Research article

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Photonic spin Hall effect of monolayer black phosphorus in the Terahertz region

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Abstract: As a two-dimensional (2D) material, black phosphorus (BP) has attracted significant attention owing to exotic physical properties such as low-energy band gap, high carrier mobility, and strong in-plane anisotropy. The striking in-plane anisotropy is a promising candidate for novel light-matter interaction. Here, we investigate the photonic spin Hall effect (PSHE) on a monolayer of BP. Due to the in-plane anisotropic property of BP, the PSHE is accompanied with Goos-Hänchen and Imbert-Fedorov effects, resulting in an asymmetric spin splitting. The asymmetric spin splitting can be flexibly tuned by the angle between the incident plane and the armchair crystalline direction of BP and by the carrier density via a bias voltage. The centroid displacements of two opposite spin components of the reflected beam along directions parallel and perpendicular to the incident plane can be considered as four independent channels for information processing. The potential application in barcode-encryption is proposed and discussed. These findings provide a deeper insight into the spin-orbit interaction in 2D material and thereby facilitate the development of optoelectronic devices in the Terahertz region.

1 Introduction

Two-dimensional (2D) materials have received a huge amount of interest in recent years due to their exciting physical properties [1–4]. Amongst them, black phosphorus (BP) has a unique bandgap that varies from around 0.3 eV in the bulk to approximately 1.5–2.0 eV in monolayer [5]. The carrier mobility in BP can reach up to $10^4 \text{ cm}^2/\text{V} \cdot \text{s}$ [6]. Thus, BP finds applications ranging from photodetector [7–9], optical modulator [10], ultrafast laser [5] to biosensor [11] etc. In monolayer BP, the phosphorus atoms form a hexagonal lattice with a puckered structure resulting in its in-plane anisotropic property [5, 7]. The striking in-plane anisotropy of BP enables novel polarization-dependent and angle-resolved optoelectronic devices [12–14]. In 2015, a polarization-sensitive broadband photo detector was demonstrated by using a BP vertical p–n junction [14]. In 2017, a BP-based wave plate was fabricated, where the polarization-plane rotation per atomic layer reached up to $\sim 0.005^\circ$ [15]. Lately, an orientation induced diode was demonstrated with a few-layer BPs [16], where large tunable current rectification and strong anisotropic photocurrent were observed [16]. Recently, BP was shown to be a prospective material for spintronics [17] due to the strong spin-orbit coupling in high quality BP. The spin relaxation time was measured to be 4 ns with a spin relaxation length exceeding $6 \mu\text{m}$ [17]. To addition, quantum Hall effect in BP was observed by embedding BP in van der Waals hetero structure [18]. High carrier Hall mobility as high as $6000 \text{ cm}^2/\text{V} \cdot \text{s}$ was achieved [18].

Here, the photonic spin Hall effect (PSHE) on a monolayer BP is investigated systematically. The PSHE originates from the spin-orbit interaction of light, which is a striking phenomenon in optics, and it has applications ranging from optical shaping to unidirectional coupling [19–21]. Due to the in-plane anisotropy of BP,

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the spin-dependent shifts originated from the PSHE are accompanied by both spin-independent Goos-Hänchen (GH) and Imbert-Fedorov (IF) shifts, resulting in an asymmetric spin splitting of the reflected Gaussian beam in directions both parallel and perpendicular to the plane of incidence [22–24]. The asymmetric spin splitting, relying on the angle between the incident plane and the armchair crystalline direction can be enhanced by the incident orbital angular momentum (OAM). The modulation of the asymmetric spin splitting by the carrier density in the monolayer BP is studied based on which the potential applications in barcode-encryption is proposed and discussed.

2 Model and theory

Let us consider a monochromatic light beam illuminating onto a monolayer BP sitting on a silicon substrate. The photonic property of BP can be described by a surface conductivity. Due to the in-plane anisotropic property, the

conductivity is different along the armchair or zigzag crystalline directions. Under the Drude model, it is [25–27]:

$$\sigma_{\text{arm,zig}} = (iD_{\text{arm,zig}}) / [\pi(\omega + i\eta/\hbar)] \quad (1)$$

where $D_{\text{arm,zig}} = \pi e^2 n / m_{\text{arm,zig}}$ is the Drude weight. The electron mass along the armchair or zigzag directions are $m_{\text{arm}} = \hbar^2 / (2\gamma^2 / \Delta + \eta_c)$, $m_{\text{zig}} = \hbar^2 / 2v_c$ respectively, where $\eta = 10$ meV, $\gamma = 4a/\pi$ eV, $\Delta = 2$ eV, $\eta_c = \hbar^2 / 0.4 m_0$, $v_c = \hbar^2 / 1.4 m_0$. The scale length of BP $a = 0.223$ nm. The electron carrier density n can be changed by electric doping via a bias voltage [9, 17].

By rotating the BP, the incident plane makes an angle of ϕ with the armchair axis of BP crystal, as shown in Figure 1A. Therefore, the conductance matrix connecting the surface current and electric light field can be given by $\sigma = [\sigma_{pp}, \sigma_{ps}; \sigma_{sp}, \sigma_{ss}]$, where $\sigma_{pp} = \sigma_{\text{arm}} \cos^2 \phi + \sigma_{\text{zig}} \sin^2 \phi$, $\sigma_{ss} = \sigma_{\text{arm}} \sin^2 \phi + \sigma_{\text{zig}} \cos^2 \phi$, and $\sigma_{sp} = \sigma_{ps} = (\sigma_{\text{zig}} - \sigma_{\text{arm}}) \sin \phi \cos \phi$ [25]. The cross conductivity σ_{sp} vanishes for isotropic 2D materials such as graphene [2]. For BP, however, σ_{sp} is generally nonzero except when the rotation angle $\phi = 0^\circ$ and 90° . The cross conductivity induces a coupling between p and s waves. Thus it will strongly affect the PSHE [28, 29].

Figure 1: Scheme of BP-Si system, the Fresnel reflection coefficients, orientation angle, polarization ellipticity and Centroid displacements of RCP and LCP.

(A) Schematic of the asymmetric spin splitting in BP-Si substrate system. (B) The Fresnel reflection coefficients with and without monolayer BP. With BP, the non-diagonal reflection coefficient emerges. (C) The orientation angle and polarization ellipticity of reflected plane wave with H incident polarization. (D) Centroid displacements of RCP and LCP components of the reflected Gaussian beam.

The Fresnel reflection coefficients of BP-Si substrate structure can be derived by using the electromagnetic boundary condition. According to Ref. [29], they can be considered as:

$$r_{pp} = (\beta_+ \alpha_- + \chi) / (\beta_+ \alpha_+ + \chi) \quad (2)$$

$$r_{ss} = -(\beta_- \alpha_+ + \chi) / (\beta_+ \alpha_+ + \chi) \quad (3)$$

$$r_{ps} = -r_{sp} = \Lambda / (\beta_+ \alpha_+ + \chi) \quad (4)$$

where, $\alpha_{\pm} = (k_{iz} \varepsilon \pm k_{iz} \varepsilon_0 + k_{iz} k_{tz} \sigma_{pp} / \omega) / \varepsilon_0$, $\beta_{\pm} = (k_{tz} \pm k_{iz} + \omega \mu_0 \sigma_{ss})$, $\chi = -k_{iz} k_{tz} \sigma_{ps}^2 / \varepsilon_0$, $\Lambda = 2k_{iz} k_{tz} Z_0 \sigma_{ps}$, $k_{iz} = k_0 \cos \theta$, and $k_{tz} = k_0 \varepsilon^{1/2} \cos \theta_t$. And θ , θ_t being the incident and transmitted angles, respectively. k_0 , ε_0 , μ_0 , ε are the wavenumber, permittivity, permeability in vacuum, and the permittivity of the silicon substrate, respectively. The non-diagonal reflection coefficients r_{ps} and r_{sp} originate from the cross conductivity σ_{sp} .

Assume that a horizontally (H) polarized Gaussian beam is illuminated on the BP-Si substrate structure. The angular spectrum of the incident beam can be represented by $\tilde{\mathbf{E}}_i = \exp[-(k_{ix}^2 + k_{iy}^2)w_0^2/4]H$ where w_0 being the beam waist. Under the paraxial condition, the angular spectrum of the reflected beam relates to the incident beam through a transformation matrix, as is detailed in Ref. [29]. In a circular polarization basis, the reflected angular spectrum is [28, 29]:

$$\tilde{\mathbf{E}}_r^{\pm} = \left[\left(r_{pp} + \frac{Mk_{ry}}{k_0} - \frac{k_{rx} \partial r_{pp}}{k_0 \partial \theta} \right) \mp i \left(r_{sp} - \frac{k_{rx} \partial r_{sp}}{k_0 \partial \theta} k_{rx} - \frac{Nk_{ry}}{k_0} \right) \right] \tilde{\mathbf{u}}_0 | \pm \rangle \quad (5)$$

Here, $M = (r_{sp} - r_{ps}) \cot \theta$, $N = (r_{pp} + r_{ss}) \cot \theta$, $k_{rx} = -k_{ix}$, and $k_{ry} = k_{iy}$. The RCP and LCP components are no longer maintaining the Gaussian envelope, and their centroids may shift along x_r - and y_r -axes. With respect to the geometric prediction, the centroid displacements can be defined as $[X_{\pm}, Y_{\pm}] = \iint [\partial_{k_{rx}}, \partial_{k_{ry}}] |\tilde{\mathbf{E}}_r^{\pm}|^2 dk_{rx} dk_{ry} / \iint |\tilde{\mathbf{E}}_r^{\pm}|^2 dk_{rx} dk_{ry}$ [30]. After some mathematical calculation, we obtain:

$$X_{\pm} = \left\{ \text{Im} \left[r_{pp}^* \frac{\partial r_{pp}}{\partial \theta} + r_{sp}^* \frac{\partial r_{sp}}{\partial \theta} \right] \pm \text{Re} \left[-r_{pp}^* \frac{\partial r_{sp}}{\partial \theta} + r_{sp}^* \frac{\partial r_{pp}}{\partial \theta} \right] \right\} / k_0 W_{\pm} \quad (6)$$

$$Y_{\pm} = \left\{ -\text{Im} [r_{pp}^* M - r_{sp}^* N] \pm \text{Re} [-r_{pp}^* N - r_{sp}^* M] \right\} / k_0 W_{\pm} \quad (7)$$

where

$$W_{\pm} = |r_{pp}|^2 + |r_{sp}|^2 \pm 2\text{Im} [r_{pp}^* r_{sp}] + \frac{1}{k_0^2 w_0^2} \left\{ \left| \frac{\partial r_{pp}}{\partial \theta} \right|^2 + \left| \frac{\partial r_{sp}}{\partial \theta} \right|^2 \pm 2\text{Im} \left[\frac{\partial r_{pp}}{\partial \theta} \frac{\partial r_{sp}}{\partial \theta} \right] + |M|^2 + |N|^2 \mp 2\text{Im} [M^* N] \right\} \quad (8)$$

The centroid displacements along x_r - and y_r -axes ($X_{\pm}$ and $Y_{\pm}$) contain two terms. The first term of $X_{\pm}$ is the GH shift, while the first term of $Y_{\pm}$ is the IF shift [30]. They are spin-independent shifts, moving the RCP and LCP components of the reflected beam together. The second terms of $X_{\pm}$ and $Y_{\pm}$ are spin-dependent, originating from the spin-orbit interaction [31–33]. These terms shift RCP and LCP components toward opposite directions [24]. In Ref. [32], only the spin-dependent terms were studied, where symmetric spin splitting was obtained, and it demonstrates great promise for detecting the parameters of anisotropic two-dimensional atomic crystals. Generally, the cooperation effect of the spin-independent and spin-dependent terms of the centroid displacements will result in asymmetric spin splitting.

For isotropic 2D materials, the second term of Equation (6) and the first term of Equation (7) vanish because of the vanishment of the non-diagonal reflection coefficients r_{ps} and r_{sp} . Thus, the reflected beam will undergo a GH shift along x_r -axis and a symmetric spin splitting along y_r -axis. No asymmetric spin splitting can be observed in isotropic 2D materials. Asymmetric spin splitting will occur in anisotropic materials [32], chiral media [28], and graphene under magnetic field [30] due to the nonzero off-diagonal reflection coefficients. As will be shown below, in the asymmetric spin splitting of monolayer BP, the displacements of RCP and LCP reflected components can be enhanced by the incident OAM and tuned flexibly by the carrier density via a bias voltage. Based on this, a novel barcode-encryption scheme is possible.

3 Results and discussion

Figure 1B shows the Fresnel reflection coefficients of air-BP-Si substrate system with and without BP, when $\phi = 45^\circ$, $f = 1$ THz, and $n = 10^{16} \text{ m}^{-2}$. The Brewster angle of the air-Si interface without BP is $\theta_B = 73.77^\circ$ where the considered permittivity of the Si substrate $\varepsilon = 11.69$. By displacing a monolayer BP on the Si substrate, the Brewster angle is perturbed [34], and it becomes $\theta'_B = 74.5^\circ$. Moreover, $|r_{pp}|$ cannot decrease to zero and a nonzero $|r_{ps}|$ emerges. For a H polarized incident plane wave, the reflected wave becomes elliptically polarized near the angle of $\theta'_B = 74.5^\circ$. The reflected plane wave contains both RCP and LCP components. As shown in Figure 1C, both the orientation angle and ellipticity of the reflected polarization state change with the incident angle. For a Gaussian incident beam, the centroids the RCP and LCP components will shift due

Figure 2: The dependences of the displacements $Y_{\pm}$ on the incident angle θ for $\phi = 0^\circ, 30^\circ, 60^\circ, 90^\circ, 120^\circ, 150^\circ$, respectively. In the calculations, $f = 1$ THz, $n = 1.2 \times 10^{17} \text{ m}^{-2}$.

to the cooperation effect of the PSHE and GH and IF shifts, as clearly shown in Figure 1D.

In the following, we focus on the asymmetric spin splitting of Gaussian incident beams. Figure 2 shows how the centroid displacements along y_r -axis ($Y_{\pm}$) changing with respect to incident angle θ for the cases of $\phi = 0^\circ, 30^\circ, 60^\circ, 90^\circ, 120^\circ, 150^\circ$, respectively. For each case, $Y_{\pm}$ takes large values near $\theta'_B = 74.5^\circ$. When the incident plane is parallel to the armchair or zigzag crystalline directions ($\phi = 0^\circ, 90^\circ$), the reflected beam undergoes symmetric spin splitting along y_r -axis, i.e. $Y_+ = -Y_-$, which is due to the vanishment of the cross conductivity. The displacements of the RCP and LCP components will intersect, where $Y_{\pm} = 0$. The maximum displacement $|Y_{\pm}|$ for the case of $\phi = 90^\circ$ is 0.73 mm, which is larger than that of $\phi = 0^\circ$. When $\phi \neq 0^\circ$ or 90° , the spin splitting is asymmetric. At the intersection points of the displacements for the RCP and LCP components, Y_+ is equal to Y_- . But they do not vanish anymore. That is, they become two opposite spin components of the reflected beam which shift together. The intersection point moves from 74.82° to 74.17° , when the rotation angle ϕ increases from 0 to 90° . When ϕ increases up to 180° , the intersection point moves back to 74.82° gradually. When the incident angle moves away from the intersection points, Y_+ and Y_- are different, where asymmetric spin splitting can be observed. However, the spin splitting becomes symmetric ($Y_+ = -Y_-$) when the incident angle moves away further.

Figure 3A and B show the displacements $Y_{\pm}$ changing with the rotation angle ϕ and carrier density n when

$\theta = 74.43^\circ$, and $f = 1$ THz. In the present case, the centroid displacements of two opposite spin components are opposite in signs. However, their absolute values are different. The largest asymmetric spin splitting takes place near $\phi = 56.4^\circ$ and 123.6° . For example, at point $(\phi, n) = (56.4^\circ, 1.2 \times 10^{17} \text{ m}^{-2})$, $Y_+ = 0.80$ mm, whereas Y_- is only -0.01 mm. Both the displacements of the RCP and LCP reflected field components vary with the carrier density. However, their variations are different. Therefore, the asymmetric spin splitting can be modulated efficiently by the carrier density.

The asymmetric spin splitting $Y_{\pm}$ changes with the frequency f . As shown in Figure 3C and D, when f increases from 1 THz to 3 THz, the displacements $|Y_{\pm}|$ decrease gradually. When the rotation angle varies from 0° to 180° , the displacement of RCP component of the reflected beam changes firstly from positive to negative values and then returns back to positive values, and vice versa for the LCP component.

Due to the absorption, the monolayer BP induces centroid displacements of the reflected beam which shifts along x_r -axis, which should vanish for an air-Si interface without BP. The reflected beam undergoes GH shift for the special cases of $\phi = 0^\circ$ and 90° , where the two spin components are not split. However, they will split generally owing to the cross conductivity σ_{sp} induced spin-dependent shifts (the second term in Equation (6)). As shown in Figure 4A and B, the displacements $X_+ = 7.43$ mm and $X_- = 4.43$ mm when $(\phi, \theta) = (35^\circ, 74.7^\circ)$. At $(\phi, \theta) = (145^\circ,$

Figure 3: Change of displacements $Y_{\pm}$ with rotating angle, carrier density and frequency.

(A, B) Changes of displacements $Y_{\pm}$ as a function of the rotation angle ϕ and carrier density n when the incident angle $\theta = 74.43^\circ$, $f = 1$ THz. (C, D) The changes of displacements $Y_{\pm}$ as a function of ϕ and f .

Figure 4: Change of displacement $X_{\pm}$ with rotating angle and incident angle, frequency and carrier density.

(A, B) The displacements $X_{\pm}$ changing with the rotation angle ϕ and incident angle θ . (C, D) The dependences of $X_{\pm}$ on the frequency f and carrier density n for $\theta = 74.1^\circ$ and $\phi = 30^\circ$.

74.69°), $X_+ = 4.43$ mm and $X_- = 7.43$ mm. Different from the displacements along y_r -axis, the displacements along x_r -axis are always positive.

The dependence of the displacements along x_r -axis on the frequency f and carrier density n for $\phi = 30^\circ$, $\theta = 74.1^\circ$ is shown in Figure 4C and D, where the asymmetric spin splitting is clearly seen. The

maximum $X_+ = 7.44$ mm is obtained at $(f, n) = (1.34$ THz, $4.89 \times 10^{16} \text{ m}^{-2})$, while the maximum $X_- = 7.21$ mm at $(f, n) = (1$ THz, $4.82 \times 10^{16} \text{ m}^{-2})$.

The centroid displacements along both x_r - and y_r -axes which will be affected by the incident OAM, due to the emerging of additional OAM-dependent terms [23, 28, 35].

An incident Laguerre–Gaussian (LG) beam carrying OAM can be given by $\tilde{\mathbf{E}}_i = [-ik_x + \text{sgn}(\ell)k_y]^{|\ell|} \exp[-(k_x^2 + k_y^2)w_0^2/4]H\rangle$. Where ℓ is topologic charge, $\text{sgn}(\ell)$ denotes the sign of ℓ [28]. The numerical results for the centroid displacements $X_{\pm}$ and $Y_{\pm}$ when $\theta = 75^\circ$ are given in Figures 5 and 6, respectively. As shown in Figure

5A and D, the spin splitting is asymmetric even for the cases of $\phi = 0^\circ, 90^\circ$. This is because the OAM induces additional spin-dependent shift as a result of the orbit-orbit interaction. This spin-dependent shift together with the GH shift leads to the asymmetric spin splitting. The asymmetric spin splitting can change with respect

Figure 5: The dependences of the displacements $X_{\pm}$ on the incident OAM ℓ for $\phi = 0^\circ, 30^\circ, 60^\circ, 90^\circ, 120^\circ, 150^\circ$, respectively.

Figure 6: The dependences of the displacements $Y_{\pm}$ on the incident OAM ℓ for $\phi = 0^\circ, 30^\circ, 60^\circ, 90^\circ, 120^\circ, 150^\circ$, respectively.

to the rotation angle, negative displacements can be obtained.

For the displacements along y_r -axis, the asymmetric spin splitting phenomenon can also be observed for the cases of $\phi=0^\circ, 90^\circ$, resulting from the OAM induced IF shift. It is worth noted that the displacement $|Y_\pm|$ increases with the incident OAM $|\ell|$, thus the OAM can enhance the asymmetric spin splitting efficiently.

Based on the above analysis, we conclude that the asymmetric spin splitting can be modulated dramatically by the carrier density via a bias voltage. The asymmetric displacements for LCP and RCP components of the reflected beam along x_r - and y_r -axes can be regarded as four independent channels for information processing. The centroid displacements larger than a certain threshold value can be considered as “1”, while smaller than that value as “0”. The encoding rule varies with the choice of the threshold values. The threshold values for the displacements along x_r - and y_r -axes can be different. Here, the threshold values are chosen respectively as 0 and 2 mm for Gaussian incident beam. As shown in Figure 7A, several different codes: “0001”, “0101”, “1101”, “1111”, “1110”, “0110”, “0010” have been obtained by tuning the carrier density. Figure 7B shows the four-channel barcode encryption for the case of high-order LG beam ($\ell=1$),

Figure 7: Schematics of barcode encryption based on the asymmetric spin splitting for the cases of $\ell=0$ (fundamental Gaussian beam) and 1 (higher-order LG beam).

where eight different codes are given. This four-channel information processing scheme with monolayer BP is superior compared to the scheme based on graphene, where there are only two independent channels [30].

The experimental measurement of the asymmetric spin splitting is possible since the spin-dependent shifts and the GH shifts of 2D materials have been observed experimentally [36, 37]. And the experimental scheme for the observation of PSEH and GH effect on 2D atomic crystals in quantum Hall regime was proposed recently [38, 39]. Here, we propose a possible experimental scheme for the asymmetric spin splitting in monolayer BP. As shown in Figure 8, a Gaussian beam from a laser source passes through a half-wave plate (HWP) and then is focused by a lens into the monolayer BP. Before the focused lens, a linear polarizer is used to choose H polarization state. The reflected beam from BP is collimated by another lens and then passes through a quarter-wave plate (QWP) which yields an angle of 45° with respect to the x_r -axis. Thus, the QWP converts circular polarization states into linear polarization ones [40]. A polarization beam splitter (PBS) is used to separate the two orthogonal polarization states, and they are recorded by two charge coupled devices, respectively. Therefore, the centroid shifts of the RCP and LCP components of the reflected beam can be obtained from the recorded intensity patterns. Figure 8B–D show the intensity distributions of the Gaussian incident beam and reflected RCP and LCP components, respectively. The

Figure 8: The possible experimental scheme and the intensity patterns of incident and reflected beams. (A) The possible experimental scheme for the asymmetric spin splitting in BP. (B–D) Intensity patterns of the Gaussian incident beam (B) and the RCP (C) and LCP (D) components of the reflected beam, respectively.

monolayer BP is separated by a SiO₂ thin layer (10 nm) from Si substrate. Thus, the carrier density of BP can be modulated by a gate voltage. To measure the asymmetric spin splitting of higher-order LG beam, a spatial light modulator is needed to convert Gaussian beam into LG beam with the desired order.

4 Conclusion

The novel PSHE has been studied systematically in monolayer BP. The in-plane anisotropy induces both spin-dependent and spin-independent shifts, which results in asymmetric spin splitting in both x_r - and y_r -directions. The asymmetric spin splitting can be enhanced by the incident OAM ℓ , and be efficiently modulated by the rotation angle ϕ and the carrier density n . Based on the tunable asymmetric spin splitting, we achieve four-channel barcode encoding for both foundational Gaussian and higher-order LG incident beams. The asymmetric spin splitting is general for anisotropic 2D materials such as BP, ReS₂, and ReSe₂ [15]. The PSHE in anisotropic 2D materials promises novel electrically tunable and angle-resolved optoelectronic devices in the Terahertz region.

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