015
Available online 2 January 2016

Keywords:
A. Graphane
A. Graphene
D. Charge distribution

ABSTRACT

Charge distribution of Lithium-doped graphane/graphene hybrid system is performed by density functional theory. It is found that almost all of transferred charges reside on the graphane layer nearest to the lithium atom, and only a few of them stay in interior layers. It indicates that the graphane layer can screen the external charge offered by lithium atom and behave like classical plate capacitor. The underlying mechanism reveals that the predominance of nearly-free electron states in band filling play an important role in determining charge distribution.

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1. Introduction

Graphene has been proposed to be a promising material for future electronic device due to its intriguing mechanical and electronic properties [1–3]. Especially graphene has extremely high carrier mobility [4], it is hoped to replace silicon as a new material for the next-generation nanoelectronic device. However, pure graphene is a zero-gap semiconductor with a linear dispersion at the Fermi level. The absence of a gap is an adverse feature for the practical application. Several methods have been carried out to modulate the electronic properties of graphene, such as chemical functionalization [5,6], slicing a graphene into nanoribbons [7,8], and uniaxial strain engineering [9,10]. Among them, functionalization of graphene with hydrogen atoms has attracted unusual attention both experimentally and theoretically [11–14]. The most attractive one is fully hydrogenated graphene named as graphane, which was first predicted theoretically by Sofo et al. [11] and then was experimentally synthesized by Elias et al. [12]. In contrast to graphene, graphane is a semiconductor with a wide direct band gap of 3.5 eV [11].

On the other hand, various graphene-based combined systems display more exotic electronic properties [15–18]. The electronic properties of graphane/fluorographene bilayer can be efficiently tuned from semiconductor to metal under the electric field [15]. Sławińska et al. have reported that graphene layer sandwiched between two hexagonal boron nitride sheets can create a band gap of over 230 meV by applying external electric field [16]. Lu et al. [17] investigate the charge distribution of K-doped graphene and h-BN combined system. They find that the outer h-BN layers, despite its insulating feature, cannot screen the external charges offered by K due to the predominant band filling of graphenes. It is consistent with the potassium-doped double-walled nanotube with BN outer wall and carbon inner wall (BNCNT) [18]. Inspired by above studies, it is worth to study the charge distribution feature of other similar graphene-based hybrid system.

In this paper, we investigate the charge distribution of the Lithium (Li) doped layered graphane/graphene hybrid system. Like two-dimensional h-BN layer, monolayer graphane is also a large band gap semiconductor. However, charge distribution exhibits different feature as Li atom is placed above it. No matter how many layers of graphane and graphenes there are, the outmost graphane layer can screen almost all of the external charges offered by Li atom. We demonstrate the mechanism of such behavior based on electrostatic theory and band filling, especially the nearly-free electronic states, in this paper.

2. Models and methods

We perform equilibrium geometries and energy band structures calculations of Li-doped graphane and graphene hybrid system by using first-principles density-functional theory (DFT). The local-density approximation (LDA) of density functional theory with the projector augmented wave potentials (PAW) is implemented within the Vienna *Ab initio* Simulation Package

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http://dx.doi.org/10.1016/j.ssc.2015.12.011
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(VASP) [19,20]. The plane wave cutoff energy is set to 450 eV and a $7 \times 7 \times 1$ Monkhorst–Pack *k*-point sampling is used for the Brillouin zone integration. Vacuum spacing of at least 15 Å is chosen in order to prevent the interaction between layer structures. All the geometrical structures are fully relaxed until force and energy are converged to 0.01 eV/Å and 10^{-5} eV, respectively. The charge amount of each atom in Li-doped graphane and graphene hybrid system is calculated by virtue of Bader charge population analysis [21]. *Furthermore, we* also *use the vdW density functional method with the optB86b -vdw functional to test calculations the structure and electronic properties of system . The results* (*not shown*) *are almost consistent with those from the LDA calculation , which indicate that the LDA is reasonable for describing the graphane /graphene system .*

The structural models we considered here are shown in Fig. 1. Increasing graphane layers (from one to four) are placed on four layer graphenes. We utilize AB-stacking of graphene layer for our calculations, while the structure of graphane layer is chosen to be the most stable A_+A_+ configuration [24], i.e. the second layer is placed on top of the first one by copying the bottom layer and moving it along vertical columns normal to the layer plane. Two adjacent graphane and graphene layers are constructed by AB stacking model. The graphene monolayer surface is simulated using a 2×2 supercell and the in-plane lattice constant of 2.45 Å is adopted, which matches well with the 2×2 supercell of graphane. One Li atom is located above the center of the hexagon of graphane due to the strongest binding compared to other high symmetry sites, and the height of Li atom is fully optimized. *Test calculations indicate that main conclusion remains unchanged when the size of supercell increases .*

3. Results and discussions

We first briefly review the electronic properties of the four-layer graphene and monolayer graphane. The electronic band structure of four-layer graphene is presented in Fig. 2(a), which exhibits four paired parabola-like bands. The innermost pair crosses at the *K*-point and the system is a zero gap semiconductor. It is quite consistent with previous study [25]. Fig. 2(b) shows the electronic band structure of monolayer graphane. According to our calculations, graphane has an approximate 3.50 eV direct gap at Γ point, as suggested by Sofo et al. [11]. The conduction band minimum (CBM) state shows a strongly delocalized feature which distributes above and below the graphane plane (see Fig. 2(c)). Such a delocalized state is classified as the nearly-free electron (NFE) state [26], and is marked in red in Fig. 2(b). When Li atom is doped in the monolayer graphane, the unoccupied NFE state shifts downward significantly in energy and crosses Fermi level becoming partially occupied (marked in red), as presented in Fig. 2 (e). It indicates that the Li-doped graphane monolayer exhibits the metallic nature. To further understand the change of the NFE state upon Li atom doped, we depict its charge density map at the Γ point in Fig. 2(f). It shows that the electron delocalized degree on

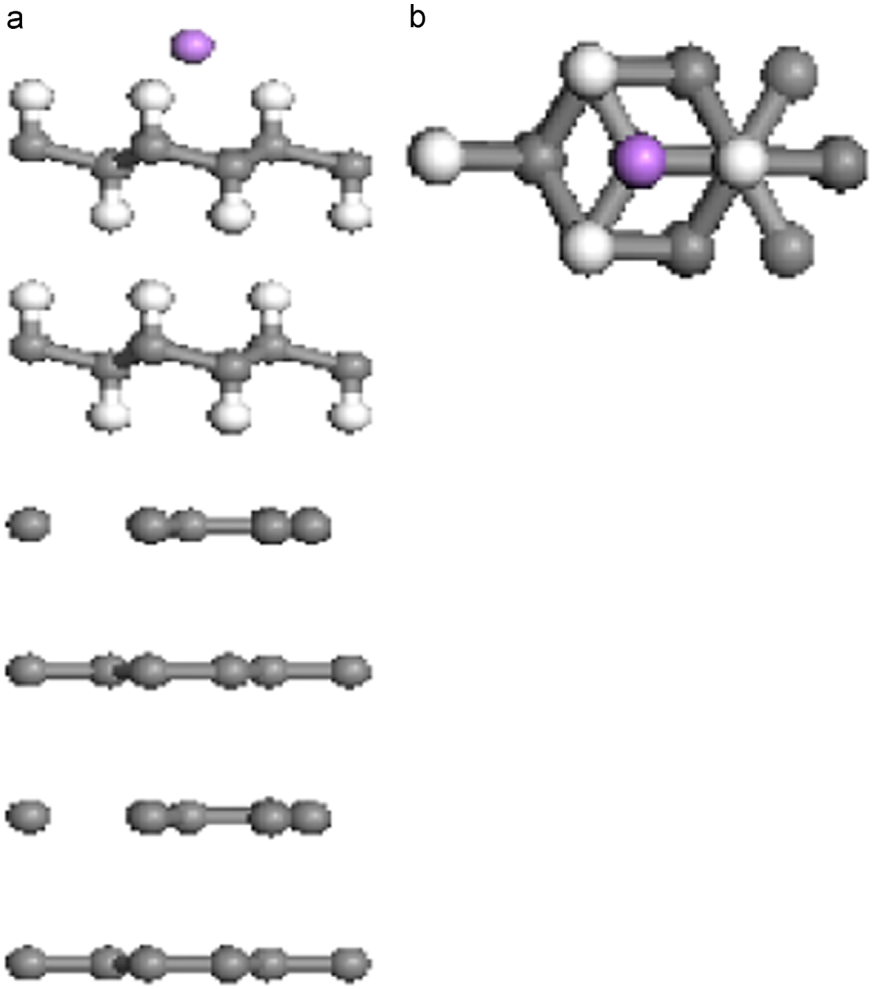

Fig. 1. (Color online) (a) Side and (b) top view of a 2×2 supercell of Li-doped two layer graphanes and four layer graphenes hybrid system. The purple, gray, and white denote lithium, carbon, and hydrogen atoms, respectively.

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