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Discussion

# Electric response of edge bands and their decay property of phosphorene ribbons

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ABSTRACT

Zigzag phosphorene ribbons can accommodate degenerate edge states that decay from edge to bulk. The electronic structure of phosphorene ribbons, both the bulk bands and the edge bands, can be tuned by normally applying an electric field. The electrical field enlarges the energy gap parabolically, which is a second order perturbation effect. The external field as a first order perturbation lifts the degeneration of the edge bands and changes their decay property. The localization of edge states is increased by the electric field and the decay length as a function of wavevector in the whole Brillouin zone can be obtained by measuring the electric response of the edge band extreme energies.



## 1. Introduction

Few-layered back phosphorus was exfoliated from its bulk counterpart recently [1]. Its field-effect transistors were proven to have large on-off current ratio at room temperatures [2–5]. Phosphorene, a mono-layer of back phosphorus, is a large gap material with high mobility and is regarded as a very promising monolayer material for its excellent electronic properties [6,7]. The phosphorene lattice has puckered structure, and its in-plane projection is a deformed honeycomb lattice as demonstrated in Fig. 1. First principle calculations imply that the electric structure can be well fitted by the tight-binding model with five types of hopping parameters [8,9]. The lattice structure and hopping parameters result in the band structure, collective excitations, and the optical response exhibit strong anisotropy [11–16]. Phosphorene sheet is super flexible and can sustain large strain [10]. By applying strain, the electronic structure and optic properties can be modified [17–19]. It was reported that there exist surface bands localized at edges of phosphorene ribbons [20–23]. The topologic origin of these edge bands was discussed recently by a few literatures [24,25].

Because the vertical spacing between the puckered-up and puckered-down atom sublayers, the normal applied electric field has effects on the band structure of phosphorene. In this paper, we investigated electronic structure of phosphorene ribbons under the influence of normally applied electric field using the tight-binding model. The electric field increases the band gap parabolically as a second order perturbation, but affects the edge bands of the zigzag ribbon as a first order perturbation. The electric field makes the two degenerate edge bands split and departure away from each other, changes the edge band dispersion, and decreases the decay length of edge states. The edge states at Γ point is the least localized ones, and those at the Brillouin zone corners are the most localized ones with zero decay length. By studying the response of the edge band split to the normally applied field, the decay length as a function of wavevector in the whole Brillouin zone can be obtained by measuring the extreme energies of edge bands.

## 2. Band structure of phosphorene ribbons

The in-plane parameters of phosphorene lattice are (in units of Å) $a = 0.8014$, $b_x = 1.515$, and $b_y = 1.674$, and the vertical distance between the two puckered-up and puckered-down sublayers is $l = 2.150$ [22]. The primitive translational cell is denoted by the rectangular in the figure, and its dimensions are $d_x = 2(a + b_x)$, and $d_y = 2b_y$. When the lattice is normally subjected by an electric field $\mathcal{E}$, a potential difference between the two sublayers $2\delta = e\mathcal{E}l$ is induced, where $e$ is the charge of electron. In this paper, we use $\delta$ to refer the electric field, and keep in mind that 1 eV of $\delta$ means 0.93 V/Å of $\mathcal{E}$. The tight-binding Hamiltonian reads

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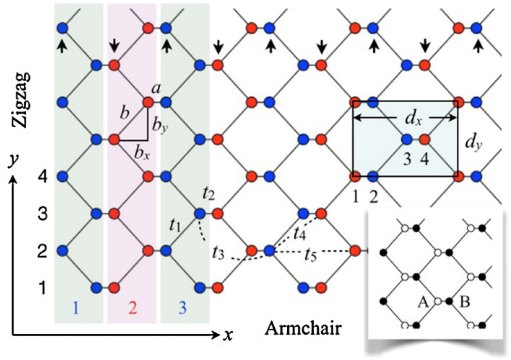


**Fig. 1.** (Color online.) Sketch of phosphorene lattice. Red- and blue-filled circles represent puckered-up and puckered-down phosphorus atoms, the rectangular shows the primitive translational cell, and the inset shows the $A$-type (empty circles) and $B$-type (filled circles) sublattice sites.

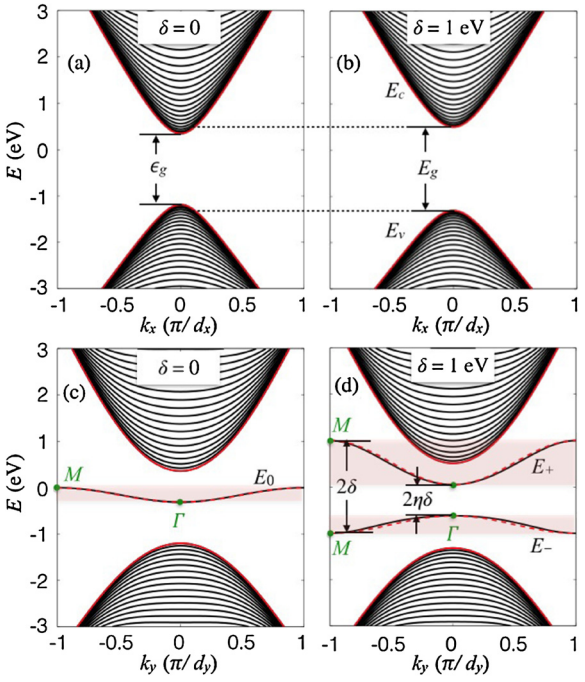


**Fig. 2.** (Color online.) Band structure of (a, b) armchair and (c, d) zigzag phosphorene ribbons of 50 lateral atoms. The atom labelling rule in armchair and zigzag directions can be found in Fig. 1.

$$H = \sum_{\langle i,j \rangle} t_{ij} c_i^+ c_j + \sum_i V_i c_i^+ c_i, \tag{1}$$

where $c_i^+(c_i)$ is the creation (annihilation) operator of electron on site $i$, $V_i$ is the on-site potential induced by the electric field, and the first summation is carried over all nonzero hoppings. The five types of nonzero hoppings, $t_1$, $t_2$, $t_3$, $t_4$, and $t_5$ (see Fig. 1), which are involved in the tight-binding model for properly describing the electronic structures, are reported to be (in units of eV) −1.220, 3.665, −0.205, −0.105 and −0.055, respectively [8]. Among them, $t_1$ and $t_2$ are the nearest-neighbor hoppings and are the largest ones in magnitude, which determine the main features of the band structure.

Fig. 2 shows the calculated band structure of armchair and zigzag ribbons without and with electric field applied. The energy gap occurs at the Γ point and becomes larger when the electric field is applied. The anisotropy between $x$-direction (armchair direction) and $y$-direction (zigzag direction) can be clearly seen. For the zigzag ribbon, there exist two cosine-like degenerate edge bands within the energy gap when no electric field applied. The degeneration is lifted by the electric field, and the two degenerated bands will departure away from each other further away when the electric field becomes larger. The two edge bands are spatially localized near the two opposite edges of the zigzag ribbon. The topologic origination of these edge bands was explained detailedly in Ref. [24] and [25] by means of winding number analysis and is not addressed here. The electric field affects the edge bands much more apparently than the bulk ones, which implies that the electric field works on the bulk and the edge bands as different order of perturbation.

The energy gap under electric field can be obtained as following. At Γ point, the $k$-space Hamiltonian in basis of $|i\rangle$ (quantum states of electron on site $i$ in the primitive cell with $i = 1, 2, 3, 4$) reads

$$h = \begin{pmatrix} \delta & c_1 & c_2 & c_3 \\ c_1 & -\delta & c_3 & c_2 \\ c_2 & c_3 & \delta & c_1 \\ c_3 & c_2 & c_1 & -\delta \end{pmatrix}. \tag{2}$$

The matrix elements $c_1$, $c_2$ and $c_3$ are defined by

$$\begin{aligned} c_1 &= t_2 + t_5, \\ c_2 &= 4t_4, \\ c_3 &= 2t_1 + 2t_3. \end{aligned} \tag{3}$$

We introduce the unitary matrix

$$U = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix} \tag{4}$$

to transform the Hamiltonian into

$$H = U^+ h U = \begin{pmatrix} \epsilon_c & 0 & 0 & \delta \\ 0 & \epsilon_v & \delta & 0 \\ 0 & \delta & \epsilon_T & 0 \\ \delta & 0 & 0 & \epsilon_B \end{pmatrix}, \tag{5}$$

where $\epsilon_c$, $\epsilon_v$, $\epsilon_T$ and $\epsilon_B$ are the energies at Γ point of conduction band, valance band, top band, and bottom band without electric field applied, respectively. The expressions of those band energies are

$$\begin{aligned} \epsilon_c &= c_2 + |c_1 + c_3|, \\ \epsilon_v &= c_2 - |c_1 + c_3|, \\ \epsilon_T &= -c_2 + |c_1 - c_3|, \\ \epsilon_B &= -c_2 - |c_1 - c_3|. \end{aligned} \tag{6}$$

The energy gap without electric field applied ($\delta = 0$) is evaluated as $\epsilon_g = \epsilon_c - \epsilon_v = 2(2t_1 + 2t_3 + t_2 + t_5) = 1.52$ eV. Eq. (5) that, at Γ point, the conduction band only couples to the bottom band, and the valence band interacts with the top band. The Hamiltonian in the equation can be decomposed into two $2 \times 2$ Hamiltonians, the band energies under the influence of electric field can be obtained analytically. After having the band energies with the electric field, we calculate the band gap as

$$E_g = 4t_1 + 4t_3 + 2\sqrt{(t_2 + t_5)^2 + \delta^2}. \tag{7}$$

The band gap as function of electric field is shown as the solid curve in Fig. 3 (a).

If $\delta$ is a small parameter, the response of the energy band to the electric field can be well understood by means of the perturbation theory. Eq. (5) is expressed in basis of the eigen states without electric field (if we set $\delta = 0$, the matrix is diagonal). Because there is no diagonal term induced by the electric field, the

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