

Electronic properties of monolayer and bilayer arsenene under in-plane biaxial strains



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ABSTRACT

Using first-principles density functional theory, we have investigated the mechanical and electronic properties of monolayer and bilayer arsenenes under in-plane biaxial strains. It is interesting to find that under large enough tensile strains, the monolayer arsenene transfers from buckled honeycomb structure to planar honeycomb phase while the interlayer distance D of bilayer arsenene maintains at about 1.371 Å. Both monolayer and bilayer arsenenes possess indirect band gaps and their electronic properties can be tuned via in-plane biaxial strains. The variations of the band gap energy are diverse with respect to the compressive and tensile biaxial strains. Under compressive strains, the band gap of both monolayer and bilayer arsenenes initially increases, and then rapidly decreases. In addition, the monolayer arsenene exhibits an indirect-to-direct band gap transition when the compressive strains reach to -10% . However, under tensile strains, the band gap of monolayer arsenene monotonously decreases with the strains, while the band gap of bilayer arsenene reduces quickly to zero under small tensile strains. Our present results will be conducive to design strain-based arsenene materials for applications in nanoelectronic and optoelectronic devices.

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1. Introduction

Recently, graphene has attracted tremendous interest due to its unusual physical properties such as high electron mobility, heat conductance and massless fermions [1,2]. It plays an important role in fundamental research and is expected to have superior performance in future electronic devices applications [3,4]. However, the zero band gap of graphene greatly restricted its applications for various needs, especially for the near blue and UV wavelength optoelectronic devices. Many efforts have been devoted to open the gap of graphene, such as cutting graphene into ribbons, and applying external electronic or strain fields, only small band gap are achieved [5–7].

The finding of graphene and its good physical performance excited people to search for graphene-like two-dimensional (2D) semiconductors with intrinsic gaps, such as MoS₂ and black phosphorene. These 2D materials have specific mechanical and optoelectronic properties which differ from their bulk counterpart, as well have wide applications in chemistry and materials science [8]. For example, AlN is a well-known group III nitride with wide direct band gap (6.2 eV), while AlN nanosheet were investigated to be an indirect band gap semiconductors [9]. Much like graphite, black phosphorus is a stable layered material in which individual atomic layer is held together by weak interlayer forces with significant van der Waals character [10]. Recently, the elemental 2D material, phosphorene, was mechanically exfoliated from black phosphorus and

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achieved excellent transistor performance at room temperature [11]. Jingsi et al. reported that phosphorene exhibited a direct band gap which can be modified by the number of layers and in-plane strains [12].

As the same group element, bulk grey arsenic shares some features with phosphorus and has stable layered structure under ambient conditions [13]. Recently, arsenene and antimonene were proposed to be new members of group-V elemental 2D nanostructures [14,15]. Yanli et al. gave a detailed investigation on the electronic structure and carrier mobility of arsenene nanosheet and nanoribbon [16,17]. Kamal et al. systematically studied the buckled and puckered monolayer arsenene in response to the uniaxial strain effects [18]. For the corresponding bilayer and monolayer arsenene, their mechanical and electronic properties under in-plane biaxial strains are still unknown. By analyzing the strain effects on the mechanical behavior and electronic properties of monolayer and bilayer arsenenes, we aim to provide a theoretical foundation for the manufacture of novel 2D arsenic materials.

The paper is organized as follows: Section 2 describes our theoretical methods and details. Section 3 presents the results and discussion. Finally, we give a brief summary in Section 4.

2. Methods and details

The calculations are performed by using the Vienna ab initio simulation package (VASP) [19] based on density functional theory (DFT) [20]. The generalized gradient approximation (GGA) given by Perdew–Burke–Ernzerhof (PBE) [21] is utilized for the exchange–correlation function. The cut-off energy for the plane-wave expansion is 450 eV to ensure a good convergence of the geometric optimization. The 4s and 3p orbitals of the arsenic atoms are treated as valence ones. The layered structures of the monolayer and bilayer arsenenes are placed in the *xy* plane. In order to reduce the interactions of neighbouring arsenenes, a vacuum of about 15 Å is added along the *z* direction. The Monkhorst–Pack scheme of $16 \times 16 \times 1$ and $16 \times 16 \times 4$ k-point mesh are used for the self-consistent Brillouin zone integration of monolayer and bilayer arsenenes, respectively. The structural optimization is allowed to relaxed until the maximum force on each atom become less than 0.01 eV/Å and maximum energy change between two steps is smaller than 10^{-5} eV.

Arsenene is a honeycomb monolayer of arsenic which is structurally similar to graphene and phosphorene. However, unlike graphene's flat structure and phosphorene's puckered structure, the arsenene uses buckled structure to keep stable which is confirmed by phonon and binding energy calculations [15,18]. The coordination number of each arsenic atom is three. The geometric structures of monolayer and bilayer arsenenes are displayed in Fig. 1. For bilayer arsenene, there are two possible stacking configurations namely AB and AA, which can be seen in Fig. 2(b) and (c). The former is the same stacking as in bulk grey arsenic. The AA stacking arrangement has also been synthesized and observed in other bilayer systems [22,23]. So the AB and AA-stacked bilayers are both considered here. To figure out the strain effects on arsenene, the arsenic systems are subjected to the in-plane biaxial strains in the following procedures: the in-plane lattice constants *a*, *b* along *x* and *y* axes are fixed at a certain value of a_1 and b_1 during the relaxation, the strains are given by the relative change of the lattice constants $\varepsilon = \varepsilon_{11} = (a_1 - a)/a = \varepsilon_{22} = (b_1 - b)/b$. $\varepsilon < 0$ represents the compressive strains and $\varepsilon > 0$ stands for the tensile strains. The in-plane biaxial strain is taken as the parameter to study the modulation of structural and electronic properties of arsenic systems.

3. Results and discussions

3.1. Structural properties

The calculated and observed structural properties and cohesive energy of strain-free monolayer and bilayer arsenene after structural optimization are summarized in Table 1. The bond length *l* of monolayer arsenene after relaxation is

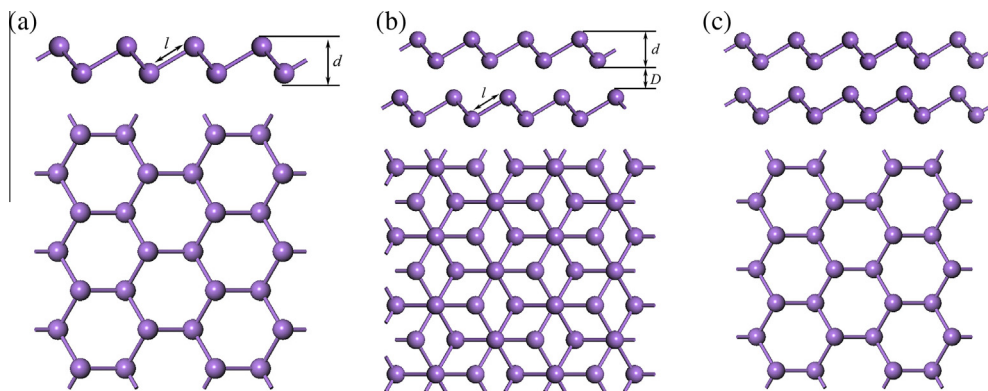


Fig. 1. Side view and top view of geometrical structures of (a) monolayer arsenene, (b) AB-stacked and (c) AA-stacked bilayer arsenene (*l* is the bond length between two As atoms, *d* represents the buckling height of monolayer arsenene and *D* is the interlayer distance of bilayer arsenene).

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