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Electronic properties of phosphorene and graphene nanoribbons with edge vacancies in magnetic field

J. Smotlacha^{a,b,*}, R. Pincak^{a,c}

^a Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, 141980 Dubna, Moscow region, Russia

^b Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University, Břehova 7, 110 00 Prague, Czech Republic

^c Institute of Experimental Physics, Slovak Academy of Sciences, Watsonova 47, 043 53 Kosice, Slovak Republic

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ABSTRACT

The graphene and phosphorene nanostructures have a big potential application in a large area of today's research in physics. However, their methods of synthesis still don't allow the production of perfect materials with an intact molecular structure. In this paper, the occurrence of atomic vacancies was considered in the edge structure of the zigzag phosphorene and graphene nanoribbons. For different concentrations of these edge vacancies, their influence on the metallic properties was investigated. The calculations were performed for different sizes of the unit cell. Furthermore, for a smaller size, the influence of a uniform magnetic field was added.

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1. Introduction

The graphene (carbon) nanostructures have been in the center of physical research for more than 10 years. In the last 5 years, the development has been enhanced with additional research on nanostructures based on phosphorus, tin, molybdenum, boron, silicon [1–4], etc. In this paper, we will be concerned with the electronic properties of the carbon and phosphorus nanostructures.

There is a basic difference between the nanostructures based on carbon and phosphorus: they are sp^2 - and sp^3 -hybridized, respectively. As a result, the smooth graphene hexagonal structure is not present in phosphorene, although it is composed of the hexagons as well. Furthermore, phosphorene can exist in 2 configurations: the black phosphorene created by an anisotropic puckered honeycomb lattice and the blue phosphorene. If nothing different follows from the context, the term “phosphorene” will usually denote “black phosphorene” here. It has the most stable crystal structure among several allotropes of phosphorus. Both large-area graphene and phosphorene are sketched in Fig. 1.

The phosphorene nanostructures are characterized by their energy band gap and high hole mobility [5]. The applicability of the black phosphorene as a field effect transistor (FET) is much more significant than that of graphene. On the one hand, the linear

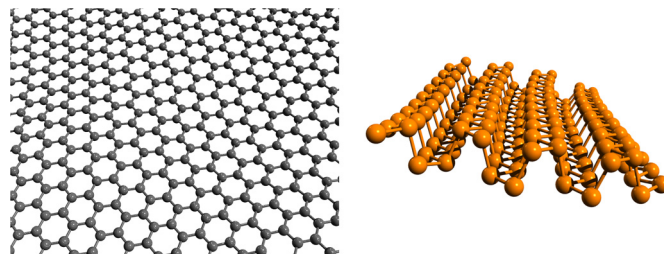


Fig. 1. Molecular structure of graphene (left) and black phosphorene (right).

dispersion in the corners of the Brillouin zone (BZ) of graphene results in the nearly relativistic velocities of the electrons (the mobility is about $10000 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ [6]). On the other hand, the lack of the band gap does not enable one to tune off the graphene channel layer in FET. For the black phosphorene, this problem is canceled, so the corresponding channel in FET can be tuned off. The structural anisotropy is present in the physical properties as well: the hole mobility in the zigzag direction is about 1.8 times higher than that in the armchair direction [7]. It is not so huge as the electron mobility in graphene, but it is still nearly relativistic in the zigzag direction: it is above $1000 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ at the temperature 120 K. Similarly to graphene, the band dispersion in the Γ -X direction of BZ is linear, unlike the parabolic band dispersion in the Γ -Y direction.

* Corresponding author.

E-mail addresses: smota@centrum.cz (J. Smotlacha), pincak@saske.sk (R. Pincak).

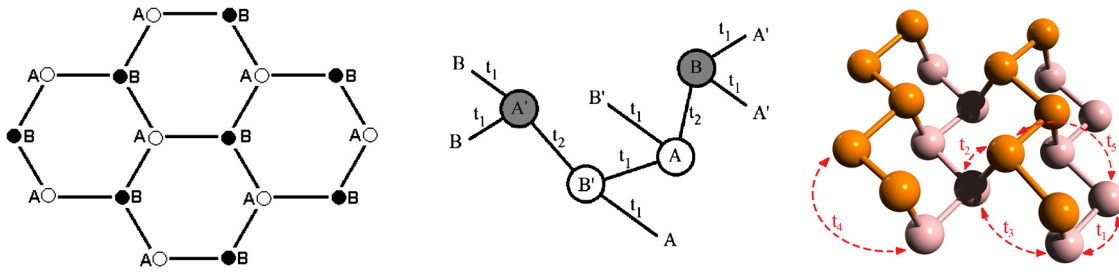


Fig. 2. Atomic sites and hopping integrals for different periodical structures: graphene (left), black phosphorene (right).

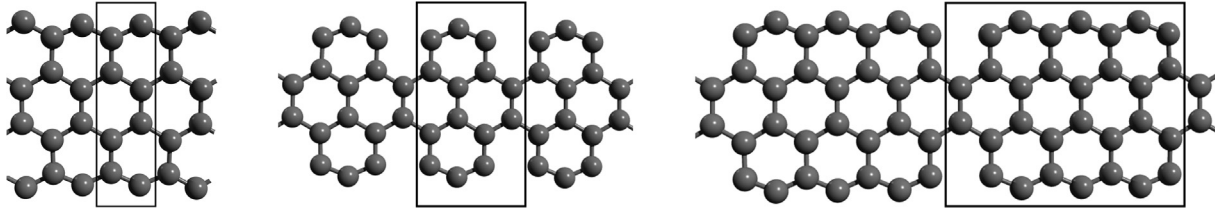


Fig. 3. Zigzag nanoribbons with different edge structures: no vacancies (left), 1 atom between 2 vacancies (middle), 3 atoms between 2 vacancies (right). The unit cells are denoted by the black frames.

The main purpose of this paper is to investigate the influence of the edge vacancies on the electronic properties of the zigzag nanoribbons, i.e., infinitely long strips of constant width that have a characteristic (zigzag) edge structure [8]. Here, they are based on the above mentioned phosphorene (zigzag phosphorene nanoribbons – ZPNR’s) and graphene (ZGNR’s). Especially, we verify the endurance of the metallic properties (typical for the zigzag nanoribbons) against the Gaussian distribution of the edge vacancies for their different concentrations. Moreover, we investigate a possible influence of the magnetic field on the metallic properties. To calculate the electronic structure, the tight-binding method is used [9–12]. Other methods based on DFT or the Green function method [11] can be used in the case of phosphorene. However, the tight-binding method is usual for the graphene-based materials [9,8] and for the inclusion of the magnetic field [13,14]. So it is sufficient for the purpose of comparing the properties of both phosphorene and graphene materials.

As mentioned above, the potential use of the black phosphorene as FET is most effective in the zigzag direction. It evokes an idea to use ZPNR’s in FET. But both ZPNR’s and ZGNR’s are metallic, so the gap for the Fermi energy is missing. However, in ZPNR’s, it can be reconstructed with the help of an external electric field [12]. In this way, the conductance is controlled by the external electric field at Fermi energy which is the transistor effect.

In this paper, after a brief description of the tight-binding method, we calculate the electronic spectrum of ZPNR’s and ZGNR’s with the atomic vacancies in the edge structure and verify the metallic properties for the Gaussian distribution of the edge vacancies and different sizes of the unit cell. Then, after comparison with the influence of the edge vacancies on the electronic structure of semi-infinite graphene, we will be concerned with the problem of how to improve the metallic properties of the zigzag nanoribbons with a smaller unit cell by the consideration of a uniform magnetic field.

2. Tight-binding method

In the tight-binding method, the calculation procedure follows from the division of the lattice into inequivalent sublattices. The sublattices are composed of the equivalent atomic sites. In the case of planar graphene or phosphorene, they are denoted by A, B or A, A', B, B' , respectively (Fig. 2). The unit cell is determined in this way – the smallest possible cell containing all the inequivalent

atomic sites. Unit cells of different structures are denoted by the black frames in Fig. 3. The interaction between the atoms is characterized by the hopping integrals – 1 for the graphene structures and 5 for the phosphorene structures [9,12]. For the graphene structures, it is $t = -2.78$ eV, and for the phosphorene structures, we have $t_1 = -1.2$ eV, $t_2 = 3.7$ eV, $t_3 = -0.205$ eV, $t_4 = -0.105$ eV, and $t_5 = -0.055$ eV.

The calculations start on the solution of the Schrödinger equation

$$\hat{H}\psi = E\psi. \tag{1}$$

This solution is expressed as the linear combination of the wave functions ψ_{A_i} , $i = 1, \dots, n$ which correspond to each of n atomic sites A_i in the unit cell. By performing some transformations, we create the matrix elements

$$H_{ab} = \int_{\mathcal{R}^3} \psi_a^* H \psi_b d\vec{r}, \quad a, b \in \{A_1, \dots, A_n\},$$

$$S = \int_{\mathcal{R}^3} \psi_{A_i}^* \psi_{A_i} d\vec{r}, \quad i = 1, \dots, n. \tag{2}$$

The resulting electronic spectrum is given by the spectrum of the corresponding matrix [9]. By using some additional assumptions [9], in the case of the nanoribbons the resulting matrix equation has the form

$$\begin{pmatrix} H_{A_1A_1} & H_{A_1A_2} & \dots & \dots & H_{A_1A_n} \\ H_{A_2A_1} & H_{A_2A_2} & \dots & \dots & H_{A_2A_n} \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ H_{A_nA_1} & H_{A_nA_2} & \dots & \dots & H_{A_nA_n} \end{pmatrix} \begin{pmatrix} C_{A_1} \\ C_{A_2} \\ \dots \\ \dots \\ C_{A_n} \end{pmatrix} = ES \begin{pmatrix} C_{A_1} \\ C_{A_2} \\ \dots \\ \dots \\ C_{A_n} \end{pmatrix}, \tag{3}$$

where $H_{A_1A_1} = \dots = H_{A_nA_n}$. In the case of ZGNR’s, the nonzero matrix elements can be written schematically as

$$H_{A_mA_n} = t\Omega_{\vec{k},m,n}^*, \tag{4}$$

where \vec{k} represents the wave vector. Then, the j -th equation of the system has the form

$$EC_j = \sum_l t\Omega_{\vec{k},j,l} C_l, \tag{5}$$

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