Strain engineering the charged-impurity-limited carrier mobility in phosphorene

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Abstract

We investigate, based on the tight-binding model and in the linear deformation regime, the strain dependence of the electronic band structure of phosphorene, exposed to a uniaxial strain in one of its principle directions, the normal, the armchair and the zigzag directions. We show that the electronic band structure of strained phosphorene, for the experimentally accessible carrier densities and the uniaxial strains, is well described by a strain-dependent decoupled electron-hole Hamiltonian. Then, employing the decoupled Hamiltonian, we consider the strain dependence of the charged-impurity-limited carrier mobility in phosphorene, for both types of carriers, arbitrary carrier densities and in both

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armchair and zigzag directions. We show that a uniaxial tensile (compressive) strain in the normal direction enhances (weakens) the anisotropy of the carrier mobility, while a uniaxial strain in the zigzag direction acts inversely. Moreover applying a uniaxial strain in the armchair direction is shown to be ineffective on the anisotropy of the carrier mobility. These will be explained based on the effects of the strains on the carrier effective masses.

Keywords: Phosphorene; Tight-binding model; Band Structure; Strain; Carrier Mobility.

1 Introduction

Since successful isolation of a single layer of graphite\textsuperscript{1} called graphene, as the first real two-dimensional lattice structure which shows novel appealing properties\textsuperscript{2, 3}, many researchers tried to synthesis or isolate new two-dimensional materials. These efforts resulted in finding other two dimensional materials such as BN\textsuperscript{4}, transition metal dichalcogenides\textsuperscript{5}, silicene\textsuperscript{6, 7, 8, 9} and recently phosphorene. Phosphorene is a single layer of black phosphorus, which can be isolated by mechanical exfoliation\textsuperscript{10, 11} of black phosphorus. In a single layer of black phosphorus, each phosphorus atom covalently couples to three nearest neighbors. This configuration of phosphorus atoms results in a honeycomb-like lattice structure. However, due to the \(sp^3\) hybridization of \(s\) and \(p\) atomic orbitals, it forms a puckered surface. The electronic band structure of phosphorene has been studied using different methods such density functional theory calculations\textsuperscript{12, 13}, \(k.p\) method\textsuperscript{14, 15} and tight-binding model\textsuperscript{13, 16, 17}. These considerations show phosphorene is a direct-band-gap insulator, but with an anisotopic band structure. This novel band structure leads to many attractive properties\textsuperscript{18, 19, 20, 21}.

Strain tuning is an effective means to tune the physical properties of two dimensional
materials (for a review, see e.g. Ref. [2, 22]). Puckered structure of phosphorene makes this easier, so one can tune and control its electronic and mechanical properties by strain, confirmed by recent studies on the effects of uniaxial and biaxial strains in phosphorene [12, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33]. These works examined effects of strains applied along three principle directions which preserve $D_{2h}$ group point symmetry of phosphorene [16], its zigzag and armchair edges and the direction normal to its plane. It has been shown that a uniaxial strain in the direction normal can decrease its band gap and even leads to an insulator to metal transition [12, 27, 34]. Moreover, the effects of an in-plane uniaxial strains along zigzag and armchair edges [28, 29, 30] on the band gap of phosphorene has been studied. Some other researchers has studied the effects of uniaxial and biaxial strains on the band structure [30, 31, 32, 33] and the optical properties [31] of phosphorene, confirming the capability of stain as an effective means to tune the properties of phosphorene. These works showed, when the uniaxial strain is applied along the armchair direction, the properties of phosphorene change further. But, recently, it has been shown [35] that the most effective direction to apply a strain and tune the band gap of phosphorene is an in-plane direction (not being along armchair nor along zigzag) with a direction angle about $0.268\pi$ counted from the armchair edge.

According to the high-potential capability of strains to tune the properties of phosphorene, driving an analytical relation for the Hamiltonian of strained phosphorene is very desirable, and can be used to examine the effects of the strains on the electric, optical and magnetic properties of phosphorene. In this paper, starting from the well-known 4-band tight-binging Hamiltonian of phosphorene [13, 16], we obtain a strain-dependent tight-binding Hamiltonian for phosphorene. In this paper we work in the linear deformation regime and only consider uniaxial strains. To benefit from the $D_{2h}$ group point symmetry of phosphorene and reduce the 4-band Hamiltonian...
to a 2-band Hamiltonian and achieve an analytical result, we restrict our consideration to the uniaxial strains applied along three principle directions of phosphorene which preserve its $D_{2h}$ group point symmetry. Thanks to this symmetry, we can obtain analytical relations for its band energies which can be used to explore easily the effects of the uniaxial strains on properties of phosphorene. Searching for low-energy structures in strained phosphorene, we use continuum approximation and derive the corresponding Hamiltonian dominating low energy excitations. Then, by taking into account the weak interband coupling of conduction and valance bands, we project the low-energy Hamiltonian into a decoupled Hamiltonian and show that for the experimentally accessible carrier density, the decoupled bands agree well the bands obtained from the tight-binding Hamiltonian. Motivated by this fact and the recent studies on the carrier mobility in phosphorene, then we apply our decoupled Hamiltonian to consider the strain dependence of the charged-impurity-limited carrier mobility in phosphorene. Our result shows that one can tune the amount and the anisotropy of the mobility in phosphorene, by making use of a uniaxial strain in the normal or zigzag direction.

The rest of this paper is organized as follows. In Sec. II we reproduce the known 4-band Hamiltonian of phosphorene. In Sec. III we explain how one can, in general, insert the effects of the strains in the Hamiltonian and obtain a general formalism for the strain-dependent Hamiltonian of phosphorene. Sec. IV devoted to consider the strain dependence of the charged-impurity-limited carrier mobility in phosphorene. We end the paper by summarizing our results in Sec. V.
2 Structure and tight-binding Hamiltonian of phosphorene

The lattice structure of phosphorene and the necessary lattice parameters to construct the tight-binding Hamiltonian of phosphorene, including the lattice constant, the bond angles and the transfer energies, have been introduced in Fig. 1. The unit cell of phosphorene (solid-line rectangle in Fig. 1) consists of four phosphorus atoms, two atoms in the lower layer represented by the grey circles (called $A$ and $B$) and two atoms in upper layer represented by the red circles (called $C$ and $D$). Hence, the tight-binding Hamiltonian of phosphorene can be written in terms of a $4 \times 4$ matrix as

$$
\hat{H}_k = \begin{pmatrix}
0 & t_{AB}(k) & t_{AC}(k) & t_{AD}(k) \\
t_{BA}(k) & 0 & t_{BC}(k) & t_{BD}(k) \\
t_{CA}(k) & t_{CB}(k) & 0 & t_{CD}(k) \\
t_{DA}(k) & t_{DB}(k) & t_{DC}(k) & 0
\end{pmatrix},
$$

acting in $(\phi_A, \psi_B, \psi_C, \psi_D)^T$ with $k$ being the two-dimensional momentum. Notice that $t_{BA}(k) = t_{AB}^*(k)$. Moreover, it has been shown\cite{13, 16} that if we only retain the transfer energies up to the fifth nearest neighbors, the tight-binding approximated band structure agrees well with its density functional theory band structure. These transfer energies are\cite{13} $t_1 = -1.220 \, eV$, $t_2 = +3.665 \, eV$, $t_3 = -0.205 \, eV$, $t_4 = -0.105 \, eV$ and $t_5 = -0.055 \, eV$. So we can rewrite the
Hamiltonian matrix as
\[
\hat{H}_k = \begin{pmatrix}
0 & f_{1k} + f_{3k} & f_{4k} & f_{2k} + f_{5k} \\
(f^*_{1k} + f^*_{3k}) & 0 & f_{2k} + f_{5k} & f_{4k} \\
(f^*_{4k}) & (f^*_{2k} + f^*_{5k}) & 0 & f_{1k} + f_{3k} \\
(f^*_{2k} + f^*_{5k}) & (f^*_{4k}) & (f^*_{1k} + f^*_{3k}) & 0 \\
\end{pmatrix},
\]\(2\)
where the matrix elements are given by
\[f_{1k} = 2t_1 e^{ik_x x_1} \cos(k_y y_1), \quad f_{2k} = t_2 e^{ik_x x_2}, \quad f_{3k} = 2t_3 e^{ik_x x_3} \cos(k_y y_3), \quad f_{4k} = 4t_4 \cos(k_x x_4) \cos(k_y y_4), \quad f_{5k} = t_5 e^{ik_x x_5}.\]
Here \(\vec{r}_i = (x_i, y_i, z_i)\) is a vector which is drawn from \(A\) (The origin of the cartesian coordinate system) to one of the \(i\)th nearest neighbors (See Fig. 1). They are \(\vec{r}_1 = (-d_1 \cos \alpha, d_1 \sin \alpha, 0), \quad \vec{r}_2 = (d_2 \cos \theta, 0, d_2 \sin \theta), \quad \vec{r}_3 = (d_1 \cos \alpha + 2d_2 \cos \theta, d_1 \sin \alpha, 0), \quad \vec{r}_4 = (-d_1 \cos \alpha - d_2 \cos \theta, d_1 \sin \alpha, d_2 \sin \theta), \quad \vec{r}_5 = (-2d_1 \cos \alpha - d_2 \cos \theta, 0, d_2 \sin \theta)\) where \(\cos \theta = \frac{-\cos \beta}{\cos \alpha} \). One can take into account the \(D_{2h}\) group point symmetry in phosphorene and project the four-band Hamiltonian into a reduced two-band Hamiltonian as[16]
\[
\hat{H}_k = \begin{pmatrix}
f_{4k} & f_{1k} + f_{2k} + f_{3k} + f_{5k} \\
(f^*_{1k} + f^*_{3k} + f^*_{2k} + f^*_{5k}) & f_{4k} \\
\end{pmatrix},
\]\(3\)
acting in \((\phi_A + \phi_C, \phi_B + \phi_D)^T/2\). The corresponding energy bands, obtained by diagonalizing the Hamiltonian matrix, are given by
\[
E_k = f_{4k} \pm |f_{1k} + f_{2k} + f_{3k} + f_{5k}|. \]
\(4\)
where \(+(-)\) denotes to the conduction(valence) band. We have shown the energy spectrum of phosphorene obtained from two-band Hamiltonian in Fig. 2. It is evident that minimum (maximum) of the conduction (valence) energy band is at \(\Gamma\) point. If we apply continuum approximation to the obtained two-band Hamiltonian and retain the terms up to the second
order in k, we can reproduce the known Hamiltonian of phosphorene \cite{16, 17},

\[
\hat{H}_k = \begin{pmatrix}
    u + \eta_x k_x^2 + \eta_y k_y^2 & \delta + \gamma_x k_x^2 + \gamma_y k_y^2 + i\chi k_x \\
    \delta + \gamma_x k_x^2 + \gamma_y k_y^2 - i\chi k_x & u + \eta_x k_x^2 + \eta_y k_y^2
\end{pmatrix},
\]

(5)

where \( u = 4t_4 = 0.42 \text{ eV}, \eta_x = -2t_4 x_4^2 = 1.03 \text{ eV} \hat{A}^2, \eta_y = -2t_4 y_4^2 = 0.56 \text{ eV} \hat{A}^2, \delta = 2t_1 + t_2 + 2t_3 + t_5 = 0.76 \text{ eV}, \gamma_x = -t_1 x_1^2 - \frac{t_2}{2} x_2^2 - t_3 x_3^2 - \frac{t_5}{2} x_5^2 = 3.51 \text{ eV} \hat{A}^2, \gamma_y = -t_1 y_1^2 - t_3 y_3^2 = 3.81 \text{ eV} \hat{A}^2 \)

and \( \chi = 2t_1 x_1 + t_2 x_2 + 2t_3 x_3 + t_5 x_5 = -5.34 \text{ eV} \hat{A} \) which agree well with the other calculations \cite{17}(Notice that in our calculations the zigzag edge lies along the x-axis.). The corresponding energy spectrums are given by

\[
E_k = u + \eta_x k_x^2 + \eta_y k_y^2 \pm \sqrt{(\delta + \gamma_x k_x^2 + \gamma_y k_y^2)^2 + \chi^2 k_x^2},
\]

(6)

where \( +(-) \) denotes to the conduction(valance) band. It is evident that the energy spectrum is linear in the \( k_x \) direction while in the \( k_y \) direction it is parabolic. Due to the large band gap, which leads to a weak interbands coupling, one can decouple the electron and the hole bands into a low energy regime. In this approximation, Eq. 6 can be written as \cite{17, 36, 37, 38}

\[
E_k \approx u + \eta_x k_x^2 + \eta_y k_y^2 \pm \delta(1 + \frac{1}{2}(2\gamma_x \frac{\delta}{\delta} k_x^2 + 2\gamma_y \frac{\delta}{\delta} k_y^2 + \frac{\chi^2 k_x^2}{\delta^2})).
\]

(7)

In this approximation the electron and hole effective masses in the \( x \) and \( y \) directions are given by,

\[
m_{ex} = \frac{\hbar^2}{2(\eta_x + \gamma_x + \chi^2/2\delta)} = 0.168 \ m_0, \ m_{ey} = \frac{\hbar^2}{2(\eta_y + \gamma_y)} = 0.852 \ m_0, \ m_{hx} = \frac{\hbar^2}{2(\gamma_x - \eta_x - \chi^2/2\delta)} = 0.184 \ m_0 \) and \( m_{hy} = \frac{\hbar^2}{2(\gamma_y - \eta_y)} = 1.146 \ m_0 \), which \( m_0 \) is the mass of a free electron, in good agreement with recent result \cite{13}. To see that in what region this approximated energy bands agree well with the other results, we have shown all three set energy bands obtained from the tight-binding, the low energy and the decoupled Hamiltonians, in Fig. 2. One can see that in the \( k_y \) direction all three set energy bands agree well in a wide range of the energy and
the momentum. Moreover, in the $k_x$ direction the tight-binding energy bands and the low-energy bands agree well too, but the decoupled bands overlap with them only up to 0.14 eV (0.13 eV) with respect to the bottom (top) of the conduction (valance) bands. This corresponds to $n = 2.20 \times 10^{13} \text{ cm}^{-2}$ and $n = 2.44 \times 10^{13} \text{ cm}^{-2}$ for the electron and hole densities. These indicate that the low energy excitations in phosphorene are well described by the decoupled Hamiltonian\cite{17, 36, 37, 38}.

### 3 Strain-dependent tight-binding Hamiltonian

In this section we rederive the tight-binding Hamiltonian of phosphorene in the presence of the uniaxial strains applied along the principle directions of phosphorene. To insert the effects of the applied strain in the tight-binding Hamiltonian of phosphorene, first we must determine the effects of the strain on the transfer energies and the bond lengths. It has been shown\cite{39} that the transfer energies between $s$ and $p$ orbitals, which construct the electronic bands of phosphorene, depend on the bond length as $t \propto \frac{1}{r^2}$. To obtain this relation, it has been supposed that the applied strain doesn’t change the bond angles and only change the bond lengths. Within the linear deformation regime, this is a reasonable assumption. Since the change in the bond angles in a strained lattice, at least, includes the terms of second order in terms of the applied strain. So they can be ignored in the linear deformation regime. Hence, we only need to determine the strain dependence of the bond lengths and the other inter-atomic distances.

Let us construct our formalism in a general case in which phosphorene is exposed to strains applied along all three principle directions of phosphorene, the armchair ($x$-direction) and the zigzag ($y$-direction) edges and the the direction normal to the phosphorene plane ($z$-direction).
So, the deformed coordinates are given by
\[
\begin{pmatrix}
x' \\
y' \\
z'
\end{pmatrix} =
\begin{pmatrix}
1 + \epsilon_x & 0 & 0 \\
0 & 1 + \epsilon_y & 0 \\
0 & 0 & 1 + \epsilon_z
\end{pmatrix}
\begin{pmatrix}
x \\
y \\
z
\end{pmatrix},
\]
where $\epsilon_x$, $\epsilon_y$ and $\epsilon_z$ are the normal strains applied along the x-, y- and z-directions respectively.

In this paper, we restrict our considerations to the linear deformation regime, so the bond lengths and the other atomic distances, in general, can be expanded in terms of all components, $\epsilon_x$, $\epsilon_y$ and $\epsilon_z$ as
\[
r' = r + \alpha_x \epsilon_x + \alpha_y \epsilon_y + \alpha_z \epsilon_z,
\]
where $r$ and $r'$ = $\sqrt{(x')^2 + (y')^2 + (z')^2}$ are the unstrained and strained bond lengths respectively and $\alpha_x$, $\alpha_y$ and $\alpha_z$ are the strain-related geometrical coefficients, given by $\alpha_x = \frac{\partial r}{\partial x} |_{\epsilon_x=0} = \frac{x^2}{r}$, $\alpha_y = \frac{\partial r}{\partial y} |_{\epsilon_y=0} = \frac{y^2}{r}$ and $\alpha_z = \frac{\partial r}{\partial z} |_{\epsilon_z=0} = \frac{z^2}{r}$. If we insert Eq. 9 into the relation $t \propto \frac{1}{r^2}$, and expand it in terms of the strains and only retain the terms up to the first order in $\epsilon$ we get
\[
t' = t - \frac{2}{r}(\alpha_x \epsilon_x + \alpha_y \epsilon_y + \alpha_z \epsilon_z)t,
\]
where $t$ and $t'$ are the unstrained and the strained transfer energies respectively.

As mentioned above, the strains applied along all three principle directions of phosphorene don’t break $D_{2h}$ symmetry. So the electronic excitations in strained phosphorene are dominated by the reduced two-band Hamiltonian, Eq. 3, but after substituting the deformed transfer energies and bond lengths into it. Recalling the relations obtained for the strained bond lengths and the transfer energies, and substituting them into the tow-band Hamiltonian, Eq. 3 we get
\[
\hat{H}_k = \begin{pmatrix}
f'^4_{4k} & f'^1_{1k} + f'^2_{2k} + f'^3_{3k} + f'^5_{5k} \\
f'^{\ast 4}_{4k} + f'^{\ast 1}_{1k} + f'^{\ast 2}_{2k} + f'^{\ast 3}_{3k} + f'^{\ast 5}_{5k} & f'^1_{1k}
\end{pmatrix},
\]
where $f'^4_{4k}$, $f'^1_{1k}$, $f'^2_{2k}$, $f'^3_{3k}$, $f'^5_{5k}$, $f'^{\ast 1}_{1k}$, $f'^{\ast 2}_{2k}$, $f'^{\ast 3}_{3k}$, $f'^{\ast 5}_{5k}$ are the transfer energies and bond lengths respectively.
where $f_{1k} = 2t_1^e e^{ik_xx_1} \cos(k_y y_1'$), $f_{2k} = t_2^e e^{ik_xx_2}$, $f_{3k} = 2t_3^e e^{ik_xx_3} \cos(k_y y_3')$, $f_{4k} = 4t_4^e \cos(k_xx_4) \cos(k_y y_4')$ and $f_{5k} = t_5^e e^{ik_xx_5'}. The corresponding electron and hole energy bands are given by

$$E_k^e = f_{4k}^e \pm |f_{1k}^e + f_{2k}^e + f_{5k}^e|.$$ 

with $+$($-$) denoting to the electron (hole) band. It easy to show that strained phosphorene has a direct band gap at $\Gamma$ point, in agreement with the recent density functional theory [12, 27, 34, 28] and tight-binding [40] calculations done in the linear deformation regime. Similar to the unstrained case, to capture the low energy physics of strained phosphorene, one can expand the matrix elements around $\Gamma$ point and only retain the terms up to second order in $k$ and first order in $\epsilon$. Hence, the low energy Hamiltonian becomes

$$\tilde{H}_k = \begin{pmatrix} u^e + \eta_x k_x^2 + \eta_y k_y^2 & \delta^e + \gamma_x k_x^2 \cos(k_y y_1') + i \chi^e k_x \\
\delta^e + \gamma_x k_x^2 \cos(k_y y_1') - i \chi^e k_x & u^e + \eta_y k_y^2 + \gamma_y k_y^2 \end{pmatrix},$$

The values of the matrix elements depends on the directions in which the strains are applied (See appendix). The applied strains can affect, by changing the energy gap and $\chi^e$, on the interband coupling. When the interband coupling is weak, one can project the low energy two-band Hamiltonian into a decoupled Hamiltonian which is given by

$$\tilde{H}_k = \begin{pmatrix} E_k^e + \frac{\hbar^2 k_x^2}{2m_{ex}} + \frac{\hbar^2 k_y^2}{2m_{ey}} & 0 \\
0 & E_k^h - \frac{\hbar^2 k_x^2}{2m_{hx}} - \frac{\hbar^2 k_y^2}{2m_{hy}} \end{pmatrix},$$

where $E_k^e = u^e + \delta^e$, $E_k^h = u^e - \delta^e$ and

$$m_{ex}^e = \frac{\hbar^2}{2(\eta_x + \gamma_x + (\chi^e)^2/2\delta^e)},$$
$$m_{ey}^e = \frac{\hbar^2}{2(\eta_y + \gamma_y)},$$
$$m_{hx}^e = \frac{\hbar^2}{2(\gamma_x - \eta_x + (\chi^e)^2/2\delta^e)),}$$
$$m_{hy}^e = \frac{\hbar^2}{2(\gamma_y - \eta_y)}. $$

(15)
In the reminder of this section we consider the effects of the strains applied along all three principle directions of phosphorene on its electronic band structure, as a key feature of crystalline materials to explore their other physical properties. We have two aims. One is to see whether our tight-binding Hamiltonian reproduces previous results\[12, 27, 34, 28, 40\] for the energy gap of strained phosphorene. The other is to show that in what energy region the decoupled energy bands agree well with the others, obtained from the low-energy and the tight-binding Hamiltonian.

**Uniaxial strain along the normal direction (z-axis)**- Let us first explore effects of a uniaxial strain in the normal direction (z-direction), $\epsilon_x = \epsilon_y = 0$ and $\epsilon_z \neq 0$. If we recall the relations obtained for the the strained bond lengths and the transfer energies, and substitute them into Eq. 12, we get

$$\Delta E_g = -(8t_1 \frac{z_1^2}{r_1^2} + 4t_2 \frac{z_2^2}{r_2^2} + 8t_3 \frac{z_3^2}{r_3^2} + 4t_5 \frac{z_5^2}{r_5^2})\epsilon_z = -12.693\epsilon_z,$$

for the strain-induced modulation in the energy gap. This shows that the energy gap of phosphorene decreases (increases) linearly when it is exposed to a uniaxial tensile (compressive) strain in the normal direction. This is in agreement with the previous first-principle\[12, 27, 34\] and tight-binding \[40\] studies on the strain-induced modulation in the energy gap of strained phosphorene, done in the linear deformation regime. This can also be seen in Fig. 3 where we have shown the energy bands of strained phosphorene for different values of $\epsilon_z$ obtained by diagonalizing Eq. 11 (black curves), Eq. 13 (red dashed curves) and Eq. 14 (green dotted-dashed curves). In this figure right (left) panels show the energy bands of phosphorene in the presence of a uniaxial tensile (compressive) strain applied in the normal direction, and in each panel the energy bands have been drown in both $\Gamma - X$ and $\Gamma - Y$ directions.
This figure also shows that a uniaxial tensile (compressive) strain in the normal direction enhances (weakens) the anisotropy of the both electron and hole energy bands slightly (See black curves in Fig. 3). This becomes more clear in the next section, where we consider the strain dependence of the carrier mobility in strained phosphorene. Moreover one can see that in the presence of a uniaxial tensile (compressive) strain, the energy range in which the decoupled bands agree well with the other bands becomes limited (extended). This is mainly due to the effect of the strain on the energy gap (See Eq. 16). When the energy gap increases (decreases), the coupling of the conduction and the valence band is enhanced (weakened) and the decoupling-band approximation becomes more (less) accurate. For a uniaxial tensile (compressive) strain about $\epsilon_z = 0.04$ ($\epsilon_z = -0.04$), the decoupled conduction band overlap well with the tight-binding conduction band up to 0.11 eV (0.18 eV) with respect to the bottom of the conduction band. By making use of $n = \frac{m^* e F}{\pi \hbar^2 E_{F}}$, where $E_{F}$ is counted from the bottom (top) of the conduction (valance) band, one can show this agreement corresponds to $n = 1.30 \times 10^{13} cm^{-2}$ ($n = 3.25 \times 10^{13} cm^{-2}$) electron density. This agreement for the valance band is up to 0.10 eV (0.16 eV) with respect to the top of the valance band, corresponding to $n = 1.48 \times 10^{13} cm^{-2}$ ($n = 3.60 \times 10^{13} cm^{-2}$) hole density.

Uniaxial strain along the zigzag edge (y-axis)- When phosphorene is exposed to a uniaxial strain along its zigzag edge, the strain-induced modulation in its energy gap is given by

$$\Delta E_g = -(8t_1 \frac{y_1^2}{r_1^2} + 4t_2 \frac{y_2^2}{r_2^2} + 8t_3 \frac{y_3^2}{r_3^2} + 4t_5 \frac{y_5^2}{r_5^2}) \epsilon_y = 5.945 \epsilon_y,$$  

which shows that a uniaxial tensile (compressive) strain in the zigzag edge increases (decreases) linearly the energy gap. This agrees well with the recent studies\cite{10, 28, 40}. Figure 4 shows that in the presence of a uniaxial tensile (compressive) strain along the zigzag edge, the anisotropy
of the band structure is weakened (enhanced). Moreover it is evident that, in the presence of
a uniaxial tensile (compressive) strain about $\epsilon_y = 0.04$ ($\epsilon_y = -0.04$), there is good agreement
between the decoupled and the tight-binding conduction bands up to 0.16 eV (0.13 eV) with
respect to the bottom of the conduction band. In the valance band the overlapping is up to
0.15 eV (0.12 eV) with respect to the top of the valance band.

Uniaxial strain along the armchair edge ($x$-axis)- In the presence of a uniaxial along the
armchair edge of phosphorene, the strain-induced modulation in its energy gap is given by

$$\Delta E_g = -(8t_1 \frac{x^2}{r_1} + 4t_2 \frac{x^2}{r_2} + 8t_3 \frac{x^2}{r_3} + 4t_5 \frac{x^2}{r_5})\epsilon_x = 3.708\epsilon_x. \quad (18)$$

which shows that the energy gap is a linear function of the applied strain, and increases (decreases) when phosphorene is exposed to a uniaxial tensile (compressive) strain in agreement
with the recent studies[10, 40]. Comparison of Eqs. 17 and 18 shows that, for same uniaxial
strains along the zigzag and armchair edges, the uniaxial strain along the zigzag edge induces a
larger band gap variation. Effects of the applied strain on the anisotropy of the band structure
can be seen in Fig. 5 which, as it is expected, is unlike the effects of the uniaxial strain along
the armchair edges. In the presence of a uniaxial tensile strain about $\epsilon_y = 0.04$ along the zigzag
edge, the overlapping of the decoupled band with the tight-binding is up 0.16 eV and 0.14 eV
for the conduction and the valance bands respectively, while for a compressive strain about
$\epsilon_y = -0.04$ they agree only up 0.13 eV for both conduction and valance bands.

We end this section by this conclusion that the electronic band structure of strained phos-
phorene, for the experimentally accessible carrier densities and the uniaxial strains applied along
all three principle directions of phosphorene, is well described by the decoupled Hamiltonian.
Motivated by this fact, we apply it to consider strain engineering the charged-impurity-limited
carrier mobility in phosphorene.

4 Strain engineering the charged-impurity-limited carrier mobility

In this section, employing our strain-dependent decoupled Hamiltonian, we investigate the strain dependence of the impurity-limited carrier mobility in phosphorene for both types of carriers, electron and hole, and along both armchair and zigzag edges. The carrier mobility, \( \mu \), is defined as \( \mu = \sigma / ne \) where \( \sigma \) is the electrical conductivity, \( n \) is the carrier density and \( e \) is the electron charge. To calculate the electrical conductivity we use the semi-classical Boltzmann transport theory combined with the relaxation time approximation. Moreover we restrict our calculation to the steady state and suppose that the two-dimensional electron gas in phosphorene is homogenous, so the electrical conductivity is given by

\[
\sigma_{ii} = -e^2 g_s \int \frac{d^2 k}{(2\pi)^2} \tau(E_k) v_i(k) \frac{\partial f(E_k)}{\partial E_k},
\]

where \( i \) is \( x, y \), \( g_s = 2 \) is the spin degeneracy, \( k = (k_x, k_y) \) is the two-dimensional momentum and \( v_i = \hbar k_i / m_i^e \) is the electron velocity in the \( i \) direction with \( k_i \) and \( m_i^e \) being the corresponding electron or hole momentum and mass. \( E_k \) is the energy band obtained from the strained-dependent decoupled Hamiltonian (Notice we have omitted the electron and hole indexes in \( m_i^e \) and \( E_k \)). \( f(E_k) \) is the Fermi-Dirac distribution function and \( \tau(E_k) \) is the relaxation time. Let us suppose that the impurities are static, of symmetric potential and have no internal excitations. So the relaxation time is given by

\[
\frac{1}{\tau(E_k)} = \frac{2\pi n_i}{\hbar} \int \frac{d^2 k'}{(2\pi)^2} \left| V_i(q) \right|^2 (1 - \cos \theta_{kk'}) \delta(E_k - E_{k'}) ,
\]
where \( n_i \) is the number of impurities per unit area, \( q = |\mathbf{k} - \mathbf{k}'| \) and \( \theta_{kk'} \) is the scattering angle between \( \mathbf{k} \) and \( \mathbf{k}' \). \( V_i(q) = \frac{2\pi e^2}{\kappa q} \) is the Fourier transform of the potential of the charge impurity and \( \kappa = (\kappa_{\text{sub}} + \kappa_{\text{enc}})/2 \) is the effective dielectric constant with \( \kappa_{\text{sub}} \) and \( \kappa_{\text{enc}} \) being the dielectric constant of the substrate (\( \kappa_{\text{sub}} = 2.5 \) for SiO\(_2\) substrate[19]) and the encapsulating layer respectively which for vacuum is zero. \( \varepsilon(q) \) is the dielectric function which within the random phase approximation is given by \( \varepsilon(q) = 1 + \frac{2\pi e^2}{\kappa q} \Pi(q) \), where \( \Pi(q) \) is the polarizability function. The polarizability function can be written[19] as

\[
\Pi(q) = \frac{\sqrt{m_x^\epsilon m_y^\epsilon}}{\pi \hbar^2} \left[ 1 - \sqrt{1 - \frac{8E_F^\epsilon/\hbar^2}{q_x^2/m_x^\epsilon + q_y^2/m_y^\epsilon}} \right],
\]

(21)

where \( E_F^\epsilon \) is the Fermi energy of strained phosphorene for a fixed carrier concentration.

If we introduce new variables as 

\[
p_x^\epsilon = \left( \frac{m_x^\epsilon}{m_x^0} \right)^{1/4} k_x \quad \text{and} \quad p_y^\epsilon = \left( \frac{m_y^\epsilon}{m_y^0} \right)^{1/4} k_y,
\]

we have \( E_p = \frac{1}{2m_{\text{eff}}} (p_x^2 + p_y^2) \) for the energy bands with \( m_{\text{eff}}^\epsilon = \sqrt{m_x^\epsilon m_y^\epsilon} \). In the new momentum, space the electrical conductivity is given by

\[
\sigma_{ii} = \frac{m_{\text{eff}}^\epsilon e^2 g_s}{2\pi \hbar^2} \int E_p dE_p \tau(E_p)(-\frac{\partial f(E_p)}{\partial E_p}),
\]

(22)

leading to \( \sigma_{ii} = \frac{g_s m_{\text{eff}}^\epsilon e^2 E_F^\epsilon \tau(E_F^\epsilon)}{\hbar} \) for the electrical conductivity of strained phosphorene at zero temperature, where \( E_F^\epsilon = \frac{\hbar^2 (p_F^\epsilon)^2}{2m_{\text{eff}}^\epsilon} \) with \( p_F^\epsilon \) being Fermi momentum in the new momentum space. \( \tau(E_F^\epsilon) \) is given by

\[
\frac{1}{\tau(E_F^\epsilon)} = \frac{n_i m_{\text{eff}}^\epsilon}{\pi \hbar^3} \int_0^\pi d\theta \left| \frac{2\pi e^2}{\sqrt{2}\kappa k_F \sqrt{1 - \cos \theta} + 2\pi e^2 D(E_F^\epsilon)} \right|^2 (1 - \cos \theta),
\]

(23)

where \( D(E_F^\epsilon) = \frac{m_{\text{eff}}^\epsilon}{\pi \hbar^2} \) is the carrier density of states at the Fermi energy and

\[
k_F = \sqrt{2\pi n \left[ \left( \frac{m_y^\epsilon}{m_x^\epsilon} \right)^{1/2} \cos^2 \theta + \left( \frac{m_x^\epsilon}{m_y^\epsilon} \right)^{1/2} \sin^2 \theta \right]},
\]

(24)

is the anisotropic Fermi momentum. In Eq. 24, \( \theta \) is counted from the x-axis, and \( n = \frac{m_{\text{eff}}^\epsilon}{\pi \hbar^2} E_F^\epsilon \) is the carrier density in strained phosphorene, being a linear function of Fermi energy as same as
the carrier density in the ordinary two-dimensional electron gas. Hence the zero-temperature carrier mobility in strained phosphorene is given by $\mu_{ii} = \frac{e\tau(E_F^c)}{m_i^e} m_{ei}^{\text{eff}}$.

In Fig. 6 we have shown our numerical results for the strain dependence of the charged-impurity-limited electron (left panels) and hole (right panels) in phosphorene exposed to the uniaxial strains in the normal direction (z-axis). The upper (lower) panels show the carrier mobility along its armchair (zigzag) edge, and orange ($n = 0.2 \times 10^{13} \text{cm}^{-2}$) to black ($n = 1.0 \times 10^{13} \text{cm}^{-2}$) curves correspond to different carrier densities with $\Delta n = 0.2 \times 10^{13} \text{cm}^{-2}$. The density of the charged impurities is supposed to be $n_i = 1.0 \times 10^{13} \text{cm}^{-1}$ which is typical of the $\text{SiO}_2$ substrate. Figure 6 shows that the carrier mobility along the armchair direction is higher than that along the zigzag direction, as same as that in unstrained phosphorene[10, 20, 37, 30]. This can be understood by this fact that, in the presence of both uniaxial tensile and compressive strains, the carrier effective mass along the armchair edge is always smaller than that along the zigzag edge. This can be tested by making use of the Eqs. 15, 25, and 26. Moreover one can see that the carrier mobility along both armchair and zigzag directions increases by increasing the carrier density. This is the familiar feature of the ordinary two-dimensional electron gas[41], arising from the linear dependence of its carrier density on the Fermi energy (In phosphorene the carrier density depends on the Fermi energy as $n = \frac{m_e^c \pi \hbar^2}{8k^2} E_F^c$). Figure 6 also shows that in the presence of a tensile (compressive) strain in the normal direction, the carrier mobility along the armchair edge increases (decreases), while the carrier mobility along the zigzag edge decreases (increases). This property originates from the effect of the strain on the anisotropy (and consequently the carrier effective mass) in phosphorene, as explained in the previous section. To explain this property further, we rewrite the relation of the carrier mobility as $\mu_{ii} = e^{m_{eff}^e} \frac{\tau(E_F^c)}{m_i^e}$. It is easy to show that the effect of the strain on $\tau(E_F^c) m_{eff}^e$ part is weak and
it mainly affects on $m_i^{\parallel}$ part. By making use of the Eqs. 15, 25, and 26, one can show that applying a uniaxial tensile (compressive) strain in the normal direction decreases (increases) both electron and hole effective masses in the armchair (zigzag) direction, and consequently their mobilities in the armchair (zigzag) direction increase (decrease).

In Fig. 7 we have compared the effect of the direction of the applied strain on the carrier mobility in phosphorene. Figure 7 shows that, unlike the strains in the normal direction, applying a uniaxial tensile (compressive) strain in the zigzag direction decreases (increases) both electron and hole mobilities in the armchair (zigzag) direction. This originates from their different effects on the anisotropy (and consequently the carrier effective mass) in phosphorene, as explained in the previous section and above. This figure also shows that applying a uniaxial strain in the armchair direction weakly change the carrier mobility in phosphorene. Moreover Figs. 6 and 7 show that applying a uniaxial tensile (compressive) strain in the normal (zigzag) direction enhances (weakens) the anisotropy of the carrier mobility in phosphorene. While in the presence of a uniaxial compressive (tensile) strain in the normal (zigzag) direction, the carrier mobility is weakened (enhanced).

5 Summary and conclusions

In Summary, we investigated the electronic band structure of strained phosphorene within the linear deformation regime and based on the tight-binding model. We restricted our consideration to the uniaxial strains applied along one of the principle directions of phosphorene, the normal, the armchair and the zigzag directions. We showed that the derived strain-dependent energy spectrums reproduce the previous results for the energy gap of strained phosphorene.
Then we applied the continuum approximation to derive the corresponding low-energy Hamiltonian. Moreover we showed, when the interband coupling is weak, the low-energy Hamiltonian can project into a decoupled electron-hole Hamiltonian. We found that the electronic band structure of the strained phosphorene, for the experimentally accessible carrier densities and the mechanical strains, is well described by the decoupled Hamiltonian. Motivated by this fact we used our strain-dependent decoupled Hamiltonian to investigate the strain dependence of the charged-impurity-limited carrier mobility in phosphorene. We examined the dependence of carrier mobility on the direction of mobility, the carrier type, the carrier density and the direction of the applied strain. We showed the dependence of the carrier mobility on the direction of mobility, the carrier type and the carrier density is same as that in unstrained phosphorene. Moreover, as a point worthy of mention, we found that applying a uniaxial tensile (compressive) strain in the normal direction decreases (increases) carrier mobility in the armchair (zigzag) direction. While in the presence of a uniaxial tensile (compressive) strain in the zigzag direction the carrier mobility is decreased (increased). We also showed that a uniaxial strain in the armchair direction don’t changed the carrier mobility approximately. These properties were explained based on the effect of the applied strain on the anisotropy of the carrier effective mass in phosphorene.
A Appendix: Calculating the elements of the strain-dependent low-energy Hamiltonian matrix

The matrix element in Eq. 13 in the linear deformation regime, depend in general on the applied strain as

\[ u' = u + \epsilon u' \]

\[ \eta_x' = \eta_x + \epsilon \eta_x' \]

\[ \eta_y' = \eta_y + \epsilon \eta_y' \]

\[ \delta' = \delta + \epsilon \delta' \]

\[ \gamma_x' = \gamma_x + \epsilon \gamma_x' \]

\[ \gamma_y' = \gamma_y + \epsilon \gamma_y' \]

\[ \chi' = \chi + \epsilon \chi' , \]  \hspace{1cm} (25)

where the coefficients of the applied strain, for a uniaxial strain in the normal direction, are given by

\[ u' = -8t_4 \frac{z_1^2}{r_4^2} = 0.32 \text{ eV} \]

\[ \eta_x' = 4t_4 \frac{z_1^2 x_1^2}{r_4^2} = -0.75 \text{ eV} \AA^2 \]

\[ \eta_y' = 4t_4 \frac{z_1^2 y_1^2}{r_4^2} = -0.43 \text{ eV} \AA^2 \]

\[ \delta' = -4t_1 \frac{z_1^2}{r_1^2} - 2t_2 \frac{z_2^2}{r_2^2} - 4t_3 \frac{z_3^2}{r_3^2} - 2t_5 \frac{z_5^2}{r_5^2} = -6.58 \text{ eV} \]

\[ \gamma_x' = 2t_1 \frac{z_1^2 x_1^2}{r_1^2} + t_2 \frac{z_2^2 x_2^2}{r_2^2} + 2t_3 \frac{z_3^2 x_3^2}{r_3^2} + t_5 \frac{z_5^2 x_5^2}{r_5^2} = 1.44 \text{ eV} \AA^2 \]

\[ \gamma_y' = 2t_1 \frac{z_1^2 y_1^2}{r_1^2} + 2t_3 \frac{z_3^2 y_3^2}{r_3^2} = 0.00 \text{ eV} \AA^2 \]

\[ \chi' = -4t_1 \frac{z_1^2 x_1}{r_1^2} - 2t_2 \frac{z_2^2 x_2}{r_2^2} - 4t_3 \frac{z_3^2 x_3}{r_3^2} - 2t_5 \frac{z_5^2 x_5}{r_5^2} = 4.74 \text{ eV} \AA. \]  \hspace{1cm} (26)
These coefficients, when the strain is applied in the zigzag edge (y-axis), become

\[ u' = \frac{-84}{2} = 0.33 \text{ eV} \]

while for a uniaxial strain along the armchair edge, they are

\[ u' = \frac{-84}{2} = 0.19 \text{ eV} \]

The lattice parameters, which we used here, are \( d_1 = 2.22 \text{ Å}, d_2 = 2.24 \text{ Å}, t_1 = -1.220 \text{ eV} \), and \( t_2 = 3.056 \text{ eV}, t_3 = -0.205 \text{ eV}, t_4 = -0.105 \text{ eV}, t_5 = -0.055 \text{ eV} \) [13], \( \alpha = 0.2675 \text{ Å} \) and \( \theta = 0.567 \text{ Å} \).
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Figure 1: (a) The top view of phosphorene lattice structure. $t_i$ indicates to transfer energies from a site to its $i$th nearest neighbors. The solid-line (dashed-line) rectangle denotes to the unit cell in the 4-band (2-band) model. The other parameters are $d_1 = 2.22 \AA$, $d_2 = 2.24 \AA$,[13] and $\alpha = 0.2675\pi$.[35] (b) The side view of phosphorene lattice structure where $\beta = 0.567\pi$.[35] (c) The coordinate system used in this work. The armchair edge is supposed to be along the $x$-axis and the zigzag edge along the $y$-axis.
Figure 2: The energy spectrums of phosphorene around Γ point obtained from the two-band tight binding Hamiltonian (solid black curve), the low-energy Hamiltonian (red dashed curve) and the decoupled Hamiltonian (green dotted-dashed curve).
Figure 3: The energy spectrums of strained phosphorene around Γ point obtained from the two-band tight binding Hamiltonian (black solid curve), the low-energy Hamiltonian (red dashed curve) and the decoupled electron-hole Hamiltonian (green dotted-dashed curve). Phosphorene is exposed to uniaxial tensile (left panels) and compressive (right panels) strains applied in the normal direction.
Figure 4: Same as Fig. 3 but for strains applied along the zigzag edge.
Figure 5: Same as Fig. 3 but for strains applied along the armchair edge.
Figure 6: The strain dependence of the charged-impurity-limited electron (left panels) and hole (right panels) mobilities along the armchair (upper panels) and zigzag (lower panels) edges of phosphorene exposed to uniaxial strains in the normal direction. Orange to black lines correspond to $n = 0.2 \times 10^{13} \text{cm}^{-2}$ to $n = 1.0 \times 10^{13} \text{cm}^{-2}$ carrier densities with $\Delta n = 0.2 \times 10^{13} \text{cm}^{-2}$ and the density of the charged impurities is $n_i = 1.0 \times 10^{13} \text{cm}^{-2}$. 
Figure 7: The strain dependence of the charged-impurity-limited electron (left panels) and hole (right panels) mobilities along the armchair (upper panels) and zigzag (lower panels) edges of phosphorene, when it is exposed to uniaxial strains along the normal (black cure), armchair (red cure) and zigzag (green cure) directions. The electron and hole densities are $1.0 \times 10^{13} cm^{-2}$ and the density of the charged impurities is $n_i = 1.0 \times 10^{13} cm^{-2}$. 