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Band-gap modulation of graphane-like SiC nanoribbons under uniaxial elastic strain

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ABSTRACT

The band-gap modulation of zigzag and armchair graphane-like SiC nanoribbons (GSiCNs) under uniaxial elastic strain is investigated using the density functional theory. The results show that band gap of both structures all decreases when being compressed or tensed. In compression, both zigzag and armchair GSiCNs are semiconductors with a direct band gap. However, in tension, the armchair GSiCNs undergo a direct-to-indirect band-gap transition but the zigzag GSiCNs still have a direct band gap. These results are also proved by HSE06 method. This implies a potential application of the graphane-like SiC nanoribbons in the future pressure sensor and optical electronics nanodevices.

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1. Introduction

Graphene with a two-dimensional (2D) honeycomb structure of carbon atoms has been one of the most important research areas since it was successfully fabricated in 2004 [1] due to its special low-energy excitations in term of dispersion relation of Dirac fermions with zero effective mass [2,3]. Furthermore, the half-integer and fractional quantization of Hall conductance has been observed in graphene [3–7]. These unusual electronic and magnetic properties have dominated graphene in variety of applications and attracted many theoretical and experimental investigations. Quasi-one-dimensional (1D) graphene nanoribbons have shown peculiar electronic, magnetic, thermal and quantum transport properties [8–15]. In addition, 2D graphene with full hydrogenation was predicted and experimentally demonstrated [14,15].

Recently, these experimental and theoretical studies on graphene created intense interest in honeycomb lattices of other group-IV elements and compounds of III–V and II–VI group elements

[16–18]. Among them, the 2D SiC honeycomb sheet is particularly concerned because the electron configuration in Si atom is more similar to that in C atom compared with other elements. Influenced by devising of the SiC nanowires and nanotubes [19, 20], there have been many works about 2D SiC honeycomb sheet. In spite of the fact that 2D SiC honeycomb sheet is not attained in experiment, many studies have demonstrated its stability based on reliable theoretical methods [16,21–24]. While the infinite periodic 2D SiC is a semiconductor with a 2.55 eV band gap, its armchair ribbons are nonmagnetic semiconductors but half metallicity has been predicted for narrow SiC zigzag nanoribbons without any chemical decoration or applied an external field [25]. Interestingly, hydrogenation of 2D SiC honeycomb sheet may directly lead to graphane-like SiC with sp³-bonding similar to graphane [14,15]. The graphane-like SiC sheet is more steady by energy calculations so that it can be more easily synthesized than graphane-like SiC one. Wang et al. studied structural stabilities and electronic properties of fully hydrogenated SiC sheet, and showed that the chair-like conformation is energetically more favored relative to the boat-like one [26]. Garcia et al. studied the structure properties of graphene- and graphane-like nanosheets and concluded that the synthesis of graphane-like SiC sheet should be feasible [27].

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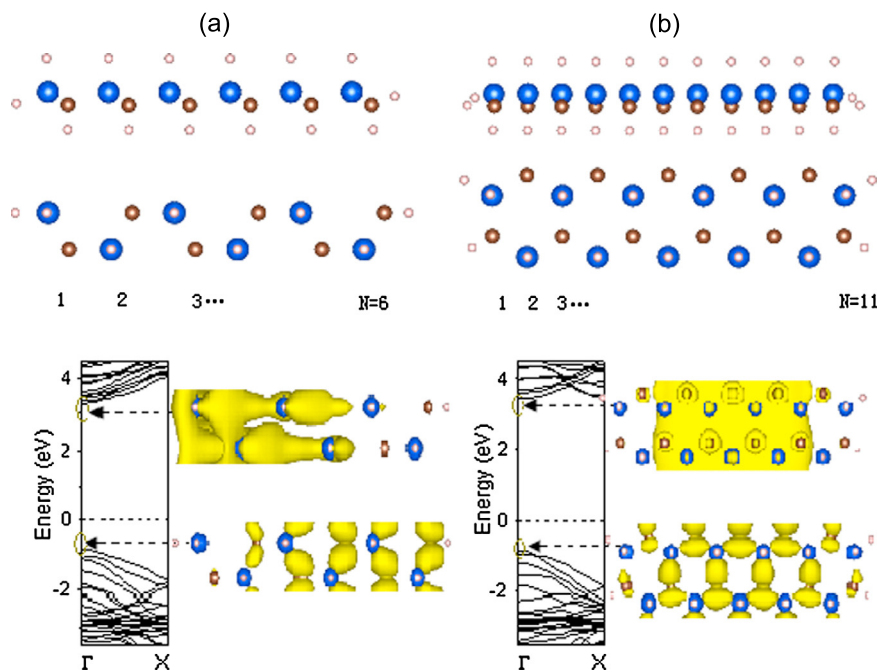*E-mail addresses:* jsblgao@gmail.com (B.-L. Gao), shke@tongji.edu.cn (S.-H. Ke).

Fig. 1. (Color online.) Side and top views of the optimized structures, the electronic band structures, and charge density of CBE, VBE at Γ point are plotted for (a) 6-zigzag and (b) 11-armchair GSiCNs, respectively. The brown, blue and pale balls represent carbon, silicon and hydrogen atoms, respectively. The Fermi energy level is plotted with a dashed line.

The reason that 2D honeycomb structures have been attracting enthusiastic attention is that their energy gaps are easily modulated by doping, adsorption, strain or cutting their shape to meet special needs, such as chemical and pressure sensor, nano-mechatronics, optoelectronic device, and nanolaser. Compared with doping impurity atom, adding vacancy and other methods, applying strain on 1D or 2D nanostructures may be a better choice in band gap engineering due to its convenience. There have been many reports in this aspect. The band-gap of graphene-like ZnO monolayer can be tunned by applying an of in-plane homogeneous biaxial strain [28]. The half-fluorinated bilayer graphene undergoes a direct-to-indirect band gap transition by applying biaxial tensile strains [29]. The calculations of first-principles density functional theory have demonstrated that band gap of zigzag BN nanoribbons can be significantly tuned under uniaxial tensile strain [30]. The band-gap modulation of graphane nanoribbons is investigated under uniaxial elastic strain [31]. The electronic properties of graphene-like SiC monolayers under many kinds of strained conditions are studied by DFT and the quasiparticle GW approximation, and the results show that the indirect-to-direct band gap transition can be tuned by strain [32]. Despite its huge importance, we are not aware of any model being able to exactly calculate the energy band properties of both 1D zigzag and armchair graphane-like SiC nanoribbons (GSiCNs) under uniaxial elastic strain. Our objective is to systemically investigate the geometric, electronic, and mechanical properties of both 1D zigzag and armchair graphane-like SiC nanoribbons (GSiCNs) under uniaxial elastic strain. The results show that the band gap decreases remarkably when GSiCNs are compressed and tensed, and in compressive case, both zigzag and armchair GSiCNs are semiconductors with direct band gap. However, in tension the armchair GSiCNs undergo a direct-to-indirect band gap transition although the zigzag GSiCNs are direct band gap. The test calculations with HSE06 method on both 6-zigzag GSiCNs and 11-armchair GSiCNs have also proved that the trend of the band gaps varying with strain is the same as that based on the GGA method. This implies a possible route of effectively using GSiCNs in mechatronics, straintronics and other nanodevices.

2. Method of calculation and computational details

Our first-principles calculations are implemented in the VASP code [33,34]. The exchange-correlation potential is described by the projector-augmented wave method for the electron–ion interaction and the generalized gradient approximation (GGA) [35] of Perdew–Burke–Ernzerhof (PBE) functional. The $2s^2 2p^2$, $3s^2 3p^2$ and $1s^1$ valence electrons for C, Si and H are included. Due to more stability of the chairlike conformer than the boatlike one [26], the graphane-like SiC nanoribbons (GSiCNs) with hydrogen atoms arranged in chairlike conformation are investigated. The zigzag and armchair GSiCNs are respectively shown as Fig. 1(a) and (b). The latest distances between any two atoms in any two adjacent nanoribbons exceed 13 Å, which is large enough to avoid the coupling between two neighboring nanoribbons. The Brillouin-zone integrations are sampled on a grid of $11 \times 1 \times 1$ Monkhorst–Pack [36] special points for geometry optimization and 21 k points for obtaining the band structures. All structures are fully optimized without any symmetry constraints. A plane wave expansion up to a 400 eV cutoff energy is used, and the convergence of energy and force are set to 10^{-5} eV and 0.02 eV/Å, respectively. In all calculations, the edge carbon (or silicon) atoms are saturated with hydrogen. In order to prove effectiveness of standard density functional theory for the calculation of magnetism, state-of-art hybrid functional calculations based on the Heyd–Scuseria–Ernzerhof (HSE06) function [37] have been also performed to examine the characteristics.

To illustrate the reliability of the calculations, the properties of a 2D graphane-like SiC monolayer are calculated for checking. The optimized Si–C bond length is 1.89 Å, and a direct energy gap of 4.04 eV appears at the $\Gamma = (0, 0, 0)$ point in the hexagonal Brillouin zone, consistent with the values of 1.89 Å and 3.84 eV in the paper [26]. Due to underestimate of the GGA method for the band gap of the semiconductor or insulator, the HSE06 screened hybrid density functional theory is used to obtain a direct energy gap of 4.71 eV because it has succeeded to reproduce the experimental band gap of many semiconductors.