Photoinduced valley-polarized current of layered MoS$_2$ by electric tuning

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Abstract

A photoinduced current of a layered MoS$_2$-based transistor is studied from first-principles. Under the illumination of circular polarized light, a valley-polarized current is generated, which can be tuned by the gate voltage. For monolayer MoS$_2$, the valley-polarized spin-up (down) electron current at $K$ ($K'$) points is induced by the right (left) circular polarized light. The valley polarization is found to reach $+1.0$ ($-1.0$) for the valley current that carried such a $K$ ($K'$) index. For bilayer MoS$_2$, the spin-up (down) current can be induced at both $K$ and $K'$ valleys by the right (left) circular light. In contrast to monolayer MoS$_2$, the photoinduced valley polarization shows asymmetric behavior upon reversal of the gate voltage. Our results show that the valley polarization of the photoinduced current can be modulated by the circular polarized light and the gate voltage. All the results can be well understood using a simple kp model.

Keywords: MoS$_2$, electric tuning, valley-polarized current, ab initio calculation

As one of the most promising two-dimensional materials, graphene has shown exceptional physical, chemical, and optical properties [1–4]. However, pristine graphene does not have a gap between the valence band and the conduction band, which hampers its applications in semiconductor devices. Although layered transition-metal dichalcogenides (TMDCs) have a similar hexagonal structure to graphene, they show distinctly different properties from graphene [5–8]. First, TMDCs have strong spin-orbit coupling (SOC), which is originated from the $d$ orbitals of the heavy metal atoms. This makes TMDCs an exciting platform for exploring spintronic applications [9–11]. Second, monolayer TMDCs, due to their inversion symmetry breaking, display physical properties that are distinct from their bulk counterpart. TMDCs cross over from an indirect band gap semiconductor at bulk to a direct band gap semiconductor at monolayer [12, 13]. Most importantly, monolayer TMDCs have six valleys at the corners of their hexagonal Brillouin zone, which can be classified into two inequivalent groups. Such valleys have large separations in momentum space, which make the valley index robust against small deformation of its lattice and low-energy scattering by a long wavelength phonon. This means that the valley index can be used as a potential information carrier. The valley properties of graphene have been extensively studied theoretically [14–16]. Recently, there has been a growing interest in the special spin and valley properties of layered TMDCs, both experimentally and theoretically [17, 18]. Xiao et al [17] found that, in a monolayer TMDC, inversion symmetry breaking and SOC lead to coupled spin and valley physics. A monolayer TMDC has opposite spins at the two inequivalent $K$ points, making the optical transition rules between the valence band and the conduction band both spin dependent and valley dependent.

Carriers with various combinations of valley and spin indices can be selectively excited by optical fields with different circular polarizations [19, 20]. Circularly polarized luminescence has been observed in monolayer MoS$_2$ and bilayer MoS$_2$ under circularly optical pumping with different...
1.7534 eVgap stands for the lead of source APs. The energy of shining light is expressed in terms of $\Delta E_{\text{gap}}$. Schottky junction were studied selection rules for optical transitions in different valleys frequencies [21, 22]. This confirms the theoretical prediction that the circular polarization originates from the contrasting selection rules for optical transitions in different valleys [19].

For the potential device application of layered TMDC, the key issue is to examine the performance of nanoelectronic devices, such as transistors. Indeed, the properties of electron–hole transport and photovoltaic effect in a gated MoS$_2$ devices, such as transistors. Indeed, the properties of electron–hole transport and photovoltaic effect in a gated MoS$_2$ were studied [23]. The phototransistor based on monolayer MoS$_2$ exhibited good photoresponsivity and prompt photoswitching, and the mechanism of the response was analyzed in the ultrathin MoS$_2$ field-effect transistors by scanning photoinduced current microscopy [24–27]. So far, most of the investigations have concentrated on the valley-polarized current through layered MoS$_2$. In this work, we calculate the photoinduced valley-polarized current in monolayer and bilayer MoS$_2$ phototransistors. As shown in figure 1, the phototransistor consists of two semi-infinite sheets of monolayer/bilayer MoS$_2$ as leads and a central scattering region. A vertical electric field $E$ along the $z$ direction is produced by applying the gate voltage $V_g$ at the bottom gate in the central scattering region. The electron–photon interaction $H_{e-ph}$ by the first-order Born approximation. Here, $H_{e-ph} = \frac{e}{m} \mathbf{A} \cdot \mathbf{P}$, where $\mathbf{A}$ is the electromagnetic vector potential and $\mathbf{P}$ is the momentum of the electron. Detailed procedures for obtaining the Green’s function have been discussed in [41].

The photoinduced valley and spin-dependent current in the lead $\alpha$ can be written as [41, 42]

$$I_{\alpha s,\tau}^{ph} = \frac{e}{h} \int \frac{dE}{2\pi} \sum_{k \in \tau} T_{\alpha s}^{ph}(E, \mathbf{k}, s).$$

Here, $\tau = \pm 1$ (corresponding to $K/K'$) is the valley index, $\mathbf{k}$ around $K$ or $K'$ is calculated starting from the point of $K$ or $K'$, and $s$ is the spin index. $T_{\alpha s}^{ph}$ is the effective transmission coefficient of lead $\alpha$ and its expression is

$$T_{\alpha s}^{ph}(E, \mathbf{k}, s) = \text{Tr} \{ i \Gamma_{\alpha s}(E, \mathbf{k}) \{ 1 - f_{\alpha s}^F \} G_{\alpha s}^{<\alpha} \} s,$$

where $f_{\alpha s}^F$ is the Fermi distribution function of lead $\alpha$, $\Gamma_{\alpha s}$ is the linewidth function that reflects the coupling between the lead and the central scattering regions, and $G_{\alpha s}^{<\alpha}$ is the Green’s function including the contribution of voltage and photons [41].

To describe the current response to the light, we examine the photoresponse, which is defined as

$$F_{\tau, s} = \frac{I_{\alpha s,\tau}^{ph}}{eF_{ph}},$$

where $F_{\tau, s}$ is the current with valley index $\tau$ and spin index $s$. $F_{ph}$ is the photon flux defined as the number of photons per unit time per unit area.

Figure 2 shows the valley and spin-polarized photoresponse versus gate voltage under bias voltage 0.3 V. The
mainly excites the spin-down electrons at the incident light. In addition, the valley light, and the red
light, and the red
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solid red line, solid blue line, dashed red line, and dashed blue line correspond to photoresponse $f_{K,\uparrow}$, $f_{K,\downarrow}$, $f_{K',\uparrow}$, and $f_{K',\downarrow}$, respectively. From panel (a), we see that the component $f_{K,\uparrow}$ is, at least, one order of magnitude larger than the other three components, indicating that the right circular polarized light $\sigma^+$ mainly excites the spin-up electrons at the $K$ point from the valence band to the conduction band in monolayer MoS$_2$. Similarly, we conclude, from figure 2(b), that the left circular polarized light $\sigma^-$ mainly excites the spin-down electrons at the $K'$ point in monolayer MoS$_2$. This phenomenon is due to the symmetry breaking in monolayer MoS$_2$ and can be explained by the optical selection rule [17]. The situation is different for bilayer MoS$_2$ where the inversion symmetry is restored. In this case, the spin-up components of the photoresponse ($f_{K,\uparrow}$ and $f_{K',\downarrow}$) are much larger than the other two components when $\sigma^+$ light is shed (panel (c)), whereas, the spin-down components ($f_{K,\downarrow}$ and $f_{K',\uparrow}$) dominate for $\sigma^-$ light (panel (d)).

To characterize valley intersection, we define valley polarization $\eta$ as

$$\eta = \frac{I_{K,\uparrow}^{\text{ph}} - I_{K',\downarrow}^{\text{ph}}}{I_{K,\uparrow}^{\text{ph}} + I_{K',\downarrow}^{\text{ph}}}$$

where $I_{K,\uparrow}^{\text{ph}} = I_{K,\uparrow}^{\text{ph}} + I_{K,\downarrow}^{\text{ph}}$. From panel (a) of figure 3, we see that almost fully polarized valley current is generated using either $\sigma^+$ or $\sigma^-$ incident light. In addition, the valley polarizations remain constant in the whole range of gate voltages from $-1.0$ to $1.0$ V, suggesting that the valley polarization of monolayer MoS$_2$ is robust against the gate voltage. In contrast, we find that the valley polarization is very sensitive to the gate voltage for bilayer MoS$_2$. As shown in panel (b) of figure 3, the valley polarization changes from $-0.25$ to $0.05$ in bilayer MoS$_2$ (blue dotted line in panel (b)) in the gate voltage window $[-1.0, 1.0]$ V when $\sigma^+$ light is shed. The valley polarization profile $\eta_\downarrow(V_g)$ satisfies $\eta_\downarrow(V_g) = -\eta_\uparrow(V_g)$. Hence, for bilayer MoS$_2$, the valley polarization can be modulated by the circular polarized light as well as the gate voltage. We also find that the modulation effect of the negative gate voltage is more significant than that of the positive one. To explain all of these phenomena, we examine the following kp model.

Due to the inversion symmetry breaking and the presence of strong SOC in monolayer MoS$_2$, spin and valley degrees of freedom couple to each other, i.e., $K$ ($K'$) valley is occupied by the spin-up (down) electrons at the top of the valence band. The electron interband transition from the top of the spin-split valence band to the bottom of the conduction band can be induced by the circular polarized light $\sigma^\pm$. If we define the coupling strength with $\sigma^\pm$ optical fields as $\mathcal{P}(\mathbf{k}, s)$, we have the following coupling intensity for transitions near $K/K'$ points [17]:

$$|\mathcal{P}(\mathbf{k}, \tau, s)|^2 = |P_0|^2 \left(1 \pm \frac{\xi'}{\sqrt{\xi^2 + 4\tau^2k^2}}\right),$$

where $|P_0|^2 = \frac{m_0^2c^2}{\tau}$, $\xi' = \xi - \tau\lambda$, $m_0$ is the free electron mass, $\lambda$ is the lattice constant, $\tau$ is the effective hopping integral, $\xi$ is the energy gap, $\tau = \pm 1$ is the valley index, $2\lambda$ is the spin splitting at the top of the valence band caused by SOC, and $s$ is for spin. To characterize the polarization of coupling, we define

$$\eta_\pm \equiv \frac{|\mathcal{P}(K')|^2 - |\mathcal{P}(K)|^2}{|\mathcal{P}(K')|^2 + |\mathcal{P}(K)|^2}.$$
maintains the inversion symmetry. To mimic the effect of the gate voltage in the \textit{ab initio} calculation, we introduce an electric field along the \( z \) direction in our kp model Hamiltonian. The kp model Hamiltonian for bilayer MoS\(_2\) with a perpendicular external electric field is expressed as follows \cite{43}:

\[
H(k, \tau, s_z) = \begin{bmatrix}
-\Delta U/2 & at(\tau k_z + ik_y) & 0 & 0 \\
0 & -\tau \xi \lambda - \Delta U/2 & 0 & t_{l} \\
0 & 0 & \xi + \Delta U/2 & at(\tau k_z - ik_y) \\
0 & t_{l} & at(\tau k_z + ik_y) & \tau \xi \lambda + \Delta U/2 \\
\end{bmatrix}
\]

(7)

where \( t_{l} \) is the intralayer hopping constant, \( \Delta U = Ed \), \( E \) is the magnitude of external electric field, and \( d \) is the distance between two monolayers. The external electric field \( E \) will induce an energy shift of \(-\Delta U/2\) at the upper layer and an energy shift \( \Delta U/2 \) at the lower layer in the bilayer MoS\(_2\). Here, all the parameters in equation (7) are taken from \cite{43}, and the basis is \( \{|d_{x^2-y^2}^{\uparrow}\rangle, \frac{1}{\sqrt{2}}(ld_{x^2-y^2}^{\uparrow})\rangle, \frac{1}{\sqrt{2}}(ld_{x^2-y^2}^{\downarrow})\rangle\rangle \)

By diagonalizing equation (7), we obtain the eigenfunctions \( |K\uparrow\rangle, |K\downarrow\rangle, |K'\uparrow\rangle \), and \( |K'\downarrow\rangle \) with \( k = 0 \) near the top valence band as follows:

\[
|K\uparrow\rangle = \begin{bmatrix} 0 \\ \sin \alpha_1 \\ 0 \\ \cos \alpha_1 \end{bmatrix} \otimes |\uparrow\rangle, \quad |K\downarrow\rangle = \begin{bmatrix} 0 \\ \sin \alpha_2 \\ 0 \\ \cos \alpha_2 \end{bmatrix} \otimes |\downarrow\rangle.
\]

(8)

\[
|K'\uparrow\rangle = \begin{bmatrix} 0 \\ \sin \alpha_2 \\ 0 \\ \cos \alpha_2 \end{bmatrix} \otimes |\downarrow\rangle, \quad |K'\downarrow\rangle = \begin{bmatrix} 0 \\ \sin \alpha_1 \\ 0 \\ \cos \alpha_1 \end{bmatrix} \otimes |\uparrow\rangle.
\]

(9)

and

\[
E_{\alpha 1} = \sqrt{t_{l}^2 + \left( \lambda + \frac{\Delta U}{2} \right)^2},
\]

\[
E_{\alpha 2} = \sqrt{t_{l}^2 + \left( \lambda - \frac{\Delta U}{2} \right)^2}.
\]

(10)

Under the illumination of circular polarized light, the coupling intensities are found to be

\[
|\mathcal{P}_Q(K, \uparrow)\rangle^2 = |P_d|^2 \cos^2 \alpha_1, |\mathcal{P}_Q(K, \downarrow)\rangle^2 = |P_d|^2 \cos^2 \alpha_2,
\]

\[
|\mathcal{P}_Q(K', \uparrow)\rangle^2 = |P_l|^2 \sin^2 \alpha_2, |\mathcal{P}_Q(K', \downarrow)\rangle^2 = |P_l|^2 \sin^2 \alpha_1,
\]

\[
|\mathcal{P}_Q(K', \uparrow)\rangle^2 = |P_d|^2 \cos^2 \alpha_2, |\mathcal{P}_Q(K', \downarrow)\rangle^2 = |P_d|^2 \cos^2 \alpha_1.
\]

In figure 5(a), we plot the valley coupling polarization versus the gate voltage using the formula above. Similar to figure 2(b), we have \( \eta_{\perp}^c(\Delta U) = -\eta_{\parallel}^c(\Delta U) \). However, we also have a relation \( \eta_{\parallel}^c(\Delta U) = -\eta_{\perp}^c(-\Delta U) \), i.e., \( \eta_{\pm}^c \) are odd functions of \( \Delta U \) which are different from our first-principles results. In fact, from equation (12) one can easily get

\[
\eta_{\pm}^c = \pm \frac{1}{2} (\cos(2\alpha_1) + \cos(2\alpha_2)).
\]
\[ \eta_\alpha^a \rightarrow \pm \frac{e^2}{(\hbar e F)^2} \Delta U \text{ when } \Delta U \rightarrow 0. \]

To understand this difference, we examine the contribution from the DOS of the valence band which is not considered in the kp model. Since the photoinduced current originates from the transition between different valence bands to the same conduction band, we will neglect the influence of the DOS of the conduction band. The DOS near the top of the valence band will be affected by the external electric field. Our \textit{ab initio} results show that the DOS of the valence band are mainly contributed by Mo atoms of bilayer MoS\textsubscript{2}. From analytical calculation, we find that \[ |P_x(K, s)\rangle^2 \langle P_x(K, s)| \] is related mainly to the DOS from the lower (upper) layer of bilayer MoS\textsubscript{2} and \[ |P_y(K', s')\rangle^2 \langle P_y(K', s')| \] is related mainly to the DOS from the upper (lower) layer of bilayer MoS\textsubscript{2}. In figure 5(b), we plot the DOS of the upper layer Mo atom (red dotted line) and lower layer Mo atom (blue dotted line) versus gate voltage obtained by the \textit{ab initio} method. From this figure, we see that the influence of the external electric field on the DOS of the Mo atom of the upper layer is different from that of the lower layer. In other words, a better definition of valley coupling polarizations should include the effect of the DOS as follows,

\[
\eta_\alpha^a = \pm \frac{D_1 \cos^2 \alpha_1 - D_u \sin^2 \alpha_1 + D_2 \cos^2 \alpha_2 - D_u \sin^2 \alpha_2}{D_1 \cos^2 \alpha_1 + D_u \sin^2 \alpha_1 + D_2 \cos^2 \alpha_2 + D_u \sin^2 \alpha_2},
\]

where \(D_1\) and \(D_u\) are the DOS of the lower and upper Mo atoms, respectively. In panel (c) of figure 5, we plot the modified coupling polarization as a function of \(\Delta U\) using equation (13) with the DOS taken from panel (b) of figure 5. In order to compare with figure 5, we changed the abscissa of panel (c) from \(-0.04\) to \(0.04\) V to \(V_g\) from \(-1.0\) to \(1.0\) V according to our \textit{ab initio} results. We see that the modified coupling polarization is no longer an odd function of the gate voltage, and the behaviors of \(\eta_\alpha^a(V_g)\) for \(V_g = [-1, 0.3]\) V are similar to the results in figure 3(b). In other words, by analyzing the polarization of the coupling, one can get the information of the valley polarization. For the monolayer MoS\textsubscript{2}, one can directly using the kp model, but for the bilayer MoS\textsubscript{2}, one has to consider the influence of the DOS of the energy bands.

In summary, we have investigated the photoinduced current of layered MoS\textsubscript{2} as a function of the external electric field. The results show that the valley polarization of photoinduced current of monolayer MoS\textsubscript{2} is independent of external electric field perpendicular to the surface of the layered MoS\textsubscript{2} which can be induced by the gate voltage, but the valley polarization of the photoinduced current of bilayer MoS\textsubscript{2} is very sensitive to the external electric field that breaks the inversion symmetry. Moreover, the valley polarization can be tuned by changing the polarity of the circular polarized light. The modulations of the valley polarization of layered MoS\textsubscript{2} transistor by gate voltages and polarities of circular polarized light provide extra knowledge for the future application of valleytronic devices.

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References

[1] Singh V et al 2011 Graphene based materials: Past, present and future Prog. Mater. Sci. 56 1178
[2] Andrei E Y, Li G H and Du X 2012 Electronic properties of graphene: a perspective from scanning tunneling microscopy and magnetotransport Rep. Prog. Phys. 75 056501
[3] Qiao Z and Ren Y F 2014 Recent progress on quantum anomalous Hall effect in graphene J. Shenzhen Univ. Sci. Eng. 31 551
[4] Ren Y, Qiao Z and Niu Q 2015 Topological phases in two-dimensional materials: a brief review arXiv:1509.09016v1
[5] Novoselov K S et al 2005 Two-dimensional atomic crystals Proc. Natl Acad. Sci. U.S.A. 102 10451
[6] Lee C et al 2010 Frictional characteristics of atomically thin sheets Science 328 76
[7] Radisavljevic B, Radenovic A, Brivio J, Giacometti V and Kis A 2011 Single-layer MoS2 transistors Nat. Nanotechnol. 6 147
[8] Korn T, Heydrich S, Hirmer M, Schmutzler J and Schuller C 2011 Electron–phonon scattering in graphene Phys. Rev. Lett. 107 106401
[9] Min H et al 2006 Intrinsic and Rashba spin–orbit interactions in graphene sheets Phys. Rev. B 74 165310
[10] Yao Y G, Ye F, Qi X L, Zhang S C and Fang Z 2007 Spin–orbit gap of graphene: First-principles calculations Phys. Rev. B 75 041401
[11] Zhu Z Y, Cheng Y C and Schwingerchlogl U 2011 Giant spin–orbit-induced spin splitting in two-dimensional transition-metal dichalcogenide semiconductors Phys. Rev. B 84 155402
[12] Mak K F, Lee C, Hone J, Shan J and Heinz T F 2010 Atomically thin MoS2: A new direct-gap semiconductor Phys. Rev. Lett. 105 136820

[13] Splendiani A et al 2010 Emerging photoluminescence in monolayer MoS2 Nano Lett. 10 1271

[14] Rycerz A, Tworzydlo J and Beenakker C W J 2007 Valley filter and valley valve in graphene Nat. Phys. 3 172

[15] Xiao D, Yao W and Niu Q 2007 Valley-contrasting physics in graphene: Magnetic moment and topological transport Phys. Rev. Lett. 99 236809

[16] Zhang F, Jung J, Fiete G A, Niu Q and MacDonald A H 2011 Spontaneous quantum Hall states in chirally stacked few-layer graphene systems Phys. Rev. Lett. 106 156801

[17] Xiao D, Liu G B, Feng W X, Xu X D and Yao W 2012 Coupled spin and valley physics in monolayers of MoS2 and other group-VI dichalcogenides Phys. Rev. Lett. 108 196802

[18] Jones A M et al 2014 Spin-layer locking effects in optical orientation of exciton spin in bilayer WSe2 Nat. Phys. 10 130

[19] Yao W, Xiao D and Niu Q 2008 Valley-dependent optoelectronics from inversion symmetry breaking Phys. Rev. B 77 235406

[20] Yuan H et al 2013 Zeeman-type spin splitting controlled by an electric field Nat. Phys. 9 563

[21] Zeng H L, Dai J F, Yao W, Xiao D and Cui X D 2012 Valley polarization in MoS2 monolayers by optical pumping Nat. Nanotechnol. 7 490

[22] Wu S F et al 2013 Electrical tuning of valley magnetic moment through symmetry control in bilayer MoS2 Nat. Phys. 9 149

[23] Fontana M et al 2013 Electron-hole transport and photovoltaic effect in gated MoS2 Schottky junctions Sci. Rep. 3 1634

[24] Lopez-Sanchez O, Lembke D, Kayci M, Radenovic A and Kis A 2013 Ultrasensitive photodetectors based on monolayer MoS2 Nat. Nanotechnol. 8 497

[25] Sundaram R S et al 2013 Electroluminescence in Single Layer MoS2 Nano Lett. 13 1416

[26] Yin Z Y et al 2012 Single-layer MoS2 phototransistors ACS Nano 6 74

[27] Wu C C et al 2013 Elucidating the photoreponse of ultrathin MoS2 field-Effect transistors by scanning photocurrent microscopy J. Phys. Chem. Lett. 4 2508

[28] Kadantsev E S and Hawrylak P 2012 Electronic structure of a single MoS2 monolayer Solid State Commun. 152 909

[29] Liu Q H et al 2012 Tuning electronic structure of bilayer MoS2 by vertical electric field: A first-principles investigation J. Phys. Chem. C 116 21556

[30] Lake R and Datta S 1992 Nonequilibrium Green’s-Function method applied to double-barrier resonant-tunneling diodes Phys. Rev. B 45 6670

[31] Henricsson L E 2002 Nonequilibrium photocurrent modeling in resonant tunneling photodetectors J. Appl. Phys. 91 6273

[32] Chen J Z, Hu Y B and Guo H 2012 First-principles analysis of photocurrent in graphene PN junctions Phys. Rev. B 85 155441

[33] Kleinman L and Bylander D M 1982 Efficacious form for model pseudopotentials Phys. Rev. Lett. 48 1425

[34] Vignale G and Rasolt M 1987 Density-functional theory in strong magnetic-fields Phys. Rev. Lett. 59 2360

[35] Taylor J, Guo H and Wang J 2001 Ab initio modeling of quantum transport properties of molecular electronic devices Phys. Rev. B 63 245407

[36] For details of the NanoDcal quantum transport package see http://nanoacademic.ca

[37] Perdew J P and Wang Y 1992 Accurate and simple analytic representation of the electron-gas correlation-energy Phys. Rev. B 45 13244

[38] Kubler J, Hock K H, Sticht J and Williams A R 1988 Density functional theory of non-collinear magnetism J. Phys. F 18 469

[39] Kubler J, Hock K H, Sticht J and Williams A R 1988 Local spin-density functional theory of non-collinear magnetism J. Appl. Phys. 63 3482

[40] Nordstrom L and Singh D J 1996 Noncollinear intra-atomic magnetism Phys. Rev. Lett. 76 4420

[41] Zhang L et al 2014 Generation and transport of valley-polarized current in transition-metal dichalcogenides Phys. Rev. B 90 195428

[42] Haug H and Jauho A P 1998 Quantum Kinetics in Transport and Optics of Semiconductors (New York: Springer)

[43] Gong Z R et al 2013 Magnetoelectric effects and valley-controlled spin quantum gates in transition metal dichalcogenide bilayers Nat. Comm. 4 2053