Solid State Communications 211 (2015) 23–28

Contents lists available at ScienceDirect

Solid State Communications

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

First-principles study on the electronic and magnetic properties of armchair graphane/graphene heterostructure nanoribbons

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ARTICLE INFO

Article history:
Received 11 February 2015
Received in revised form
16 March 2015
Accepted 17 March 2015
Communicated by Ralph Gebauer
Available online 26 March 2015

Keywords:
A. Graphene nanoribbon
D. Electronic properties
E. First-principles

ABSTRACT

In this paper, the electronic and magnetic properties of electronic and magnetic properties of armchair graphane/graphene heterostructure nanoribbons (AGA/GNRs) have been systematically investigated by first-principles calculations based on density functional theory. The calculated results indicate that 13-armchair graphane nanoribbon (13-AGANR), 13-armchair graphene nanoribbons (13-AGNR) and hybrid armchair graphane/graphene nanoribbons (AGA_{13-x}/G_xNRs) are all direct semiconductors (13, $13-x$ and x are denoted as the nanoribbons' widths). The band structures near the Fermi level of AGA_{13-x}/G_xNRs are mainly determined by the graphene section and the atomic charge transfers in the interface of AGA_{13-x}/G_xNRs are stronger. AGA_7/G_6NR with DB defects at AGANR edge obviously affect the magnetic properties. These diverse and tunable electronic and magnetic properties can be a theoretical guidance for the design of novel nanoelectronic devices.

1. Introduction

Graphene consists of a hexagonal monolayer network of sp^2-hybridized carbon atoms. Since graphene was first experimentally fabricated in 2004 [1], graphene monolayers has motivated considerable interest in variety of one-atom-thick two-dimensional (2D) crystals [2–4], especially after large-scale synthesis methods like chemical vapor-deposition [6] and epitaxial growth [7] on metal and SiC substrates are developed. The quasi-one-dimensional (1D) graphene ribbons (GNRs) with armchair or zigzag edges have attracted much attention because of their electronic [8–11], magnetic [12,13], and quantum-transport properties [14,15]. A graphene nanoribbons (GNRs) can be realized by cutting mechanically exfoliated graphene or patterning epitaxially grown graphene structures [16,17]. Recently, the fascinating electronic properties associated with one-dimensional (1D) fully and partially hydrogenated graphene [18,19], graphane [20], BN [21], ZnO [22], SiC [23], GaN [24], and AlN [24,25] nanoribbons derived from either monolayer or multilayer sheets heavily depend on the ribbons' width, thickness and edge modification. The fully and partially hydrogenated nanoribbons exhibit completely distinct properties from their pristine forms. The high quality graphane nanoribbons GANRs can be fabricated by selectively hydrogenating graphene or by carving GNRs on a graphane sheet [26,27]. Furthermore, hybrid graphane/graphene nanoribbons (GA/GNRs) could exhibit unique electronic properties that differ from the pristine armchair (AGNRs) and zigzag GNRs (ZGNRs) [28,29]. These suggest such ribbon-hybridized graphene-like materials as promising candidates for applications in future electronic and optoelectronic nanodevices. Therefore, serious efforts are highly warranted to explore the physical properties of GNR for various technological applications.

Yet a systematically theoretical understanding of electronic properties of these functionalized armchair graphane/graphene nanoribbons (AGA/GNRs) remains unclear. How and to what extent does the ratio of GA affect the electronic properties of different GA/GE NRs systems? Because the interaction of hydrogen with graphene is of great technological interest, compared with the unsaturated nanoribbon, how would its band gap change in a hydrogenated AGNRs? Therefore, the above questions are discussed in this paper. The structural, electronic properties of hybrid AGA/GNRs with the variation of the proportion are extensive carried out based on first-principles calculations with density functional theory (DFT). Meanwhile, Band structure distribution (BS), the Density of States (DOS), atom Mulliken charges and the population analysis are performed to determine changes of atomic and electronic structures of hybrid AGA/GNRs. These studies provide us a deep understanding of the novel properties of AGA/GNRs, which is essential to employ them as building blocks for future nanodevices.

2. Computational methods

The simulation is calculated by first-principles DFT, which is provided by DMOL^3 [30–32]. The generalized gradient approximation (GGA) with the Perdew–Burke–Ernzerhof scheme (PBE) [33] is

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http://dx.doi.org/10.1016/j.ssc.2015.03.014
0038-1098/

employed to optimize geometrical structures and calculate properties. The all-electron relativistic Kohn–Sham wave functions are expanded in the local atomic orbital basis set for DMOL^3 [30]. Pseudopotentials with C–$2s^2 2p^2$, and H–$1s^1$ valence electron configurations are used for C and H atoms. Similar functional have been successfully used to study the structural and electronic properties of water, Si and Cu nanowires [34,35]. The nearest distance between for edge–edge and layer–layer in neighboring cells is greater than 15 Å to ensure no interactions. For geometry optimization, both the cell and the atomic positions are allowed to fully relax. The Brillouin

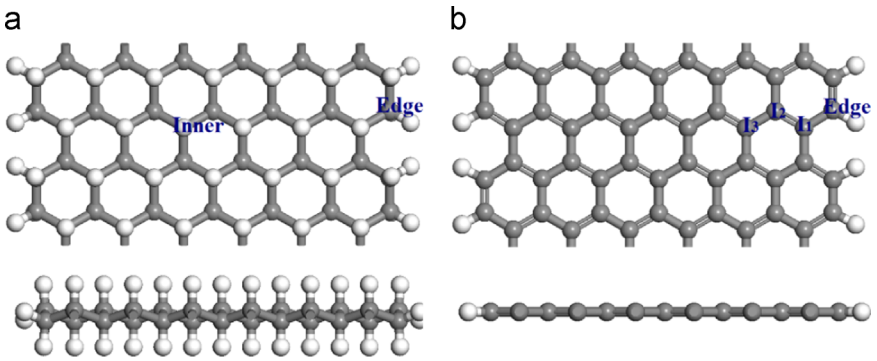

Fig. 1. Schematic illustration of supercell 13-AGANR (a) and 13-AGNR (b) arrangements, where the gray and white spheres are C and H atoms, respectively.

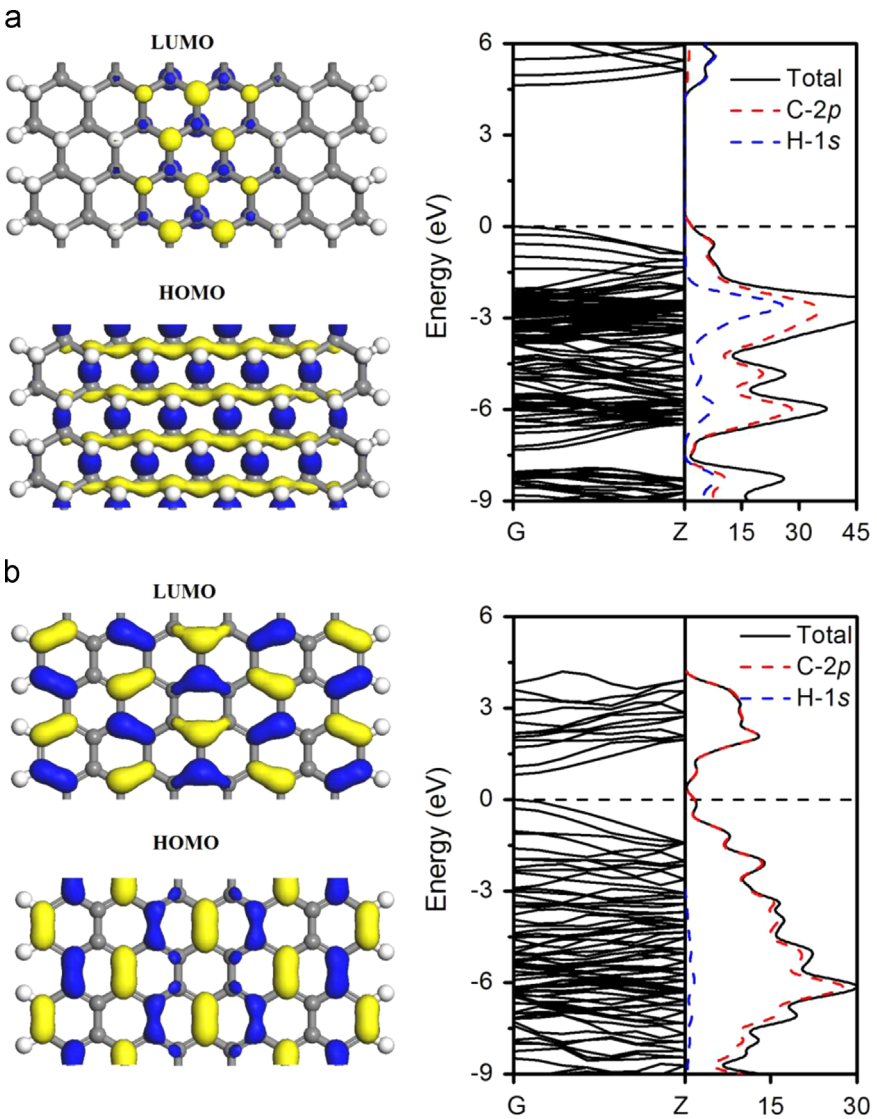

Fig. 2. Band structure, Partial DOS and charge density isosurfaces of LUMO and HOMO at Gamma point of 13-AGANR (a) and 13-AGNR (b). The E_f is set to zero. Blue and yellow denote the positive and negative wave function contours, respectively, and the value of the isosurfaces is 0.025 e/Å^3. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)