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# Atomistic quantum transport simulation of multilayer phosphorene nanoribbon field effect transistors

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ABSTRACT

Few-layer black phosphorus is a semiconductor material, where its allotrope is called phosphorene; a new two-dimensional material which is discovered in 2014. In this paper, first we use the tight-binding method to implement a matrix representation for single-layer and multilayer structures of phosphorene nanoribbon (PNR) to define the Hamiltonian of the system. Second, we investigate the band structure and the band gap of multilayer PNRs. The band gap of armchair PNRs with 16 atoms across the width of PNR for single-layer, bilayer, and three-layer structures are obtained as 1.899, 1.224, and 0.937 eV, respectively. Third, we use the atomistic description of structure to simulate the performance characteristics of single and multilayer PNR field effect transistors (PNRFETs) by employing the non-equilibrium Green's function (NEGF) formalism. Based on the properties of the material and device structures, $I_d$-$V_{gs}$, $I_d$-$V_{ds}$ characteristics, energy band diagram in the channel, and $I_{ON}/I_{OFF}$ are analyzed. The ON to OFF current ratio for single-layer, bilayer, and three-layer PNRFETs are increasing when the channel length increases from 5 nm to 15 nm. The current ratio for single-layer increases from 1277 for $L_{ch}$=5 nm to $216.7\times10^6$ for $L_{ch}$=15 nm. The $I_{ON}/I_{OFF}$ in single-layer PNRFET is higher in comparison with those values in bilayer and three-layer PNRFETs due to very small off-current in the single-layer PNRFET which in turn resulted from its larger band gap. The results show that the performance of PNRFET changes significantly depending on the number of phosphorene layers and the length of the channel of device.

## 1. Introduction

Since 2004, a number of two-dimensional (2D) materials have been discovered such as Graphene, Molybdenum Disulphide ($MoS_2$), Arsenene, and Black Phosphorus (BP). Graphene as a 2D sheet of carbon atoms with thickness of only one atom was the first 2D material discovered in 2004, which has attracted a great attention in the semiconductor industry, particularly in electronic devices, interconnects, and energy storage [1–5]. The main issue for graphene is its lack of energy bandgap which, limits its application as a material for electronic devices such as field effect transistors (FETs), because graphene devices cannot be turned OFF completely. BP in its layered form which is named "*phosphorene*", is a 2D semiconductor material discovered in 2014. It shows interesting electronic, semiconducting and optical properties [6–9]. Phosphorene, like graphene, can be produced as thin as one single atomic layer. In fact, BP bulk crystal is composed of many individual layers stacked up over together by van der Waals force; however, unlike graphene layers which are perfectly flat, phosphorene layers form a puckered surface due to the $sp^3$ hybridization [10].

The phosphorene nanoribbons (PNRs) can be obtained by cutting a single-layer phosphorene along its armchair or zigzag directions in the same way as the graphene nanoribbon (GNR) is produced. Therefore, the armchair PNRs (A-PNRs) or zigzag PNRs (Z-PNRs) can be identified by the number of dimer lines or the zigzag chains across the ribbon width, respectively [8]. Both A-PNRs and Z-PNRs have positive and much smaller formation energies compared to the GNRs, which means that the experimental synthesis of PNRs is fully accessible [11]. According to the research history of the previous 2D materials such as graphene and $MoS_2$, the theoretical and simulation research studies of PNRs are necessary for future experimental works. Edge disorder is a problem in GNRs and therefore, patterning will be

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relatively difficult due to significant changes in the band gap of GNRs by different numbers of atoms across its widths, especially in narrower GNRs [12]. However, it should be mentioned that recently a group of scientists found a way to yield atomically precise zigzag graphene nanoribbon edges [13]. The band gap of GNR changes significantly by changing the number of carbon atoms within the width of ribbon, however by changing the number of phosphorous atoms within the width of the ribbon, the variation of band gap of PNR becomes very small and thus negligible. This makes the fabrication of PNRs more convenient [14–19].

Theoretical and experimental studies have been carried out on few-layer phosphorene transistors. Various articles on phosphorene have been published since Liu et al. discovered phosphorene as a new 2D semiconductor material in 2014 [7,9,20–23]. For example, doped contact multilayer (ML) phosphorene FETs are simulated by self-consistently solving the 2D Poisson's equation and Schrodinger's equation based on NEGF in mode space [23]. FETs which use phosphorene as the channel material with a thickness of a few nanometers (meaning a few layers of phosphorene) were fabricated [7,20,24,25]; however, in most of these experimental research articles, Schottky barriers junctions are used as the source and drain contacts [7,9,20,26]. Multilayer Schottky barrier phosphorene FETs are also simulated using NEGF and 2D Poisson's equation based on atomistic structure of the channel calculated from the k.p model with a band gap of 1.52 eV. The results show ambipolar behavior with a high leakage current in multilayers that can be reduced by several orders of magnitude in single- and bilayer phosphorene FETs [22]. The effect of layer stacking orders (similar to layer stacking of AA, AB, and AC in GNR) of bilayer black phosphorene on the device properties of MOSFETs create possible chances to immunize FETs against short channel effects [27]. Single-layer BP FETs outperform both $MoS_2$ and SiFETs, either n- or p-type devices, due to higher carrier velocity in the armchair direction [21]. Wan et al. simulated single-layer phosphorene tunneling FETs (TFETs) via a self-consistent atomistic quantum transport based on the recursive scattering matrix approach using the density functional theory (DFT), where the band structure calculation resulted in a 0.93 eV band gap [22]. The proposed TFET exhibits a subthreshold slope (SS) below 60 mV/dec. Their results show that the on-current, $I_{ON}$, is dependent on the transport direction due to highly anisotropic band structure of phosphorene [19]. It also shows $I_{ON}$ three orders of magnitude larger at the same $I_{ON}/I_{OFF}$ ratio compared to that of the single-layer $MoTe_2$ TFETs, where it suggests superiority of phosphorene for TFETs application [19].

Cao et al. demonstrated that single-layer phosphorene FETs are promising candidates for the International Technology Roadmap for Semiconductors (ITRS) for the 2024 horizon [23]. Authors used the old version of tight-binding parameters which resulted in a band gap energy of 1.6 eV [23]. Another way to define the Hamiltonian of the system is to use the k.p method [22,23]. However, the k.p method is based on the effective mass approximation whose applicability is not well justified for BP and its Hamiltonian is not well suited for studying real space problems even in the low-energy range [28]. The tight-binding method [29] shows fairly accurate energy band structures for phosphorene materials compared to the results based on the k.p method. More importantly, the results from tight-binding method are comparable to the first-principle calculations based on the DFT approach, especially in the low energy regime. Thus, we use the new tight-binding parameters to determine the Hamiltonian of the system. The parameters of tight-binding model for BP with an arbitrary number of layers were derived from partially self-consistent GW0 approach and presented for the first time by Rudenko et al. [28,30].

To the best of our knowledge, there is no quantum transport simulation study on SL- and ML-PNRFETs that uses NEGF with new TB parameters in literature so far. Our paper overcomes this limitation by utilizing new tight-binding parameters to form a matrix representation for single-layer and multilayer PNR structures. The defined matrix representation is used in the quantum transport simulation of PNRFETs using the NEGF formalism and 2D Poisson's equation [31,32]. We explore the A-PNRs because of anisotropic properties of band structure of phosphorene, which enable electrons to travel faster in the direction of the armchair. This suggests that the armchair direction in the 2D plane has the highest carrier mobility [17,22].

## 2. Theoretical method

In this section, we have presented realistic matrix representations of SL- and ML-PNRs. The modified tight-binding parameters are introduced and used to simulate the PNR FETs based on the non-equilibrium Green's function formalism. Fig. 1 shows the view, the hopping parameter and the ball-stick model of the atomic structure of multilayer black phosphorus. In order to implement the tight-binding method, we use the atomic structure of (SL) layer phosphorene as shown in Fig. 1(c). We supply all the model definitions in order to construct the Hamiltonian of the system for both the band structure calculation and the device simulation. The unit cell of phosphorene is composed of four atoms named as $P_1$-$P_4$ as shown in Fig. 1(c). The basis vectors are $a_1$ and $a_2$ along the armchair and zigzag directions, respectively. The length of $a_1$ and $a_2$ are 4.43 A° and 3.27 A°, respectively [6]. In order to have a direct bandgap material, we add hydrogen atoms to passivate the edge phosphorus atoms as shown in Fig. 1(c) [8].

In our previous paper, we used the simple five-element TB parameters to investigate the electronic properties of phosphorene nanoribbons under the external modulated electric fields [16]. However, in this work, we apply the new ten-element TB parameters to determine the Hamiltonian of an A-PNR-FET for implementation of the quantum transport method in the NEGF formalism. The proposed matrix representation of phosphorene structures can be applied to all SL- and ML-PNRs with an even number of phosphorus atoms in the width of the layer. The tight-binding model of phosphorene is given by the effective four-band Hamiltonian, considering one electron per lattice site. The tight-binding formula for SL- and ML- phosphorene materials is defined as follows [28]:

$$H = \sum_{i \neq j} t_{ij}^{\parallel} c_i^{\dagger} c_j + \sum_{i \neq j} t_{ij}^{\perp} c_i^{\dagger} c_j \tag{1}$$

Where i and j run over the lattice sites, $t^{||}$ ($t^{\perp}$) is the inlayer (interlayer) hopping parameter between the sites i and j, and $c_i^{\dagger}$ ($c_j$) is the creation (annihilation) operator of electrons at site i (j). The first term stands for the inlayer interactions between phosphorus atoms, and the second term describes the interactions between atoms belonging to different layers. We note that the Hamiltonian given by (Eq. (1)) does not contain on-site terms, meaning that electrons have equivalent energies at all the sites.

First, we define a unit cell including four phosphorus atoms as shown in Fig. 1(c). The 4-atom unit cell is distributed in the transverse direction ($y$-direction) to make a large unit cell which makes the width of the ribbon. Then, we distribute the new large unit cell along the transport direction (x-direction) in order to construct the full Hamiltonian matrix, H, of the A-PNR structure. The new tight-binding parameters for inlayer and interlayer interactions in phosphorene multilayer structures are introduced in Fig. 1(b) and the values are given in Table 1 [28].

Using the phosphorene structure and the unit cells shown in Fig. 1(c), we have the Hamiltonian matrix $\alpha_u$ for each individual unit cell as follows: