Chemical Physics Letters 708 (2018) 130–137

Contents lists available at ScienceDirect

Chemical Physics Letters

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

Research paper

Antimonene nanosheet device for detection of explosive vapors – A first-principles inspection

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HIGHLIGHTS

- The antimonene nanosheet device (AMD) is designed and used for adsorption of explosive vapors.
- The magnitude of current varies in the order of 10^{-11}–10^{-7} A upon adsorption of vapors on AMD.
- The results suggest that the distinction of four explosive vapors is possible using AMD device.

ARTICLE INFO

Keywords:
Antimonene
Nanosheet
Molecular device
Adsorption
Explosive device

ABSTRACT

The recent advances in the molecular device fabrication have outstretched the exciting applications in vapor sensing devices. This report investigates the explosive vapor detection using the antimonene molecular device (AMD) implemented with the first-principles study. The adsorption of four different explosive vapors namely hexanitrostilbene, M-dinitrobenzene, picric acid, and 2,4,6-trinitrotoluene on AMD device is examined. The adsorption configurations, charge transfer, band gap variation of antimonene nanosheet upon adsorption of explosive vapors on AMD are studied. The adsorption of vapors on AMD device is supported with the transmission spectrum and current-voltage features. Further, the results suggest that next-generation nanosensor is conceivable using antimonene nanosheets.

1. Introduction

In recent days, several two-dimensional (2D) monolayers such as graphene, graphane, silicene, germanene, and stanene are in focus among the research community [1–5]. Besides, flat graphene exhibits excellent electron mobility and allows electrons to flow freely along its surface. However, the zero band gap restricts its application to chemical and bio sensors. The recent advancement in the technology leads to the exfoliation of monolayer and few layers of group-V materials such as phospherene, arsenene, and antimonene. The exfoliation of thin layers from its bulk crystals leads to substantial changes in the band structure, which in turn results in tuning the band gap of monolayer materials [6]. The 2D Sb monolayer, antimonene, possesses a semiconducting property. The free-standing α and β antimonene allotropes are geometrically stable. The α-antimonene has puckered structure, whereas β-antiomene owns the buckled hexagonal structure [7]. The literature report shows that antimonene has the indirect band gap of 2.28 eV [8]. The fascinating properties of antimonene include high thermal conductivity, strain induced band shift, excellent carrier mobility and favorable spintronic properties [9]. Moreover, under the influence of biaxial strain, antimonene gets converted from indirect to direct band gap semiconductor [6]. In addition, antimonene holds large on-site spin-orbit coupling [10]. These unique properties of antimonene lead to number of applications such as optics, chemical sensors and electronic devices [11]. Zeng group have extensively studied the electronic properties of arsenene and antimonene, which opens the path for their application in the nanoelectronic device and chemical sensors [12,13]. Ji group [14] synthesized 2D antimonene single crystals grown by van der Waals epitaxy. The authors synthesized few layer antimonene polygons through van der Waals epitaxy. Mao et al. [15] synthesized antimonene grown on Ag (1 1 1) via molecular beam epitaxy. The authors reported that Sb deposited on $AgSb_2$ surface alloy results to the formation of antimonene with the buckled honeycomb structure. Xie et al. [16] reported that van der Waals bilayer antimonene as excellent thermophotovoltaic cell. The authors achieved the radiation-to-electricity efficiency of 31%. Wang et al. [17] theoretically studied the various allotropes of antimonene namely α, β, γ and δ forms with its structural parameters and properties.

Recently, security concern is a critical issue owing to the advances in explosives, and its trafficking requires rapid detection of explosives

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https://doi.org/10.1016/j.cplett.2018.08.016
Received 30 May 2018; Accepted 6 August 2018
Available online 06 August 2018

effectively to detect its presence. Moreover, solid state chemical sensors play an essential role in the detection mechanism of explosive vapors. Besides, the older methods of explosive detection include spectroscopic techniques, electrochemical sensors, olfactory type sensors, luminescence sensors [18]. The challenging task is in finding the unexploded ordinance including the traditional explosive materials such as trinitro toluene, the chemical used in improvised explosive devices (IEDs) such as ammonium nitrate. Furthermore, the vapors emanating from the bulk explosives in the trace level indirectly infers us the possible presence. Hence, it is crucial to detect the trace level of vapors evolved from the explosive material. Nevertheless, the advancement in the chemical sensors leads to the improvement of the existing techniques and results in the development of novel sensors. Traditionally metal oxide based chemical sensors are used to detect the presence of explosive volatiles [19]. Lefferts and Castell [20] detailed regarding the vapor sensing mechanism of explosive materials. The authors extensively described the traditional methods and new sensing methods, which involve nanomaterials, microcantilevers, and polymer materials. Nowadays the advancement in the low-dimensional materials especially 2D materials opened the inroads for its possible application in explosive detection. In that direction, the present work leaves its footprint in the development of chemical sensor based on 2D group-V monolayer material, antimonene. The novel prospect of the present work is to study the adsorption behavior of explosive volatiles on to antimonene nanosheet, which is used as the base material for explosive detection.

2. Computational details

In this report, the adsorption behavior of explosive vapors are investigated using the antimonene nanosheet, The density functional theory (DFT) based simulations in combination with non-equilibrium Green's function (NEGF) method is implemented using the SIESTA package [21]. The generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof (PBE) and the Troullier-Martins pseudopotentials are used in the calculations [22–24]. In order to take into count the weak dispersive interactions, the van der Waals corrections along with GGA-PBE are implemented [25,26]. The double-ζ with polarization basis set (DZP) is adopted for expanding the Kohn-Sham states [27,28]. Moreover, the chosen basis set and exchange-correlation functional are proven effective for studying similar systems [29,30]. Besides, the energy shift of 0.01 Ry with 15 × 15 × 1 k-points using Monkhorst-pack scheme is used [31]. Further, the complete geometrical optimization was carried out with conjugate gradient (CG) algorithm until the Hellmann–Feynman force was converged to 0.01 eV/Å. The TranSiesta code is used to study the electronic transport calculation for antimonene device. The basic idea behind the quantum transport computations is to split the antimonene nanosheet into three regions namely two probes and scattering region. The quantum transport calculations for antimonene nanosheet in this work are adopted as reported by Amorim and Scheicher [32] group.

3. Results and discussion

3.1. Structural details of antimonene sheet molecular device

The antimonene nanosheet exhibits low buckled nanostructures with anisotropic corrugation, in that the adjacent row antimony atoms are crumpled successively through zigzag direction. We thus performed the passivation of hydrogen element at the terminated end of antimonene nanosheet. The relaxed buckled structure of pristine antimonene nanosheet is shown in Fig. 1. The lattice constant for the fully relaxed unit cell is found to be a = b = 4.12 Å. The bond length and buckled height amongst antimony atoms in the proposed structure is found to be 2.89 Å and 1.50 Å, respectively, which is validated with already reported work [33]. The monolayer antimonene nanosheets

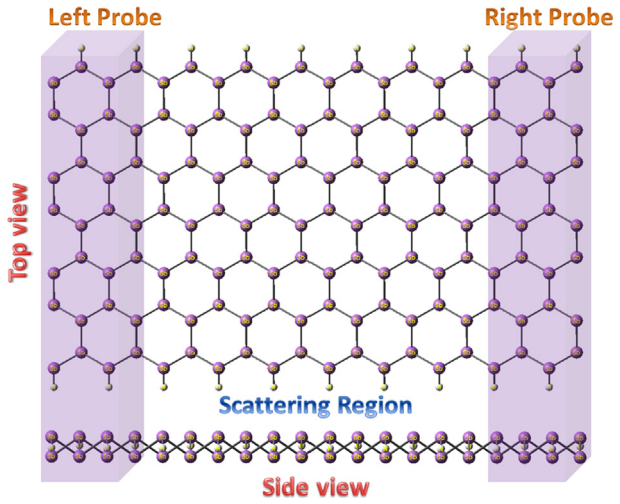

Fig. 1. Pictorial representation of antimonene molecular device (AMD).

consist of a thin hexagonal layer of Sb atoms, which has a super cell size of 10 × 10 [34]. Further, the emergence of nanoelectronics utilizing the monolayer materials opens the gate for the design and development of the molecular device. The size of the scattering and electrode region is in the order of nanometric regime, which is sufficient for the vapor molecules to get adsorbed/desorbed during the sensing process. The pictorial representation of isolated antimonene nanosheet molecular device (AMD) with the left and right leads along with the scattering region is shown in Fig. 1. First of all, the stability of antimonene sheet should be ensured, which is facilitated with the formation energy [35,36].

The calculated formation energy of antimonene is found to be −4.157 eV that is calculated from the following equation,

$$\mathbf{E_f = (1/n)[E(SbNS) - nE(Sb)]}$$

where 'n' is the number of antimony atoms in the nanosheet, E(SbNS) is the energy of antimonene nanosheet and E(Sb) is the energy of bulk antimony. Since the formation energy is found to be −4.157 eV, the negative magnitude ensures the stable structure. Now turning the attention towards the electronic properties of antimonene nanosheet, the energy band gap is found to be 1.28 eV as depicted in Fig. 2, showing the semiconductor property.

Also, peaks are noticed along the conduction band in the energy interval of 1–3 eV. Moreover, the semiconductor nature and the availability of free electrons in the conduction band infer the antimonene nanosheet is a suitable candidate for the chemical sensor [37,38]. As mentioned earlier, the AMD comprises of left, right leads with scattering region. The scattering region of AMD is exposed to the explosive vapors, which in turn changes the transport properties of AMD, indicating the presence of explosive vapors. Moreover, the explosive vapors such as hexanitrostilbene, M-dinitrobenzene, picric acid and 2,4,6-trinitrotoluene evolved from the explosive are studied through the adsorption on to AMD device. The adsorption of hexanitrostilbene, M-dinitrobenzene, picric acid and 2,4,6-trinitrotoluene on AMD device is named as E1, E2, E3 and E4 positions, respectively. Fig. 3a–d represents the adsorption positions E1–E4 of vapors on to AMD device. The interaction sites of positions above are the global minima (GM) positions, which refer the highly reactive sites. At the starting stage, various possible orientation (complex) of explosive vapors on AMD including perpendicular to the hexagonal ring, normal to the Sb-atom and bridge sites are simulated and based on the lowest energy, the GM interaction sites are reserved for discussion, and the remaining other adsorption sites are ignored. The interaction sites of explosive vapors on AMD are identified as performed and reported by Ralph H Scheicher group [39,40].