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Electric field effects on electronic characteristics of arsenene nanoribbons

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ABSTRACT

By using the first-principles calculations, we investigate the effects of electric field on electronic structures of armchair and zigzag arsenene nanoribbons (AsNRs) with different widths. The results show that for each case, quantum size effects induce a smaller band gap in larger AsNRs. Moreover, electric field can reduce effectively the band gap of AsNRs. In addition, the electric field can induce only the transition of band structures in the A-AsNRs or Z-AsNRs with narrow size. The band gap decrease more rapidly and the threshold electric field induced metal becomes smaller in the wider AsNRs.

1. Introduction

Since single-layer graphene was fabricated successfully in 2004 [1], Graphene has become a noticeable nanometer material because of its unique electronic, mechanical and transport properties. Recently, different kinds of graphene-like two-dimensional (2D) nanomaterials, such as silicene [2–5], stanene [6–8], phosphorene [9–13], C_2N [14–16], transition metal dichalcogenides [17–20], and SnS_2 [21–25], GaN [26,27], have attracted plentiful attentions duo to their novel physical and chemical properties, practical applications in nanoelectronic devices. More recently, a new-type 2D nanomaterial, arsenic monolayer (arsenene) is also attaching ever-increasing attentions because it possess some typical electronic characteristics [28–33].

Previous results have shown that gray arsenene possesses buckled and puckered honeycomb structures with two atoms per unit cell and the structure is high stabilized. Interestingly, a indirect-to-direct band gap transition occurs in the arsenene nanosheets when slight biaxial strain is applied [29,30], which can be used as a precursor for mechanical sensors and optoelectronic devices. More recently, research groups investigated theoretically the electronic band structures of bilayer arsenene [31]. The exciton states and carrier mobility of arsenene have also been studied theoretically [32]. In addition, the electronic structures of hydrogenated arsenenes have also been studied [33]. All these studies show that arsenene can be a new promising 2D semiconductor materials for the applications in the optoelectronic devices.

However, as we all know, there are few studies involved on the studies of arsenene nanoribbons. More recently, Wang et al.'s results demonstrated that AsNRs still retain semiconducting properties, which is not relevant to edge type [34]. In this work, we focus on the electric field effects on the electronic structures of arsenene nanoribbons (AsNRs). Our results show that the band structures and band gap can be tuned effectively by the applied electric field. Moreover, the effects of electric field have more obvious influences on the larger size nanoribbons. We expect that these results are useful to understand the underlying physical mechanism of AsNRs and related device applications.

2. Computational methods

In this work, all the geometric optimization and electronic structure calculations are carried out using the Atomistix ToolKit (ATK) software package [35], which is based on density-functional theory (DFT) in combination with the non-equilibrium Green's function (NEGF) [36]. During the calculations, the generalized gradient approximation (GGA) within the Perdue-Burke-Ernzerhof (PBE) [37] scheme is used with

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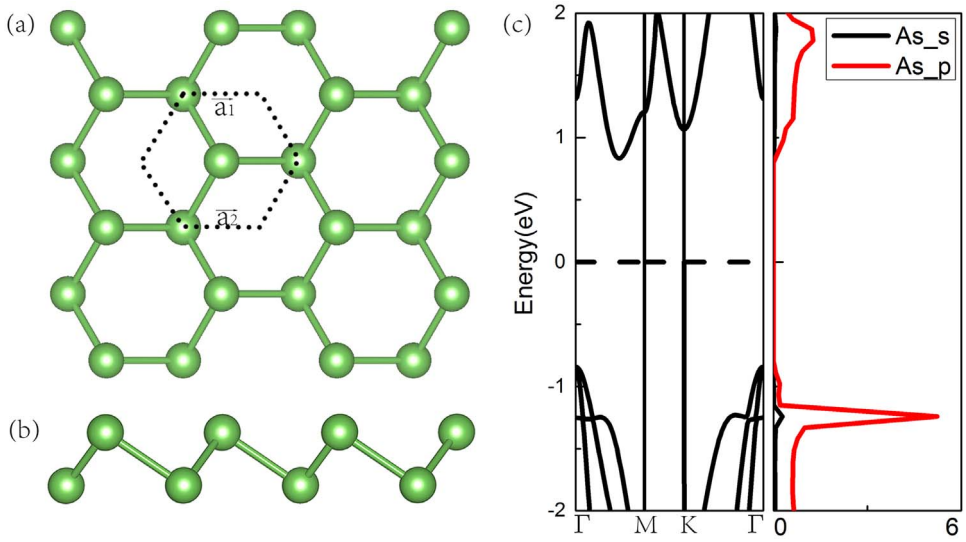

Fig. 1. The top (a), side (b) view and (c) electronic structures of pristine arsenene nanosheets.

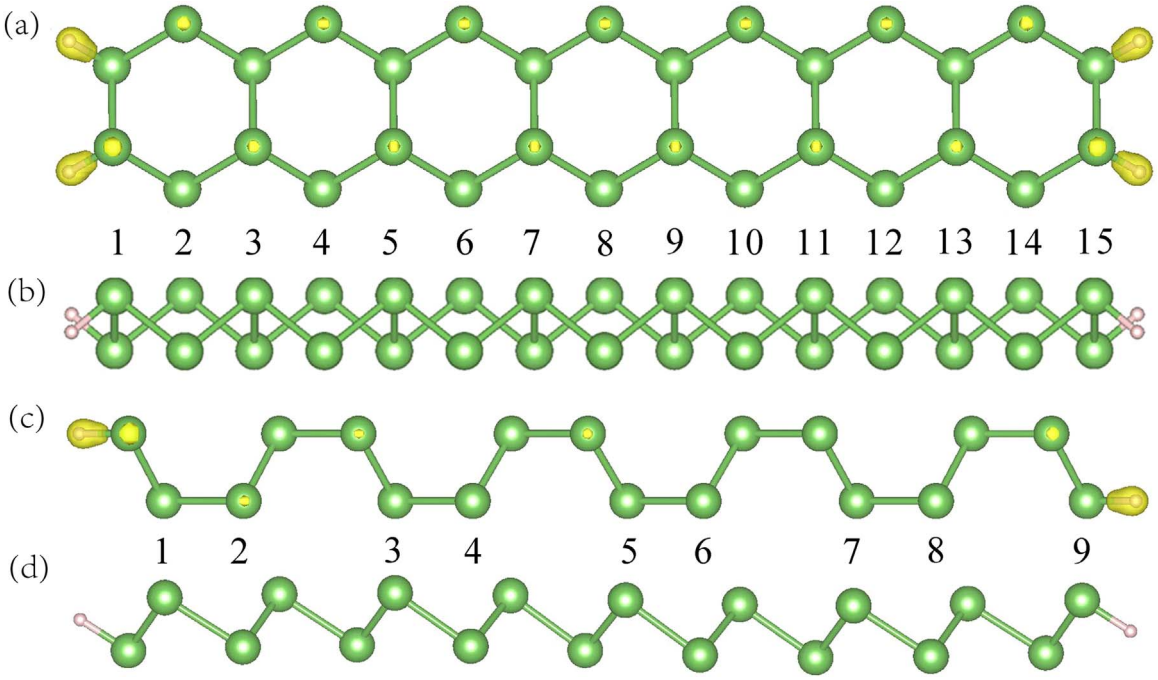

Fig. 2. The top (a) and side (b) view of A-15 A-AsNRs. The top (c) and side (d) view of Z-9 Z-AsNRs. The yellow area represents the electron density distribution, while the green and pink globules represent arsenic and hydrogen atoms, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

double-zete polarized numerical atomic-orbital basis set chose for As and H atoms. Edges of all nanoribbons are saturated with hydrogen atoms to eliminate dangling bonds. The vacuum layers of 15–20 Å are used in the non-periodic directions, which is large enough to neglect interactions with their periodic replicas. The geometries are optimized until all residual force on each atom is smaller than 0.01 eV/Å. The convergence criterion for the density matrix is chosen to be 10^{-5} eV. A cutoff energy of 180 Ry and a Monkhorst-Pack k-mesh of 1 × 1 × 15 are chosen.

3. Results and discussions

3.1. Electronic structures

To testify the accuracy of the used calculation methods, we calculate firstly the structural parameters and electronic structures of pristine arsenene nanosheets, as shown in Fig. 1. The relaxed arsenene structure has a buckled hexagonal lattice symmetry and the lattice parameters (3.608 Å). In addition, the calculated electronic structure demonstrates that

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