



# Investigation on electronic properties of functionalized arsenene nanoribbon and nanotubes: A first-principles study



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## ARTICLE INFO

### Article history:

Received 28 May 2017

In final form 20 August 2017

Available online 24 August 2017

### Keywords:

Nanoribbon

Nanotube

Arsenene

Stability

Band structure

## ABSTRACT

The electronic properties of arsenene nanotubes and nanoribbons with hydrogenation along the zigzag and armchair edges are studied using density functional theory (DFT) technique. The structural stability of hydrogenated zigzag and armchair arsenene nanostructures are confirmed with formation energy. The electronic properties of arsenene nano-conformers are described in terms of energy band structure and projected density of states spectrum. Furthermore, owing to the influence of hydrogen passivation, buckled orientation and width of arsenene nanostructures, the band gap widens in the range of 0.38–1.13 eV. The findings of the present work confirm that the electronic properties of arsenene nanomaterial, can be fine-tuned with the influence of passivation with hydrogen, zigzag or armchair border shapes and effect of the width of nanoribbons or nanotubes, which can be utilized as spintronic device and chemical sensor.

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## 1. Introduction

Like graphene, other two-dimensional materials have attracted great interest due to their chemical and physical properties, which depends on their electronic, thermal and structural properties [1–3]. In the beginning stage, graphene is found to be a good candidate for potential application in future nanoelectronic devices owing to its ultra-high charge carrier density and mobility. Even though, the lack of energy band gap obstructs its use in Boolean logic applications, which requires a high current on/off ratio. While different techniques have been reported to open the energy band gap in graphene [4], most of the works infer the complexity in the fabrication of device and opening the band gap. Owing to this reason, presently the research mainly focuses on other 2D-materials with fascinating properties. Phosphorene, a single-layer of black phosphorus (BP), have been recently initiated new possibilities. The sizable band gap of phosphorene is found to be approximately 2 eV [5] and it has high anisotropic transport [6], negative Poisson's ratio [7], high carrier mobility [8], thermo-electric and optical responses [9].

Theoretical and experimental investigations on single-layer and thin film structures of blue and black phosphorus [8] have originated the search for analogous phosphorus nanostructures and in other group-V pnictogens. Recent computational studies revealed

that phosphorus [10], nitrogen [11], bismuth [12], antimony [13] and arsenic [14] can form washboard, buckled honeycomb or single-layered structures. Preferably, arsenic, phosphorus, bismuth and antimony have stable three-dimensional layered crystallographic nanostructures, which confirm efforts to prepare very thin or mono-layer of these specified elements. These deeds prompt researchers to think whether the antimony and arsenic elements can also exhibit stable 2D nanosheets owing to their electronic configuration very similar to that of phosphorus element. The chair- and stirrup-shaped monolayer conformers of antimonene [13] and arsenene [14] are also found to be stable in structure. Like layered black-phosphorene, antimonene and arsenene also have unique properties, including ultra-high mechanical stretch ability, high carrier mobility, negative Poisson's ratio and controllable topological-phase-transition [15,16]. In contrast to high-carrier-mobility observed in 2D arsenene [15], extracting 2D antimonene and arsenene into nanoribbons would give small carrier mobilities [17]. Recently, Kamal et al. [14] reported about the first-principles study on monolayers of arsenic with buckled honeycomb structure and symmetric arsenic washboard structures, named as arsenene. They also confirmed that these single-layer conformers are more stable in structure and showed a semiconductor nature with the band gaps observed to be around 1.5–2.10 eV. At present, density functional theory (DFT) study provides a good understanding of arsenene (As) [14,18], even then the electronic properties of arsenene are still to be explored.

Arsenene a single-layer arsenic conformer was computationally reported by Kamal and Zhang et al. in the year 2015 [14,19]. It is

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more stable in two kinds of hexagonal nanostructures, the so-called puckered and buckled phases. In addition, the buckled phase hexagonal structure is slightly more stable rather than puckered phase [14]. Hsu-Sheng Tsai et al [20] synthesized arsenene nanoribbons on InAs substrate using plasma assisted technique. The authors report that the thickness of layers can be controlled by plasma exposure time. A. J. Mannix et al [21] reported about the synthesis and chemistry of elemental two-dimensional materials using physical vapor deposition (PVD), micromechanical cleavage, and chemical vapor deposition (CVD). M. Pumera and Z. Sofer [22] studied two-dimensional arsenene, antimonene and bismuthene. The authors have given detailed insights on preparatory methods, size effects, doping and device development. Xiaotian Sun et al [23] studied the structures, mobility and electronic properties of arsenene, antimonene and antimony arsenide alloy with point defects. M. Noei and A.A. Peyghan [24] have extensively studied the adsorption behavior of formaldehyde on BC<sub>2</sub>N nanotubes, synthesis of aluminium nitride nanotubes [25], adsorption of para-nitrophenol on pristine and Al-doped boron nitride (BN) sheets [26] and sensing properties of 4-chloroaniline on BN nanotubes [27]. These reports provide the possible application of nanosheets and nanotube for various applications in chemical sensors. Recent DFT studies confirmed its indirect-to-direct band gap transition under oxidation [28] and biaxial strain [14,19]. On hydrogenation [29] or by tensile strain [30], it is transformed into a quantum-spin-Hall insulator [QSHI] and interstitial or substitution doping prominently change its magnetic and electronic properties [18]. Wang and co-workers [17] observed that the band gap characteristics of arsenene were highly related to directions and edge shapes of arsenene nanoribbon. Kou et al. [31] described that the layered arsenic configuration possesses stable, low-buckled 2D nanostructure. Kecik et al [32] proposed the structural stability, electronic and mechanical properties of single and multilayered arsenene nanostructures using DFT study. In the present study, the electronic properties of functionalized buckled arsenene nanoribbon with hydrogen and for the first time functionalized arsenene nanotubes are investigated and reported.

## 2. Computational details

The first-principles calculations on bare and hydrogenated nanoribbon and nanotube form of arsenene are studied with density functional theory (DFT) method using Atomistix Toolkit (ATK) package [33], which utilizes SIESTA code [34]. For all calculations, local structural relaxation was performed with the help of DFT technique implemented by generalized gradient approximation (GGA) in combination with Perdew-Burke-Ernzerhof (PBE) exchange correlation functional in ATK package [35,36]. This exchange correlation functional is prominent for studying arsenene, which is also validated with reported work [14]. The dispersion corrected density functional theory technique demonstrated by Grimme has been utilized in order to achieve the chemical functionalization on arsenene nanoribbon by hydrogen element [37]. Preferably, a plane-wave basis set along with energy cutoff of 500 eV is used and a vacuum slab of minimum ~18 Å was taken. The hydrogenated arsenene nanoribbon and nanotube were optimized until force and energy is converged to 0.01 eV/Å and 10<sup>-6</sup> eV respectively. The Brillouin zones of arsenene are sampled with 13 × 13 × 1 Monkhorst-pack k-points with 6 × 6 × 1 super cell size of 64 atoms. The electronic band structures, electron localization function (ELF) and projected density of states of hydrogenated arsenene nanoribbon and nanotubes for zigzag and armchair conformers were calculated with SIESTA code. In the present work, double zeta polarization (DZP) basis set [38] is utilized, while relaxing arsenene nanoribbon and nanotube.

## 3. Results and discussion

### 3.1. Geometric structures of hydrogenated nanoribbon and nanotube arsenene conformers

The hydrogenated zigzag and armchair arsenene nanoribbon and nanotube possess low buckled conformers with high anisotropic corrugation, in which the adjacent row As atoms are buckled alternatively along zigzag and armchair directions respectively. We, therefore, passivated each terminated end of arsenene nanoribbon with hydrogen. The optimized buckled structure of pristine arsenene nanoribbon of armchair and zigzag conformers is shown in Fig. 1(a) & (b) respectively. In the relaxed unit cell, the calculated lattice constant  $a = b = 3.60$  Å. The As-As-As bond angle, As-As bond length and buckling height, were found to be 92.1°, 2.52 Å and 1.40 Å, respectively, which is in good agreement with reported theoretical works [14,19]. The armchair buckled arsenene conformer is analogous to silicene and blue phosphorene [39–41]. Succeeding the previous agreement of nanoribbons [42], the zigzag and armchair arsenene nanoribbons are constructed by slicing the sheets along  $\langle 2\bar{1}10 \rangle$  and  $\langle 1\bar{1}0 \rangle$  directions. In Fig. 1(c) & (d), the corresponding terminated end atoms of armchair and zigzag arsenene nanoribbons are chemically functionalized by H atoms for removing dangling bonds and reinforce the stabilities of terminated edges [43].

In order to construct the arsenene nanotube, first the above mentioned pristine arsenene nanoribbons were constructed. Next by wrapping-up the two-dimensional nanoribbon towards a chiral vector direction, the arsenene nanotubes are formed through joining its terminating edges as shown in Fig. 1(e) & (f). Furthermore, like carbon nanotube (CNT), arsenene nanotube possesses two forms of edge conformers, namely armchair and zigzag edges as shown in Fig. 1(e) & (f) respectively. From the previously reported work of silicene nanotube, the electronic properties get modified with respect to the value of chiral vector ( $n, m$ ). The main focus of the present work is to calculate the formation energy, energy band structure, projected density of states and electron density of arsenene nanoribbons and nanotubes (both zigzag and armchair) in order to study the electronic properties and structural stability of the system Co-ordinates of various arsenene nanoribbon and nanotubes are given in the [supplementary information](#).

### 3.2. Structural stability and electronic properties of arsenene nano-conformers

The structural stability of pristine arsenene nanotubes, bare and hydrogenated arsenene nanoribbons is described in terms of formation energy [44,45] as shown in Eqs. (1) & (2),

$$E_{\text{form}} = 1/n[E(\text{bare} - \text{As}) - nE(\text{As})] \quad (1)$$

(for bare arsenene nanotubes and nanoribbons)

$$E_{\text{form}} = 1/n[E(\text{H} - \text{As}) - xE(\text{As}) - yE(\text{H})] \quad (2)$$

(for hydrogenated arsenene nanoribbons)

where  $E(\text{bare-As})$  and  $E(\text{H-As})$  represent the total energy of bare and hydrogenated arsenene nano-conformers respectively.  $E(\text{As})$  and  $E(\text{H})$  refers the energy of As and H atoms respectively. 'n' is the total number of atoms in arsenene conformers, including passivated hydrogen atoms. In addition, x and y infer the number of As and H atoms respectively. In the first case, bare arsenene conformers ( $n = x$ ) and for the second case of hydrogenated arsenene nanoribbons ( $n = x + y$ ). The formation energies of arsenene nanotubes and nanoribbons are tabulated in Table 1. The formation

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