Anisotropic RKKY interaction and modulation with mechanical strain in phosphorene

Houjian Duan, Shuai Li, Shi-Han Zheng, Zhenlong Sun, Mou Yang and Rui-Qiang Wang

Guangdong Provincial Key Laboratory of Quantum Engineering and Quantum Materials, School of Physics and Telecommunication Engineering, South China Normal University, Guangzhou 510006, People’s Republic of China

E-mail: rqwanggz@163.com

Abstract

We investigate the Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction between two magnetic impurities placed on a phosphorene surface based on the tight-binding model. It is found that the RKKY interaction exhibits strong anisotropy along different lattice directions and is sensitive to the deformed direction. The RKKY interaction is largest for impurities distributed in the armchair direction while the strain effect is strongest for the deformation exerted along the zigzag direction. Applied linear strain can increase the RKKY magnitude nonlinearly, and observably prolong the decay rate from the exponent to the $1/R^2$ law with the impurity distance. Most interestingly, near the strain-induced closing point of the bandgap, we find that the RKKY interaction is no longer simply ferromagnetic or antiferromagnetic, but presents oscillatory behavior, exhibiting the transition from ferromagnetism to antiferromagnetism. This originates from the combination effect of negative energy in the conduction band due to modification of the Fermi surface and the narrowing bandgap, and importantly both of them are reached simultaneously just by tuning the strain. Therefore, the strain effect proves to be an alternative approach to engineering impurity interactions in phosphorene materials.

Keywords: phosphorene, RKKY interaction, impurity effect

1. Introduction

Phosphorene, which is a monolayer of black phosphorus with a large direct energy gap, has attracted intensive attention since its mechanical exfoliation was achieved successfully in the laboratory [1], because of its unique electronic properties and potential applications in nanoelectronics. Compared to other two-dimensional materials, besides the large bandgap, phosphorene forms a puckered surface due to the $sp^3$ hybridization, which lowers the primitive symmetry and generates a highly anisotropic band structure. The high anisotropy and large bandgap make phosphorene a promising material in electronic and optical devices [2, 3]. It has a higher on-off current ratio than graphene, even at room temperature [4, 5], and exhibits a higher carrier mobility and a larger optical conductivity than transition metal dichalcogenides [1, 4–8].

An another most surprising characteristic of phosphorene is its strong response to strain fields. Phosphorene has better elastic properties than graphene. In armchair and zigzag directions, it can sustain a large amount of strain up to about 30% [9, 10]. A large amount of uniaxial strain in the direction normal to the phosphorene plane can lead to a gapless band in the elastic limit [10–15] and even induce a semiconductor–metal transition [14–17]. Modification of the in-plane uniaxial strains on the bandgap has also been analyzed in [9, 18, 19]. This suggests that the exerted strain can act as an efficient means of changing the electronic and optical properties of phosphorene, such as magneto-optical transport [20], tunable optical properties [2], anisotropic excitons [21], quantum oscillations [22] and thermoelectric behavior [23].

Adding magnetic atoms or defects has opened up the possibility for great application potential in spintronics. Among these aspects, the Ruderman–Kittel–Kasuya–Yoshida (RKKY) interaction, which measures the effective coupling between two magnetic moments mediated by a background of electrons, is an important
characteristic of the electron system. This coupling is crucial for magnetic ordering of the impurities and has recently been extensively studied in topological insulators [24–26] and three-dimensional Dirac/Weyl semimetals [27]. Much previous literature has focused on the RKKY interaction of graphene [28–35], due to its unique linear band structure around the Dirac point. It was reported that the exchange interaction between the magnetic adatoms is ferromagnetic if the adatoms belong to the same sublattice, and is antiferromagnetic if the adatoms belong to different sublattices [32–35], which is guaranteed by the particle–hole symmetry. The RKKY interaction also presents isotropic decay with an impurity distance as $R^{-3}$, whether in the armchair direction or in the zigzag direction [32–35]. Unlike graphene, phosphorene possesses a strong anisotropic band, the symmetry breaking of electron–hole pairs, and in particular a tunable strain effect, and it is naturally expected that the RKKY interaction of phosphorene will exhibit more interesting behavior, which is our motivation for carrying out this study.

In this paper, within the tight-binding model we investigate the RKKY interaction between two magnetic impurities placed on the same/different sublattices of phosphorene. We analyze in detail the spatial variation of the exchange interaction for different impurity configurations. We find that there exists strong RKKY anisotropy along different lattice directions. The strain effect deforming along the zigzag direction is most prominent. More importantly, the large amount of deformation can lead to oscillation of the RKKY interaction around the zero value with the impurity distance, exhibiting the transformation from ferromagnetism to antiferromagnetism. The rest of the paper is organized as follows. In section 2 we start from the tight-binding model and give the formula for the calculation of the RKKY interactions in the imaginary time representation based on the second order perturbation theory. In section 3, we analyze the strain-induced change in the energy bandgap. In section 4, we discuss the anisotropic RKKY interaction and its response to the in-plane strain. A short summary is given in the last section.

2. Model and method

The top view of the monolayer structure of black phosphorus is illustrated in figure 1, where each unit cell of phosphorene contains four phosphorus atoms, two atoms located in the upper sublattice (red squares) and the other two in the lower sublattice (blue squares). In the momentum representation, a four-band Hamiltonian is needed to describe it. As addressed in [37], the four-band model can be reduced to a two-band model due to the $D_{3h}$ point group invariance, where only two points in the unit cell are considered where the puckering structure is not concerned. In the planar view of the black phosphorene structure, the unit cell with two atoms (a and b) is circled by an ellipse in figure 1, which can traverse the whole lattice space by the lattice constant $d = (a + b_x, b_y)$ with $a = 0.8014, b_x = 1.515$, and $b_y = 1.674$ [14] in units of Å. In the tight-binding model, one can perfectly describe the band of phosphorene by considering just five hopping parameters describing the electronic band structure, and $a$ and $b$ are the in-plane bond lengths.

Figure 1. (a) The top view and (b) the side view of the monolayer structure of black phosphorus. The ellipse encircles the pair of atoms (a and b) belonging to the unit cell, where the puckering is not taken into account. $t_j (j = 1, 2, 3, 4, 5)$ are the five hopping parameters describing the electronic band structure, and $a$ and $b$ are the in-plane bond lengths.
nearest-neighbor hopping parameters dominate the others, and in general play the main role in constructing the electronic structure.

With the aforementioned two-atom unit cell and hopping energies, we write the two-band Hamiltonian in the momentum space as \( H_0 = \sum_k \varepsilon_k \ket{k} c_k \bra{k} \), where \( \varepsilon_k = (\varepsilon_g(k), \varepsilon_v(k))^T \) is the annihilation operator of electrons for the \( A \)- and \( B \)-sublattice, the spin indices are suppressed, and the Hamiltonian [37]

\[
H_0(k) = \begin{pmatrix}
g_g(k) & e^{i \mathbf{k} \mathbf{a}_1} g_v^*(k) \\
e^{-i \mathbf{k} \mathbf{a}_1} g_v(k) & g_v(k)
\end{pmatrix}
\]

with

\[
g_g(k) = 4t_4 \cos(k_x d_x) \cos(k_y d_y) \\
g_v(k) = t_2 + t_5 e^{-i k_x d_x} + 2(t_5 e^{-i k_y d_y} + t_5 e^{i k_x d_x}) \cos(k_y d_y).
\]

By diagonalizing the matrix Hamiltonian \( H_0(k) \), one can obtain its band energies \( E_{g,v}(k) = g_g(k) \pm |g_v(k)| \) and the corresponding eigenvectors

\[
u_{g,v}(k) = \frac{1}{\sqrt{2}} \begin{pmatrix} \pm e^{i \mathbf{k} \mathbf{a}_1} \\ 1 \end{pmatrix}
\]

where \( e^{i \mathbf{k} \mathbf{a}_1} = g_v(k)/g_g(k) \) and the subscript \( g (v) \) denote the conduction (valence) band. It is obvious that \( g_g(k) \) and in turn the hopping energy \( t_4 \) play a role in breaking the electron–hole symmetry.

When two magnetic impurities are separately placed at the sites \( \mathbf{r}_1 \) and \( \mathbf{r}_2 \) on the phosphorene and interact with conducting electrons, the system Hamiltonian is

\[
H = H_0 - [S(\mathbf{r}_1) \cdot \mathbf{s}(\mathbf{r}_1) - S(\mathbf{r}_2) \cdot \mathbf{s}(\mathbf{r}_2)],
\]

where \( S(\mathbf{r}_1) [s(\mathbf{r}_1)] \) is the spin of impurities (itinerant electrons), and \( J \) is the spin–exchange coupling strength, which is set to be weak and equal for simplicity. Performing the perturbation theory for the thermodynamic potential and eliminating the degrees of freedom of itinerant electrons [38], we obtain an effective RKKY interaction

\[
H_{\text{RKKY}} = -J^\lambda \chi_{ij} \mathbf{S}(\mathbf{r}_i) \cdot \mathbf{S}(\mathbf{r}_j),
\]

where the static spin susceptibility \( \chi_{ij} \) characterizes the indirect exchange interaction between the spins of two impurities, located at \( \mathbf{r}_i \) and \( \mathbf{r}_j \) and mediated by the free electrons, and is given by

\[
\chi_{ij}^{\lambda \chi} = -\frac{1}{4} \int_0^{1/4kT} G^{\lambda \chi}(\mathbf{r}_i, \mathbf{r}_j, \tau) G^{\chi \lambda}(\mathbf{r}_j, \mathbf{r}_i, -\tau) d\tau.
\]

Here, \( \lambda, \chi = A \) or \( B \), \( T \) is the temperature, and \( G^{\lambda \chi}(\mathbf{r}_i, \mathbf{r}_j, \tau) \) is the Matsubara Green function in real space, defined by \( G^{\lambda \chi}(\mathbf{r}_i, \mathbf{r}_j, \tau) = - (T \int_{\tau} [\chi_{ij}(\mathbf{r}_i, \tau) \psi_{ik}(\mathbf{r}_j) \psi_{ik}^*(\mathbf{r}_j)] \). In the representation of \( H_0 \), Green’s function can be expressed as [35]

\[
G^{\lambda \chi}(\mathbf{r}_i, \mathbf{r}_j, \tau) = -\text{sgn}(\tau) \sum_{k,n = c,v} \psi_{nk}^\dagger(\mathbf{r}_i) \psi_{nk}(\mathbf{r}_j) e^{-E_n(k)\tau} f \left[ -\text{sgn}(\tau) E_n \right]
\]

where \( \text{sgn}(\tau) \) is the sign function of \( \tau \), \( f(x) = \left[ e^{x-\mu}/kT + 1 \right]^{-1} \) is the Fermi distribution function, and \( \psi_{nk}(\mathbf{r}) = e^{i k \cdot \mathbf{r}} u_{nk}(\mathbf{k}) \) is the Bloch wave function.

3. Band structure modulated by mechanical strain

Phosphorene has much better elastically deformed properties than graphene since it can sustain a tensile strain of up to about 30% along the armchair or zigzag direction. With the strain applied, the electronic band structure is deformed. Thus, before studying the strain effect on RKKY interaction, we need to discuss the variation of the band structure with the applied strain first.

For simplicity, we only consider the in-plane strain in the present discussion due to the quasi-two-dimensional nature of the phosphorene. The mechanical strain effect is reflected in the changing of the length of the bond vector, whose coordinate \((x', y')\) for deformation is related to the undeformed \((x, y)\) coordinate in the form

\[
\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} 1 + \epsilon_x & \gamma \\ \gamma & 1 + \epsilon_y \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}.
\]

Here, \( \epsilon_i \) \((i = x, y)\) is the applied mechanical strain and \( \gamma \) is the weak shear component due to the twist of the lattice [13]. The hopping energy \( t \), which is contributed mainly by the overlapping of the wave-functions between the \( s \) and \( p \) orbitals in the phosphorene, is proportional to the bond length as \( t \propto |\mathbf{r}|^{-2} \). This is a reasonable
approximation when the principal directions of the two neighboring Wannier orbits are kept along the bond vector of the two neighboring atoms, and so the angular dependence does not play a role in the strain effect [13, 39, 40]. Thus, the five hopping energies $t'_j$ ($j = 1, \cdots, 5$) for the deformed situation can be written as

$$t'_j = \left| \frac{t}{r} \right|^2 t_j$$

By substituting $t'$ for $t$ in the Hamiltonian $H_0(k)$ and setting $\gamma = 0.2\epsilon_{y/f}$ throughout, we obtain the energy band structure of the deformed lattice, which is shown in figures 2(a) and (b). For the pristine phosphorene, i.e. $\epsilon_i = 0$, there is a well-known large energy bandgap $E_g = 2(t_2 + t_3 + 2t_4 + 2t_5) = 1.52$ eV. With finite compressive strain ($\epsilon_i < 0$) applied, the conduction band moves down but the valence band moves up, thus narrowing the bandgap $E_g = E_v(0) - E_c(0) = 2|\epsilon_i(0)|$. For a certain critical value of $\epsilon_i$, the bandgap closes up completely. Interestingly, the pronounced anisotropic response of the bandgap appears in the same strain, which can be seen by comparing figures 2(a) and (b). Obviously, the same deformation can cause more sensitive band movement along the zigzag direction ($\gamma$ axis) than the armchair direction ($x$ axis). This strain effect anisotropy originates from the high anisotropy of the lattice structure, which can be seen in $g_i(k)$ in equation (2). This special lattice structure also manifests itself in the asymmetry of the energy dispersion along $k_x$ and $k_y$. In particular, for a critical strength of $\epsilon_i$ to close the bandgap, a unique semi-Dirac dispersion is exhibited, namely, a linear energy dispersion along $k_x$ and a parabolic one along $k_y$. Another feature is the breaking of the electron–hole symmetry due to the energy band being shifted downwards overall, which is attributed to a finite $g_6(k)$ or $t_k$. This manifests itself as the appearance of negative energy in the conduction band, which becomes more and more prominent with the increase of the strain. It is expected that this strain–induced change in the energy dispersion will produce interesting effects in the RKKY interaction.

4. RKKY interaction modulated by mechanical strain

In this section, we perform the numerical calculations for RKKY interaction with equations (6) and (7). In $G^{AA}(\mathbf{r}, \mathbf{r'}, \tau)$, the summation of momentum $\sum_k$ is replaced with the integration $\int d^2k \int dk$. We set the temperature $T = 0$ and the chemical potential $\mu = 0$, and discuss first the RKKY interactions in the phosphorene subjected to small amounts of strain. For this situation, the conduction band energy is positive while the valence band energy is negative, as shown in figure 2, which allows us to simplify the Green function specifically to

$$G^{AA}(\mathbf{r}, \mathbf{r'}, \tau) = -\text{sgn}(\tau) \frac{2d x dy}{(2\pi)^2} \int e^{ik \cdot \mathbf{R}_y - g_\tau(k)\tau - |g_\tau(k)|\tau^2} |\mathbf{k}| \, dk,$$

$$G^{AB}(\mathbf{r}, \mathbf{r'}, \tau) = -\frac{2d x dy}{(2\pi)^2} \int e^{ik \cdot \mathbf{R}_y - g_\tau(k)\tau - |g_\tau(k)|\tau^2} |\mathbf{k}| \, dk.$$  

Inserting equations (10) and (11) into equation (6) and carrying out the numerical calculation in the full tight-binding band, we display the results in figures 3(b) and (c). Due to the anisotropic structure of phosphorene, the
relative positions $\mathbf{R}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ between the magnetic impurities have four configurations, i.e. typical zigzag (ZZ), asymmetric ZZ, typical armchair (AC), and asymmetric AC, as illustrated in figure 3(a), where the specific $\mathbf{R}_{ij}$ are listed. The corresponding RKKY interaction as a function of the spatial distance $R_{ij}$ is shown in figure 3(b) for two impurities placed on the same sublattices and in figure 3(c) on opposite sublattices. On the whole, the RKKY curves dominate approximately by an exponential decay $e^{-\eta R}$ where $\eta$ is the slope of the curves. By comparing four configurations, we find that the RKKY interaction is greatest along the typical AC direction with a slowly decaying rate and is smallest in the typical ZZ direction accompanied by fast decaying. These descriptions are suitable for the case of no matter, whether two impurities inhabit the same or different sublattices. Comparing figures 3(b) with (c), it is obvious that the impurity interaction on the same sublattice $\chi^{AA}$ is somewhat less than $\chi^{AB}$ on the opposite one. The exhibited strong anisotropy is close to the anisotropy of energy dispersion and the anisotropy of the phosphorene structure. In order to understand the above behavior, in the low-energy approximation we expand $E_{c/v}(k)$ at the center of the Dirac cone (the $\Gamma$ point in the Brillouin zone) and keep them to the order of $k^2$,

$$E_{c/v}(k) = 4t_4 \left(1 - \frac{d_z^2 k^2}{2} - \frac{d_y^2 k^2}{2}\right) \pm \left(\frac{E_g}{2} + \gamma k^2_z + \zeta k^2_y \right),$$

with

$$\gamma = -2(t_2 t_5 + 8t_3 t_3 + t_3 t_5 + 2t_2 t_5 + 9t_3 t_5) d_z^2 / E_g,$$

$$\zeta = -(t_1 + t_2) d_y^2.$$  

Proceeding with the integrals, we can obtain analytical expressions of the RKKY for $t_4 = 0$ as

$$\chi^{AA} = -\frac{C \sqrt{E_g} K_0(\sqrt{E_g} R)}{\gamma \zeta R},$$

$$\chi^{AB} = \frac{C}{\gamma \zeta R} \sqrt{E_g} \left(\frac{\lambda R}{\gamma \zeta R^2} \right) K_0(\sqrt{E_g} R) + \frac{2C \lambda R}{\gamma \zeta R^2} \left(\frac{\lambda R}{E_g R^2} - \gamma \right) K_0(\sqrt{E_g} R),$$

where $C = \frac{d_z^2 d_y^2}{32 \pi^2}, \lambda = \frac{E_g a}{2} + 2d_y(3t_3 - t_1 - t_2)$, and $K_0$ is the $0$th order modified Bessel function of the second kind. For a large distance $R$, the Bessel function $K_0(\sqrt{E_g} R) \to \frac{\left(\gamma \zeta R^2 \right)^{1/2} e^{-\sqrt{E_g} R}}{\sqrt{\pi E_g}},$ and thus $\chi$ produces an exponential factor $e^{-\sqrt{E_g} R}$ depending on the distance between two impurities. The exponential
factor, which dominates over large distances, explains the linear limit in figures 3(b) and (c), where a different slope originates from the anisotropy in the phosphorene structure $\mathcal{E}$. Compared with the undeformed case (solid lines), the strain (seeing dashed lines) cannot only increase the RKKY strength but also slow the RKKY decay rate (shrinking the slope) with distance by narrowing the bandgap $E_g$.

In equations (14) and (15), we also note that the RKKY is always ferromagnetic $\chi^{AA} < 0$ for impurities placed on the same sublattices, and interacts antiferromagnetically $\chi^{AB} > 0$ on the opposite sublattices. No transition appears from ferromagnetism to antiferromagnetism. This scenario resembles that of graphene \[32–35\]. At the same time, we find that $g(\mathbf{k})$ or $t_4$ plays a negligible role on $\chi$ for this weak strain. With the further increase in strain, the electron–hole asymmetry is enhanced and $E_c(\mathbf{k})$ enters the negative energy regime.

In this situation, the formulas in equations (10) and (11) fail and we need to perform numerical calculations by inserting equation (7) into equation (6). Since the strongest RKKY interaction occurs in the typical AC direction, in the following we focus on this configuration only.

We find that once $E_c(\mathbf{k})$ enters the negative energy regime, the effect of $t_4$ is visible by causing RKKY oscillations around $\chi = 0$, as shown in figure 4. This oscillating behavior is very interesting because it raises the possibility of switching the magnetic interaction between ferromagnetism and antiferromagnetism. The oscillating RKKY with slow decay dominates over a long distance and can be fitted roughly with a sinusoidal function $\alpha \sin(\beta R + \xi) / R^2$, which is similar to the behavior of impurities in two-dimensional metals \[41, 42\]. The fitted parameters $\alpha$, $\beta$ and $\xi$ are dependent on the strain strength. For example, the oscillation period $2\pi / \beta$ becomes short with an increasing strain magnitude, as shown in the inset of figure 4(a). The underlying physics of the oscillation is the interference effect between contributions from positive and negative energy in the conduction band. We also find that the oscillating amplitude is sensitive to the bandgap $E_c$. With the strain increase $\epsilon_y = -0.05, -0.08, -0.12, -0.16$ as shown in figures 4(a) and (b), the oscillation amplitude becomes more and more significant due to the narrowed gap (see figure 2(b)), accompanied by a shortened period. For

![Figure 4. The oscillation effect of RKKY interaction for two impurities, distributed (a) on the same sublattices $\chi^{AA}$ and (b) on opposite sublattices $\chi^{AB}$. The strain is exerted along the typical ZZ direction $\epsilon_y = -0.05, -0.08, -0.12, -0.16$; the inset is the change in oscillation period $2\pi / \beta$ with $\epsilon_y$.](image-url)
other impurity configurations in figure 3(a), our numerical calculations show that similar results can be obtained but with a weaker oscillation amplitude. For the same impurity configuration—but with the strain exerted along the x direction—a larger $\epsilon_x$ is needed to narrow the bandgap and then to generate the oscillation. One can recall that RKKY oscillation has also been reported in doped graphene [35] but with different physics. In their study, the oscillation phenomenon stems either from the interference between two Dirac cones $K$ and $K'$ and the factor $\cos[(K - K') \cdot R_y]$, or from the finite size of the Fermi surface. However, the present scenario is essentially different because the phosphorene possesses only a single Dirac cone without doping ($\mu$ located at the Γ point). Here, the essential role is played by the hopping parameter $t_4$, which was also once reported to cause interesting effects such as the quasi-flat edge band on the phosphorene zigzag edge [37].

The above numerical results show that $t_4$ plays a determined role in generating the RKKY oscillation by modifying the Fermi surface of strained phosphorene. In order to clarify this point, in figure 5(a) we plot the exchange interaction $\chi^{AA}$ versus $R$ for different values of $t_4$. Without $t_4$, the oscillation of $\chi^{AA}$ quickly vanishes and is replaced by a monotonous decay. With the increase in $t_4$, the oscillation becomes stronger. From here, we know that the strain-induced oscillation in figure 4(a) is realized through increasing the size of $t_4$. Here, we want to point out that the appearance of a negative energy conduction band, which is caused by $t_4$ through the breaking of the electron–hole symmetry, is critical to the formation of the oscillation. The strain dependence of the RKKY interaction is shown in figure 5(b), where different distances between two impurities are chosen. It is shown that the RKKY interaction is nonmonotonously dependent on the linear strain. For a fixed spatial distance between impurities, the strain can reverse the RKKY from antiferromagnetism to ferromagnetism. This proves to be an alternative approach to tuning the impurity interactions in phosphorene materials.

Figure 5. (a) The dependence of $\chi^{AA}$ on parameter $t_4$ as a function of $R$ with the strain $\epsilon_x = -0.12$ applied. (b) The variation of $\chi^{AA}$ with strain $\epsilon_y$ for a different distance $R$. 

![Image of figure 5](image-url)
5. Summary

We have studied the RKKY interaction and its tunability with strain in the tight-binding model when two magnetic impurities are positioned on the same/opposite phosphorene sublattices. First, we analyze the variation of energy dispersion and find the strain can cause the closing of the large bandgap, semi-Dirac dispersion, and negative energy in the conduction band. Then, we compare the RKKY interaction for impurities distributed in four different structural configurations. It is found that although they all fall exponentially in all directions, their decay patterns are different from each other due to the strong anisotropic structure of phosphorene. When an in-plane strain is applied, the decay rate of the exchange coupling can be weakened, and in the meantime, the strain effect is also anisotropic. The strongest strain effect is the deformation along the typical ZZ direction and the weakest one is along the typical AC. Interestingly, although we use the linear strain to deform the phosphorene structure, the response of the RKKY interaction is not simply a linear change with the strain. More importantly, we find that large amounts of strain within the elastic limit can switch the RKKY interaction from ferromagnetism to antiferromagnetism, exhibiting spatial oscillatory behavior around the zero value. The RKKY oscillation becomes more and more prominent with the increasing strength of the strain. This is the joint effect of the negative energy of the conduction band due to the modification of the Fermi surface of strained phosphorene and the narrowing gap, which can be reached simultaneously by using the strain. The underlying mechanism is different from that reported previously in graphene. Therefore, the strain effect provides the possibility of tuning the impurity interactions in phosphorene materials.

Acknowledgments

This work was supported by the National Natural Science Foundation of China (grant nos. 11474106 and 11774100), by Key Program for Guangdong NSF of China (grant no. 2017B030311003), by GDUPS(2017), and by the Innovation Project of Graduate School of South China Normal University.

References

[1] Xia F, Wang H and Jia Y 2014 Nat. Commun. 5 4458
[2] Low T, Rodin A S, Carvalho A, Jiang Y, Wang H, Xia F and Castro Neto A H 2014 Phys. Rev. B 90 075434
[3] Youngblood N, Chen C, Koester S J and Li M 2015 Nat. Photon. 9 247–52
[4] Li L, Yu Y, Ye G J, Ge Q, Ou X, Wu H, Feng D, Chen X H and Zhang Y 2014 Nat. Nanotechnol. 9 372–7
[5] Koenig S P, Doganov R A, Schmidt H, Neto A H and Özyilmaz B 2014 Appl. Phys. Lett. 104 103106
[6] Liu H, Neal A T, Zhu Z, Luo Z, Xu X, Tománík D and Ye P D 2014 ACS Nano 8 4033
[7] Qiao J, Kong X, Hu Z X, Yang F and J H W 2014 Nat. Commun. 5 4475
[8] Cai Y, Zhang G and Zhang Y 2014 Sci. Rep. 4 6677
[9] Peng X, Wei Q and Coppée A 2014 Phys. Rev. B 90 085402
[10] Wei Q and Peng X 2014 Appl. Phys. Lett. 104 251915
[11] Guo H, Lu N, Dai J, Wu X and Zeng X C 2014 J. Phys. Chem. C 118 14051
[12] Elahi M, Khalili K, Tabatabaei S M, Pourfath M and Asgari R 2015 Phys. Rev. B 91 115412
[13] Jiang J W and Park H S 2015 Phys. Rev. B 91 235118
[14] Rodin A S, Carvalho A and Castro Neto A H 2014 Phys. Rev. Lett. 112 176801
[15] Han X, Stewart H M, Shevlin S A, Catlow C R A and Guo Z X 2014 Nano Lett. 14 4607
[16] Qin G, Yan Q B, Qin Z, Yue S Y, Cai H J, Zheng Q R and Su G 2014 Sci. Rep. 4 6946
[17] Manjanath A, Samanta A, Pandey T and Singh A K 2015 Nanotechnology 26 075701
[18] Elahi M, Khalili K, Tabatabaei S M, Pourfath M and Asgari R 2015 Phys. Rev. B 91 115412
[19] Li Y, Yang X and Li J 2014 J. Phys. Chem. C 118 23970
[20] Tahir M, Vasilopoulos P and Peeters F M 2015 Phys. Rev. B 92 045420
[21] Tran V, Soklaski R, Liang Y and Yang L 2014 Phys. Rev. B 89 235319
[22] Chen X, et al 2015 Nat. Commun. 6 7315
[23] Li H Y, Lu W J, Shao D F and Sun Y P 2014 Phys. Rev. B 90 085433
[24] Zhu J J, Yao D X, Zhang S C and Chang K 2013 Phys. Rev. Lett. 106 097201
[25] Abanin D A and Pesin D A 2011 Phys. Rev. Lett. 106 136802
[26] Biswas R R and Balatsky A V 2010 Phys. Rev. B 81 233405
[27] Chang H R, Zhou J, Wang S X, Shan W Y and Xiao D 2015 Phys. Rev. B 92 241103
[28] Pozzobon M A H, Lopez-Sancho M P, Stauber T and Guinea F 2005 Phys. Rev. B 72 155121
[29] Dugaev V K, Litvinov V I and Fal'ko V I 2009 Phys. Rev. B 80 233409
[39] Harrison W A 1999 Elementary Electronic Structure (Singapore: World Scientific)
[40] Tang H, Jiang J W, Wang B S and Su Z B 2009 Solid State Commun. 149 82
[41] Fischer B and Klein M W 1975 Phys. Rev. B 11 2025
[42] Béal-Monod M T 1987 Phys. Rev. B 36 8835