Applied Surface Science 423 (2017) 566–570

Contents lists available at ScienceDirect

Applied Surface Science

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

Arsenic carbide monolayer: First principles prediction

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ARTICLE INFO

Article history:
Received 26 March 2017
Received in revised form 25 May 2017
Accepted 13 June 2017
Available online 16 June 2017

Keywords:
First principles calculation
As_2C monolayer
Indirect band gap
Electronic properties
Optical properties

ABSTRACT

Using the first principles calculation, a new pentagonal indirect band gap semiconductor namely arsenic carbide monolayer (As_2C) is predicted. The calculated cohesive energy of −5.69 eV/atom the thermodynamic stability of the predicted monolayer. Furthermore, the kinetic stability of the monolayer is examined by phonon dispersion calculation, where the absence of imaginary modes and high value of maximum phonon frequency confirms the high dynamic stability of the proposed monolayer. Investigating in the electronic properties of the As_2C monolayer indicates that it is a semiconductor with an indirect band gap of 1.62 eV. Analyzing the optical properties of the As_2C monolayer imply that the monolayer has high UV light absorption, however, it has an almost zero absorption in visible region of electromagnetic spectra. The specific electronic and optical properties imply that As_2C monolayer may be used in new generation of nano-optoelectronic technology design.

1. Introduction

The prediction of new materials is an essential step to syntheses new materials. Since the discovery of two dimensional graphene in 2004 [1], due its unique layered structure, unique band structure, high mobility, heat conductance, and mechanical strength, much attention has been paid to investigate graphene and predict and propose new possible two dimensional structures.

By using first principles calculation, a new two dimensional carbon allotrope named penta-graphene composed of pentagon network of carbon was proposed in 2014 [2]. Followed by the prediction of penta-graphene, in recent years, a number of pentagonal two dimensional materials have been proposed [4–7].

Lopez et al. purposed a 2D pentagonal silicon carbide with unusual electronic behavior in 2015 [4]. Afterwards, Li et al. [5], computationally predicted a new stable two dimensional inorganic material called pentagonal B2C monolayer (penta-B2C). Also, a pentagonal carbon-nitride sheet with has been predicted by Zhang et al. [6], where an energy band gap of 6.53 eV was calculated for the proposed material.

On the other hand, recently, a new indirect band gap 2D material semiconductor with ultra high carrier mobility named arsenene, has been developed based on first principles calculations [8,9]. The arsenene is a monolayer of Arsenic atoms in a buckled honeycomb structure. Due to its semiconducting nature, arsenene has a good potential applications in design of transistors with high on/off ratios, blue LEDs and photodetectors [8].

Inspired by these two novel prediction, in this paper, by using density functional theory (DFT), a new buckled monolayer of As_2C is predicted. Our calculation indicates that the As_2C monolayer is thermodynamically stable. Furthermore, the kinetic stability of the monolayer is confirmed by phonon depression calculation. Investigating on the electronic properties of the predicted As_2C monolayer shows that it is semiconductor with an indirect band gap of 1.62 eV. In addition, analyzing the optical properties of the monolayer indicates that it has a good potential application in optoelectronic devices.

The rest of the paper is organized as follows. The computational details are given in Section 2. The stability and the structural properties of the proposed monolayer are discussed in Section 3. The electronic and optical properties of the predicted As_2C monolayer are discussed in Section 4. Finally, the conclusion is discussed in the last section.

2. Computational details

In the present article, for the aim of the electronic and the optical properties calculation, the density functional theory (DFT) implemented in WIEN2k code [10] is employed. The Kohn-Sham wave functions are expanded by applying the full potential linear augmented plane waves plus local orbital (FPLAPW+*lo*), and by utilizing the generalized gradient approximation presented by Perdew–Burke–Ernzerhof (GGA-PBE) [11], the exchange-correlation term is produced. Based on Monkhorst–Pack

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http://dx.doi.org/10.1016/j.apsusc.2017.06.142
0169-4332/

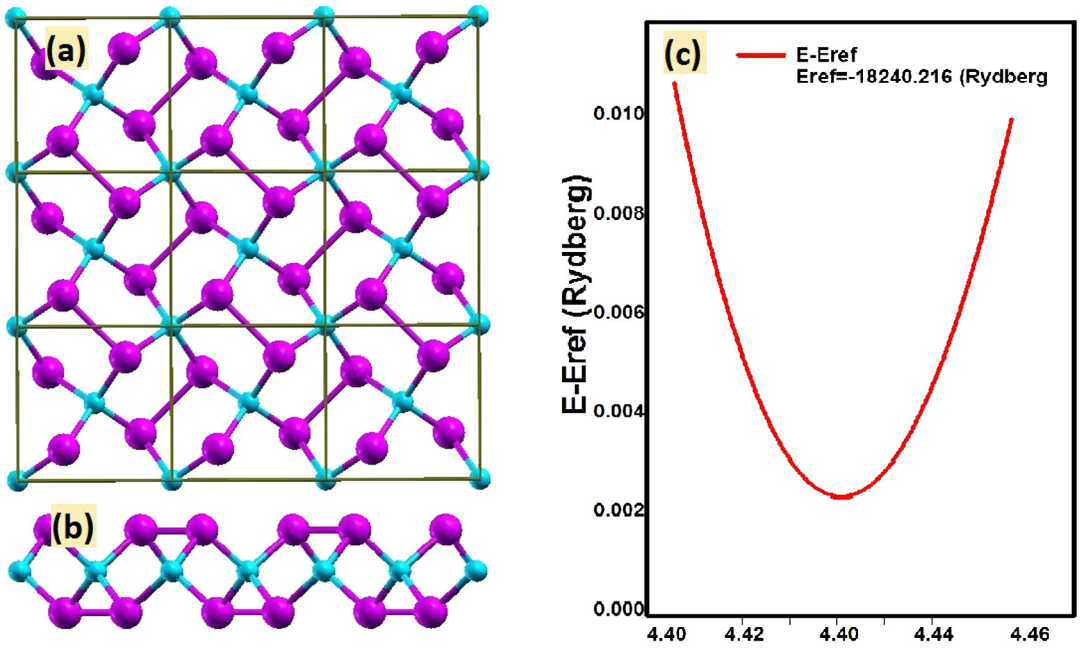

Fig. 1. (a) Top view of the As_2C monolayer. (b) Side view of the As_2C monolayer. (c) The energy vs unit cell volume of SiS_2 monolayer.

approximation [12], $10 \times 10 \times 1$ and $20 \times 20 \times 1$ k-mesh have been considered in the first Brillouin zone for electronic and optical calculations, respectively. The input parameters of $R_{MT}K_{max}$=7, G_{max}=14 $Ry^{1/2}$ and l_{max} = 10 is considered. To gain the complex dielectric function components, the random phase approximation (RPA) method and the Kramers–Kronig relations are employed [13]. Furthermore, to avoid neighboring layers interactions, a vacuum layers of 12 Å in non-periodic direction (z-axis) is considered.

3. Structural properties and stability of the As_2C monolayer

As mentioned in the introduction, inspired by the prediction of penta-graphene [2], a number of new two dimensional pentagonal compounds with the general form of X2Y was predicted. Generally, in these type of pentagonal monolayers there are four X and two Y atoms in a unit cell. The Y atom is four-coordinated with four X atoms, and the X atoms are three coordinated with two Y and one Y atoms, forming a buckled network. For penta-graphene there are four sp^3- and two sp^2-hybridyzed carbon atoms as X and Y atoms respectively. In 2016, a new two dimensional pentagonal SiC2 (penta-SiC2) has been obtained by replacing the two sp^3 carbon atoms in penta-graphene with silicon atoms and a two dimensional pentagonal SiN2 is obtained by replacing the carbon atoms in penta-SiC2 with nitrogen atoms [3]. Here we try to find an optimized structure of the possible As_2C monolayer.

To find an optimized structure, using Birch–Murnaghan [14] thermodynamical equation state of the total energy versus lattice constants of considered unit cell for a the As_2C monolayer is calculated. According to the Birch–Murnaghan equation of state:

$$E(V) = E_0 + \frac{9B_0V_0}{16}\left\{\left[\left(\frac{V_0}{V}\right)^{2/3} - 1\right]^3 B_0'\right\} + \frac{9B_0V_0}{16}\left\{\left[\left(\frac{V_0}{V}\right)^{2/3} - 1\right]^2 \left[6 - 4\left(\frac{V_0}{V}\right)^{2/3}\right]\right\}, \quad (1)$$

in which V_0 is the initial considered volume, V is the deformed volume, B_0 is the bulk modulus, and B_0' is the derivative of the bulk modulus with respect to pressure. The minimum point of the E-V curve provides the equilibrium lattice constant of the crystal cell. The total energy versus lattice constants of considered cubic unit cell for a unit cell of As_2C monolayer is plotted in Fig. 1(c). As seen in Fig. 1(c), the optimized lattice constant of $a = b = 4.42$ Å is calculated. The top view and the side view of a 3×3 supercell of the optimized As_2C monolayer is shown in Fig. 1(a) and (b) respectively. As seen in Fig. 1(a), a unit cell of the possible stable structure of As_2C monolayer is consists of four arsenic and two carbon atoms, in which each carbon atoms are bonded to four arsenic atoms and each arsenic atoms are bonded to a carbon atom and its two neighboring arsenic atoms. There are three different atomic planes, the carbon atoms are in a same plane. The arsenic atoms are buckled into two different atomic planes, 1.25 Åabove and below the carbon atomic plane respectively. The atoms form a buckled pentagon network a with a buckling thickness of about 2.5 Å. As seen in Fig. 1(a), there are two different bonds, the As—As bonds and the As—C bonds with the length of 2.65 Å and 2.02 Å respectively. Furthermore, the calculation shows that the angles of As—C—As, As—As—C and C—As—C are 112.5°, 99.98°, and 101.28° respectively.

Now, it is needed to check if the As_2C monolayer is stable or not?

To examine the thermodynamic stability of the proposed structure, the cohesive energy of the optimized cell is calculated as:

$$E_{coh} = \frac{mE_{As}^{isolated} + nE_{C}^{isolated} - E_{As_2C}^{total}}{m+n} \quad (2)$$

where $E_{As_2C}^{total}$, $E_{As}^{isolated}$ and $E_{C}^{isolated}$ are the total energy of As_2C unit cell, the energy of isolated arsenic and the energy of isolated carbon atoms, respectively. Also, m and n indexes are the number of arsenic and carbon atoms in the unit cell, respectively (here m = 4, n = 2).

By following this equation, we obtained the value of −5.69 eV/atom for the cohesive energy of As_2C monolayer, which a good confirmation of the thermodynamic stability of the monolayer. Although the relative stability of different materials with different composition or structure cannot be determined directly by the cohesive energy, the calculated value of −5.69 eV/atom is clear evidence that the proposed monolayer is strongly bonded.

Next, to evaluate the kinetic stability of the proposed monolayer, the phonon dispersion spectra is calculated by using density functional perturbation theory (DFPT) as implemented in QUANTUM