Physica E: Low-dimensional Systems and Nanostructures 105 (2019) 146–150

Contents lists available at ScienceDirect

Physica E: Low-dimensional Systems and Nanostructures

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

Adsorption of ozone gas molecule on armchair phosphorene nanoribbons with different edge passivation types

Zahra Teymoori[a], Somayeh Fotoohi[a,*], Mansoureh Pashangpour[b]

[a] Department of Electrical Engineering, Islamshahr Branch, Islamic Azad University, Islamshahr, Iran
[b] Department of Science, Islamshahr Branch, Islamic Azad University, Islamshahr, Iran

ARTICLE INFO

Keywords:
Non-equilibrium Green's function
Density functional theory
Armchair phosphorene nanoribbons
Sensitivity

ABSTRACT

The effects of ozone (O_3) gas molecule adsorption on the electronic structures and transport properties of armchair phosphorene nanoribbons (APNRs) with different edge passivation types (H, Cl, F) as well as unpassivated APNR are investigated by density functional theory (DFT) combined with non-equilibrium Green's function (NEGF) method. Our results show that the adsorption of O_3 on APNRs with different edge passivation induces sensible changes to electronic properties. Besides, the systems exhibit p-type semiconducting behavior after O_3 adsorption. Moreover, Cl-passivated APNR shows the highest adsorption energy with O_3 molecule. Furthermore, the sensitivity of APNRs is determined by electrical conductivity changes after the adsorption. The results reveal that maximum sensitivities are 81.39%, 55.87% and 56.40% for H, Cl and F-passivated APNRs at bais voltage of 2 V, respectively. It is obtained 35% for unpassivated APNR at bais voltage of 1.2 V. Therefore, this newly developed passivated APNR would be an excellent candidate for sensing O_3 gas.

1. Introduction

Two dimensional materials (2D) such as graphene [1–3], graphyne [4,5], g-C_3N_4 [6], MoS_2 [7], antimonene [8,9], etc. have attracted enormous attention. The properties of 2D materials can be tuned by several feasible methods such as doping [8], edge modification [10], defect [8] and strain [6,9,11]. Besides, the external electric field could tailor the electronic properties of nano structures for multiple applications. Recently, Li et al. have investigated the interaction of CO gas on different types of antimonene using first-principles calculations. The results show that the collection and storage of CO gas can be controlled by external electric field [8].

2D materials are appropriate for sensor applications because of their high surface-to-volume ratio and porous surfaces which makes them suitable for gas molecules adsorption. The main sensing mechanism in nano devices relies on change in electrical conductivity due to their interaction with the adsorbed molecules. That originates from the induced charge transfer between the adsorbed molecules and substrate [12].

Phosphorene, a distinctive 2D material, has attracted much attention because of its excellent properties such as high charge carrier mobility around 1000 cm^2/V [10,13–15], on/off ratio up to 10^4 [16,17], transport anisotropy and linear dichroism [18]. Unlike the zero-bandgap graphene, phosphorene has a direct bandgap [19] ranged from about 0.3 eV (multilayer phosphorus) to 1.5 eV (mono-layer phosphorene) [20]. The results exhibit anisotropic optical, mechanical and electronic transport properties because of its puckered geometry [21]. Similar graphene, phosphorene can be patterned into narrow ribbons that its charge carriers become confined in one-dimensional systems, known as phosphorene nanoribbons (PNRs). PNRs have many specific properties similar to graphene nanoribbons [1,2]. For PNRs, the energy gap depends on the widths and the edges' configuration of the ribbons. The number of P-P dimers perpendicular to the ribbon length defines the ribbon width.

Alike to graphene, PNRs are classified as either armchair PNRs (APNRs) or zigzag PNRs (ZPNRs) [20,21] depending on their edge orientation.

Xie et al. have investigated the electronic transport properties of PNRs by DFT calculation combined with NEGF method. The results show the edge shape and edge defects can affect the electronic transport properties of PNRs [20].

Guo et al. have studied the electronic and transport properties of C, Si, Ge-doped APNRs by employing first-principles calculations. The results indicate that C, Si, Ge dopants can induce the transition occur from semiconductor to metal in the APNRs [22].

Peng et al. have investigated different edge functionalization groups such as H, F, Cl, OH, O, S, and Se, in addition to a pristine case for a series of ribbon widths up to 3.5 nm. It was found that the APNRs are

* Corresponding author.
E-mail address: s.fotoohi@iiau.ac.ir (S. Fotoohi).

https://doi.org/10.1016/j.physe.2018.09.009
Received 25 March 2018; Received in revised form 30 July 2018; Accepted 11 September 2018

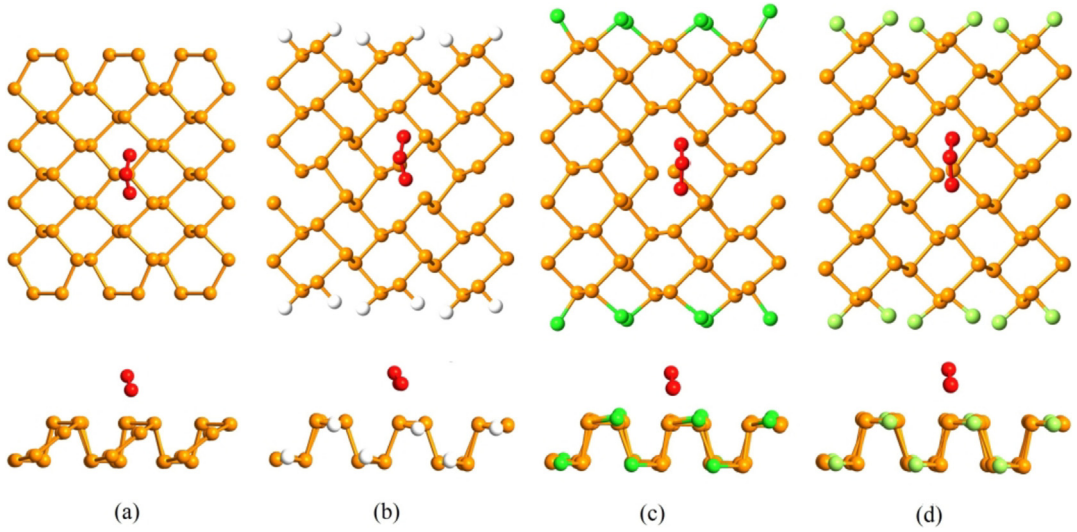

Fig. 1. Top views and side views of the adsorption of O_3 on (a) unpassivated APNR, (b) H-passivated APNR, (c) Cl-passivated APNR and (d) F-passivated APNR after relaxation.

semiconductors for all edge groups considered in this work. However, the ZPNRs have either semiconductor or metallic behavior in dependence on their edge chemical types [10].

Adsorption of various chemical types on phosphorene has been investigated using the experimental [23] and ab initio [24,25] methods including density functional theory. Kou et al. have studied the adsorption of CO, CO_2, NH_3, NO and NO_2 gas molecules on a mono-layer phosphorene. Transport calculations indicate that the gas molecule adsorption on phosphorene can either decrease or increase the current, hence changing the resistance can be directly observed in experiment [26].

Ozone (O_3) is a pale blue gas with a distinctively pungent smell. This chemical needs to be consistently monitored since its toxicity. Incidence of asthma, a decreased lung function growth, lung cancer and mortality are important effects of O_3 on human health. Therefore, monitoring of O_3 concentration in the environment and the development of O_3 gas sensor are very important.

Theoretical studies of O_3 interaction with carbon nanotubes (CNT) show that the binding energy of ozone on CNT is 0.2–0.3 eV depending on the diameter and chirality [27].

So far, the interaction of ozone with APNRs has not been reported theoretically. So, in this paper, we investigate ozone adsorption effects on the electronic and transport properties of 9-APNRs (9 refers to the number of dimer lines along their width) with different edge passivation types including of H, Cl and F atoms as well as unpassivated 9-APNR.

The organization of this paper is as follows: computational methods are presented in section 2. In this section, density functional theory (DFT) calculations within generalized gradient approximation (GGA) combined with non-equilibrium Green's function (NEGF) method are used to study electronic and transport properties of passivated and unpassivated 9-APNRs before and after ozone adsorption. In section 3, the results of simulation are presented and compared. The results show that H-passivated APNR is more sensitive to ozone adsorption than the other structures. The consequences of this work can provide helpful information to make a device which is sensitive ozone molecule adsorption.

2. Computational methods

Ab-initio calculations have been performed by SIESTA package [28] that uses numerical atomic orbitals as the basis sets and Troullier-Martin type [29] norm-conserving pseudopotentials. The exchange-correlation functional of the generalized gradient approximation (GGA) is represented by the Perdew-Burke-Ernzerhof approximation [30]. Each basis set is assumed to be double-ζ polarized. Self-consistent calculations are performed with a mixing rate of 0.01 and the convergence criterion for the density matrix is taken to be 10^{-4}. The cutoff energy is 500 eV, a $1 \times 1 \times 30$ Monkhorst-Pack grid is used for the integration of the Brillouin zone and a Gaussian smearing with a width of 0.03 eV is used in the calculations. In our simulations, an orthorhombic supercell with 9 dimers in width direction is considered. Generally, periodic boundary condition should be used in order to define APNR in SIESTA package along the ribbon length (i.e., z-direction). We have considered a large vacuum to eliminate interaction between the mirror images in other two directions the neighboring APNR in x- and y-direction. Hellmann–Feynman force tolerance is chosen to be smaller than 0.02 eV/Å for each atom after full relaxation of all structures.

Band structure, projected density of states (PDOS) and density of states (DOS) have been calculated within DFT [31] framework for investigation of electronic properties. Quantum conductance and current-voltage characteristic have been studied for transport properties by NEGF technique [32] based on DFT as implemented in the TranSIESTA module within the SIESTA package.

The ability to simulate open boundary conditions for a two-probe system at different potentials is provided in the TranSIESTA module. The current through the central region is evaluated by the Lundauer-Büttiker formula [32]:

$$I(V_b) = G_0 \int_{\mu_R}^{\mu_L} T(E, V_b) dE \quad (1)$$

where μ_L and μ_R are the electrochemical potentials in left and right leads connected to both sides of the conductor, related through the externally applied bias ($V_b = (\mu_L - \mu_R)/e$), $G_0 = 2e^2/h$ is the minimum quantum conductance and $T(E, V_b)$ is the transmission function determined by the probability that an electron with energy E is injected from one side of the conductor, transmitting to the other side under the bias V_b.

3. Results and discussion

There are different possible adsorption positions of O_3 molecule on the APNRs surfaces with various edge types. To find the most stable position of the molecule in each simulated system, the whole systems is fully relaxed for each possible case and get their total energies. Fig. 1