

# Electronic structure and optic absorption of phosphorene under strain



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## HIGHLIGHTS

- Evolution of the band structure when applying strain.
- Evolution of energy gap and effective mass when applying strain.
- Strain-induced semi-Dirac band and band inversion.
- Optic absorption and its anisotropy under strain.

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## ABSTRACT

We studied the electronic structure and optic absorption of phosphorene (monolayer of black phosphorus) under strain. Strain was found to be a powerful tool for the band structure engineering. The in-plane strain in armchair or zigzag direction changes the effective mass components along both directions, while the vertical strain only has significant effect on the effective mass in the armchair direction. The band gap is narrowed by compressive in-plane strain and tensile vertical strain. Under certain strain configurations, the gap is closed and the energy band evolves to the semi-Dirac type: the dispersion is linear in the armchair direction and is gapless quadratic in the zigzag direction. The band-edge optic absorption is completely polarized along the armchair direction, and the polarization rate is reduced when the photon energy increases. Strain not only changes the absorption edge (the smallest photon energy for electron transition), but also the absorption polarization.

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## 1. Introduction

Exfoliated thin-layer black phosphorus has been realized recently [1]. Phosphorene, a monolayer of black phosphorus with a finite direct gap, is expected to be a new candidate of the family of pure two-dimensional materials. Phosphorene has attracted widespread interest due to its excellent electronic, optical and mechanical properties. Compared to graphene, phosphorene field-effect transistors have higher on-off current ratio at room temperature [2,3], which gives phosphorene a great potential for switching device fabrication. In contrast with transition metal dichalcogenides, phosphorene exhibits a higher carrier mobility [1–6]. Phosphorene has a strongly anisotropic band structure, which allows phosphorene to act as optical polarized-sensitive device [7,8]. Due to the puckering lattice structure, phosphorene possesses a superior flexibility and sustains a tensile strain up to about 30% in either the zigzag or the armchair direction and shows a great power in practical strain engineering [9,10]. By applying in-plane

or vertical strain, the energy gap can be tuned gradually [11–13], and the semiconductor-to-metal transition can be induced [9,13–15]. A considerable increase of effective mass induced by the strain suggests a great potential for switching devices [14,15]. Furthermore, strain is regarded as an efficient method to enhance the thermoelectric performance of phosphorene [16].

Most literatures about the strain effects on phosphorene are based on first-principle calculations. Numerical methods can handle the complexity of real materials while lack of clear understanding in physics. Recently, tight-binding parameters were obtained from *ab initio* calculations, and the dispersion fits well with the numerical one [17]. The tight-binding model allows one to get simple solutions to predict various properties of phosphorene under strain and sheds more insight on the strain-induced physics.

In this paper, we studied the electronic structure and optic absorption of phosphorene under strain. The band gap depends positively on the in-plane strain and negatively on the vertical strain. By adjusting uniaxial strains in three principle directions, the band gap can be reduced to zero and for this situation, the dispersion is linear in the armchair direction and is quadratic in

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the zigzag direction. In other words, the semi-Dirac band structure turns up when band gap is closed by strain. A tensile strain along armchair direction increases the effective mass components in both directions, the strain in zigzag direction changes them in two directions in opposite ways, and the vertical strain only has significant effect on the effective mass along armchair direction. The band-edge optic absorption is completely polarized along the armchair direction, and the polarization rate decreases when the photon energy increases. Strain changes the absorption polarization as well as absorption edge.

## 2. Electronic structure under strain

Fig. 1 shows the lattice of phosphorene. The in-plane geometry parameters (in units of Å) of the phosphorene lattice are  $a_0 = 0.8014$ ,  $(b_{0x}, b_{0y}) = (1.515, 1.674)$ , and the thickness (the distance between sublayers that is not shown in the figure) is  $l_0 = 2.150$  [18]. The hopping energies  $t_{01}$ ,  $t_{02}$ ,  $t_{03}$ ,  $t_{04}$  and  $t_{05}$  are  $-1.220$ ,  $3.665$ ,  $-0.205$ ,  $-0.105$  and  $-0.055$  respectively [17], all in units of eV. The former two hopping energies are the nearest-neighbor ones and play the most significant role in constructing the electronic structure, other smaller ones only modulate the band structure slightly.

When a strain is applied, the lattice mesh is deformed. The deformed coordinates  $(x, y, z)$  are related with the undeformed coordinates  $(x_0, y_0, z_0)$  by

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 1 + \epsilon_x & 0 & 0 \\ 0 & 1 + \epsilon_y & 0 \\ 0 & 0 & 1 + \epsilon_z \end{pmatrix} \begin{pmatrix} x_0 \\ y_0 \\ z_0 \end{pmatrix}, \quad (1)$$

where  $\epsilon_i$  is the strain in  $i$ -direction. In the equation and from here on, we use the subscript 0 to denote quantities of undeformed phosphorene, and those without the subscript 0 means they are for strained phosphorene. The deformed bond length  $r$  can be expressed as

$$r/r_0 = 1 + \alpha_x \epsilon_x + \alpha_y \epsilon_y + \alpha_z \epsilon_z. \quad (2)$$

where the coefficients  $\alpha_i = \partial_{\epsilon_i} r/r_0$  are calculated as

$$\alpha_x = \frac{x_0^2}{r_0^2}, \quad \alpha_y = \frac{y_0^2}{r_0^2}, \quad \alpha_z = \frac{z_0^2}{r_0^2}. \quad (3)$$

The change of the bond length leads to the corresponding modulation of the hopping energy. In phosphorene, the hopping

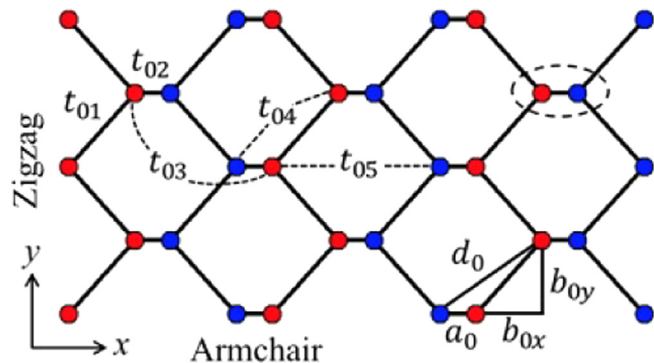


Fig. 1. The in-plane projection of phosphorene lattice. The red- and blue-filled circles represent the puckled up and puckled down phosphorus atoms. The ellipse denotes the translational cell of the in-plane lattice. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this paper.)

**Table 1**  
The coefficients  $\alpha_i$  for strained hopping energies.

	$t_1$	$t_2$	$t_3$	$t_4$	$t_5$
$\alpha_x$	$b_{0x}^2 r_{01}^{-2}$	$a_0^2 r_{02}^{-2}$	$(d_{0x} + a_0)^2 r_{03}^{-2}$	$d_{0x}^2 r_{04}^{-2}$	$(d_{0x} + b_{0x})^2 r_{05}^{-2}$
$\alpha_y$	$b_{0y}^2 r_{01}^{-2}$	0	$b_{0y}^2 r_{03}^{-2}$	$b_{0y}^2 r_{04}^{-2}$	0
$\alpha_z$	0	$l_0^2 r_{02}^{-2}$	0	$l_0^2 r_{04}^{-2}$	$l_0^2 r_{05}^{-2}$

energy is determined by the coupling between  $s$  and  $p$  orbitals of different phosphorus atoms. Detailed consideration of the coupling reveals that the hopping energy magnitude depends on the bond length in a relation  $t \propto r^{-2}$  [19,20]. By means of this relation and Eq. (2), we have the dependence of hopping energy on the strain components,

$$t/t_0 = (r/r_0)^{-2} \approx 1 - 2(\alpha_x \epsilon_x + \alpha_y \epsilon_y + \alpha_z \epsilon_z). \quad (4)$$

In the equation, the expression behind the approximation symbol is the linear version of that following the equals sign. The linear approximation, which is usually adopted for electronic structure calculation under small strains, is only used for qualitative analysis in this work. The linear coefficients  $\alpha_i$  for five strained hopping energies  $t_1 \sim t_5$  are listed in Table 1.

The tight binding Hamiltonian is

$$H_{TB} = \sum_{i,j} t_{ij} c_i^\dagger c_j \quad (5)$$

where  $t_{ij}$  is the hopping energy between  $i$ th and  $j$ th atoms, and  $c_i^\dagger (c_j)$  is the creation (annihilation) operator of electrons on atom  $i$  ( $j$ ), and the summation runs over the lattice sites with nonzero hoppings. Since there is no on-site potential difference of puckered-up and puckered-down atoms, the primitive translational cell consists of two adjacent atoms [22], as labelled by the ellipse in Fig. 1. The  $k$ -space Hamiltonian based on the choice of unit cell reads

$$H = \begin{pmatrix} g_0 & g_1 e^{ik_x a} \\ g_1^* e^{-ik_x a} & g_0 \end{pmatrix} \quad (6)$$

with

$$g_0 = 4t_4 \cos k_x d_x \cos k_y d_y,$$

$$g_1 = t_2 + t_5 e^{-i2k_x d_x} + 2(t_1 e^{-ik_x d_x} + t_3 e^{ik_x d_x}) \cos k_y d_y,$$

where  $\mathbf{d} = (a + b_x, b_y)$ . Solving the eigen problem of the Hamiltonian, we have the conduction and valence band energies,

$$E_{c/v} = g_0 \pm |g_1|. \quad (7)$$

The energy gap, which is the difference between  $E_c$  and  $E_v$  at  $\Gamma$  point, is obtained as

$$E_g = 2(t_2 + t_5 + 2t_1 + 2t_3). \quad (8)$$

The energy gap depends on all hopping energies except for  $t_4$ , which only accounts for the small asymmetry between the conduction and valence bands. Among these hoppings,  $t_2$  and  $t_1$  are the largest and second largest ones in amplitude, and have most important influence on the gap. If there is a tensile strain along  $z$ -direction,  $r_2$  is elongated,  $t_2$  becomes smaller, and the gap shrinks. If the tensile strain is in  $y$ -direction,  $r_1$  is elongated,  $t_1$  is smaller in amplitude, and the gap increases because  $t_1$  is negative. When the tensile strain is applied in  $x$ -direction, both  $r_1$  and  $r_2$  become longer, which induces opposite effects on the energy gap, so it is difficult to tell how the gap changes. Fig. 2(a) shows the band gap as function of strain, which verifies the above analysis of  $E_g$  when

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