

Spin photocurrents in semiconductors

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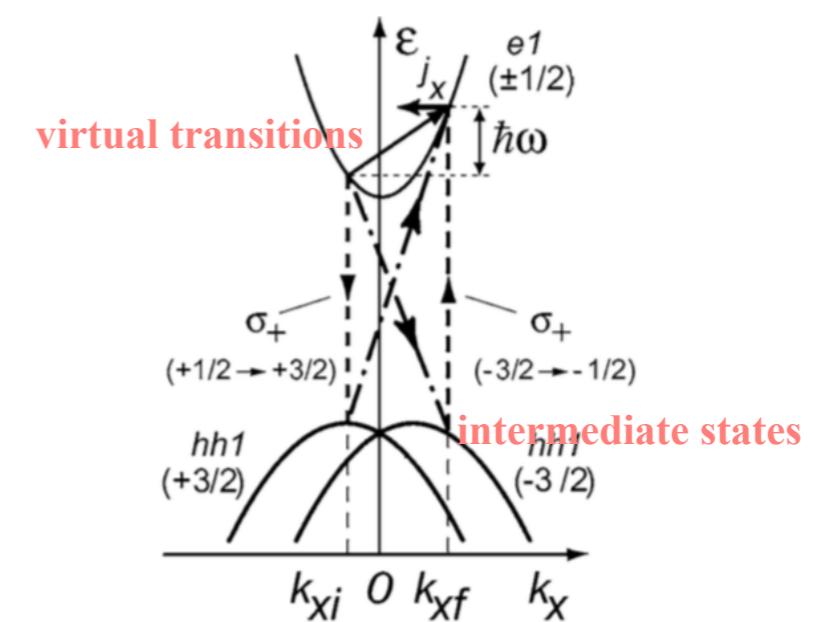
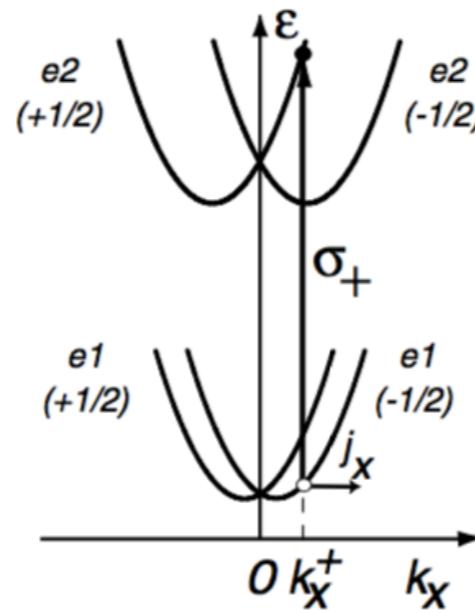
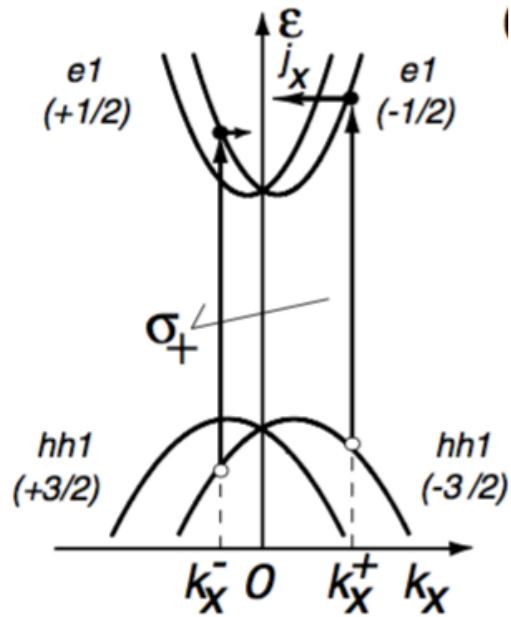
2017-12-7

Main outline:

- *The ordinary spin photocurrents in semiconductors
- *Symmetry analysis of CPGE
- *Some special CPGE in semiconductors
- *Some personal thoughts

The origination of CPGE in semiconductors

*The microscopic model for CPGE



1. **Inter-band transitions:** between conduct band and valence band

2. **Inter-subband transitions**(infrared and far infrared):between size-quantized subbands in the conduction band

3. **Intra-subband transitions**(far-infrared range):phonon needed

Phenomenology theory of CPGE

*The macroscopic model for CPGE

$$j_\lambda = \sum_\mu \gamma_{\lambda\mu} i(\mathbf{E} \times \mathbf{E}^*)_\mu,$$

$$i(\mathbf{E} \times \mathbf{E}^*)_\mu = \hat{\mathbf{e}}_\mu E_0^2 P_{circ}$$

γ is a second-rank pseudo-tensor; P_{circ} is the radiation helicity

Sub problem (Solved)

$$P_{circ} = \frac{I_{\sigma+} - I_{\sigma-}}{I_{\sigma+} + I_{\sigma-}}$$

$$i(\vec{E} \times \vec{E}^*) = E_0^2 P_{circ} \vec{e}_K$$

\vec{E} 为电磁波的复电矢量. \vec{e}_K 为电磁波传播方向

$$\vec{E}_{\sigma+} = a_1 e^{i(\phi_1 + \frac{\lambda}{2})} \vec{x}_0 + a_2 e^{i\phi_1} \vec{y}_0$$

$$\vec{E}_{\sigma-} = a_2 e^{i(\phi_2 - \frac{\lambda}{2})} \vec{x}_0 + a_1 e^{i\phi_2} \vec{y}_0$$

$$\vec{E} = \vec{E}_{\sigma+} + \vec{E}_{\sigma-}$$

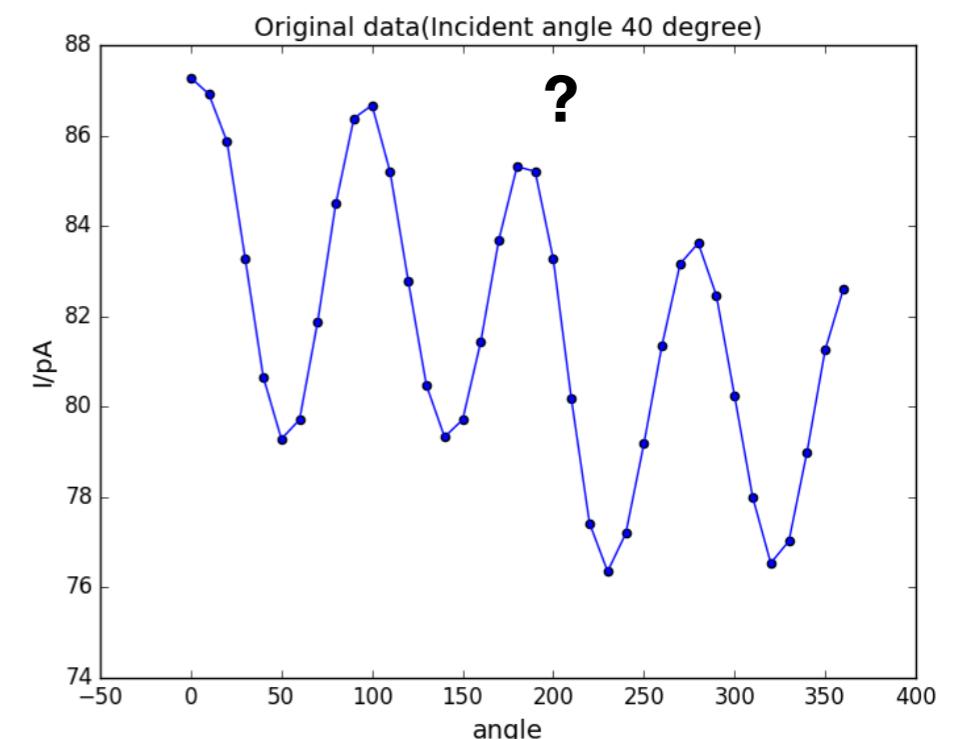
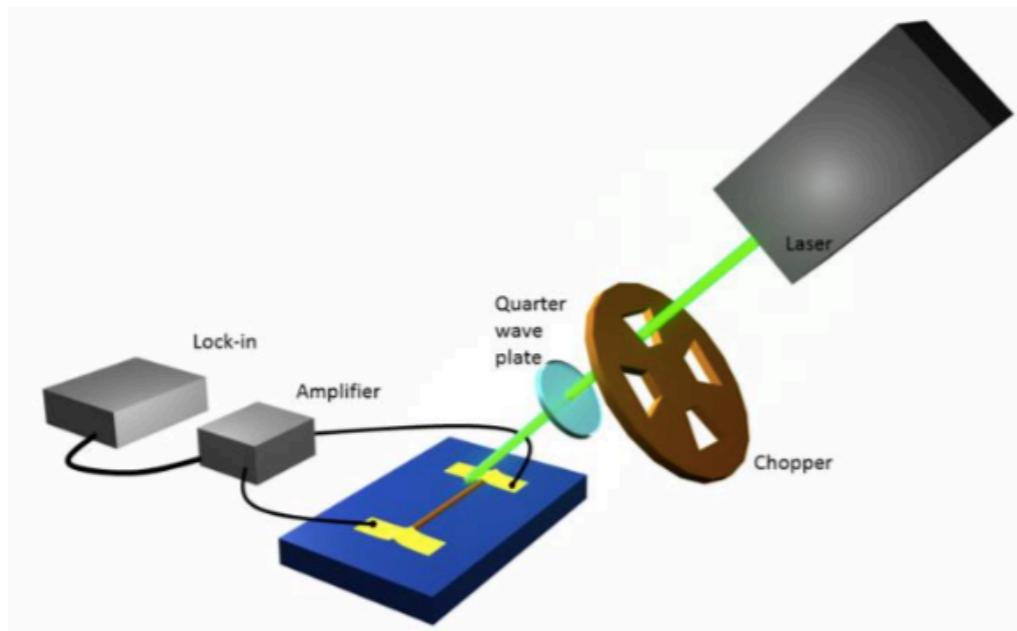
$$\vec{E} \times \vec{E}^* = 2i(a_1^2 - a_2^2) = 2i(I_{\sigma+} - I_{\sigma-})$$

$$P_{circ} = \frac{I_{\sigma+} - I_{\sigma-}}{I_{\sigma+} + I_{\sigma-}} = \sin 2\varphi$$

The definition of P_{circ}

The Experiment of measuring CPGE

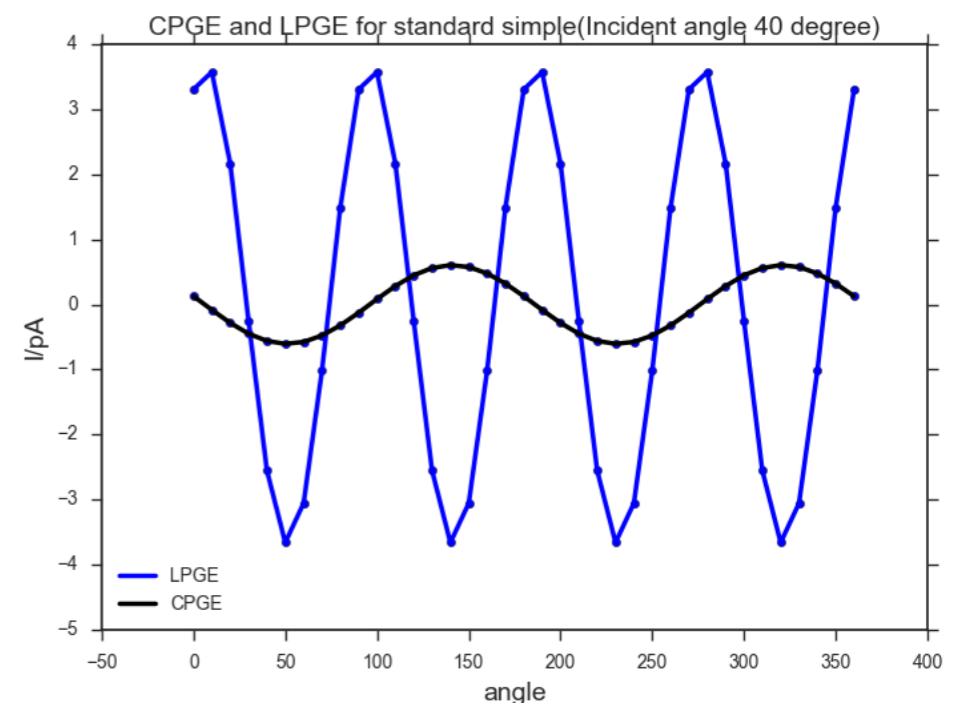
*The measuring system



The equation used to fit the experimental datas:

$$\mathbf{j} = j_c \sin 2\varphi + j_L \sin 2\varphi \cos 2\varphi + j_0$$

j_L is the Linear photogalvanic originating from the spin selective scattering by phonons, defects, etc



Multi-layer MoS₂/should be zero theoretically

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The symmetry analysis of CPGE in semiconductors

*The properties of matter tensor in Crystals

1.The First-Rank matter Tensor(vector)

$$V_j' = R_{ji} V_i$$

2.The second-Rank matter Tensor

$$T_{ij}' = R_{ik} R_{jl} T_{kl}$$

For pseudo-tensor the $\det(R)$ should be added

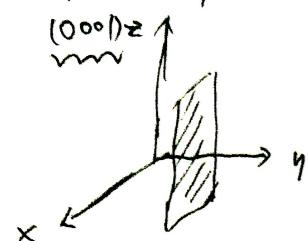
*The symmetry analysis of CPGE

$$j_\lambda = \sum_\mu \gamma_{\lambda\mu} \mathbf{i}(\mathbf{E} \times \mathbf{E}^*)_\mu,$$

Considering the symmetry of semiconductors ,many component of the second-rank pseudo-tensor will be zero

The symmetry analysis of CPGE in semiconductors

C_s point group (仅多个镜像及旋转操作)



$$R = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\chi = \begin{pmatrix} \chi_{xx} & \chi_{xy} & \chi_{xz} \\ \chi_{yx} & \chi_{yy} & \chi_{yz} \\ \chi_{zx} & \chi_{zy} & \chi_{zz} \end{pmatrix}$$

$$\chi \xrightarrow{R} \chi' = R \chi R^T \det R$$

$$= \begin{pmatrix} -\chi_{xx} & \chi_{xy} & -\chi_{xz} \\ \chi_{yx} & -\chi_{yy} & \chi_{yz} \\ -\chi_{zx} & \chi_{zy} & -\chi_{zz} \end{pmatrix}$$

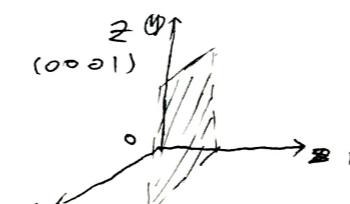
$$\chi' = \chi \Rightarrow \chi_{xy}, \chi_{yx}, \chi_{yz}, \chi_{zy} \text{ 为零}$$

其它均为零

$$\begin{aligned} j_\lambda &= \sum_\mu \chi_{\lambda\mu} E_\mu^\lambda \vec{P}_{circ} \hat{e}_\mu & j_x &= \chi_{xy} \hat{e}_y |E^2| \vec{P}_{circ} \\ j_y &= (\chi_{yx} \hat{e}'_x + \chi_{yz} \hat{e}'_z) |E^2| \vec{P}_{circ} & j_z &= \chi_{zy} \hat{e}'_y |E^2| \vec{P}_{circ} \end{aligned}$$

(\hat{e}' 光轴坐标系)

C_{2v} point group



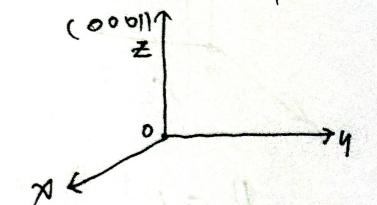
二阶轴 + σ_v

$$R(C_2) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad R(\sigma_v) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$\begin{aligned} \chi &\xrightarrow{R(C_2)} \chi' = \chi \\ \chi &\xrightarrow{R(\sigma_v)} \chi' = \chi \end{aligned} \Rightarrow \chi = \begin{pmatrix} 0 & \chi_{xy} & 0 \\ \chi_{yx} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

C_{6v}/C_{3v} GaN, ZnO

AlGaN/GaN 异质结



$$R(C_3) = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$R(C_6') = \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$R(\sigma_v) = \begin{pmatrix} 0 & 1 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$\chi \xrightarrow{R(C_3), R(C_6'), R(\sigma_v)} \chi'$

$$\chi = \begin{pmatrix} 0 & \chi_{xy} & 0 \\ -\chi_{xy} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

*The information we can get from the symmetry analysis

1. For C_{3v} or higher symmetry: The CPGE is perpendicular to the direction of light propagation.

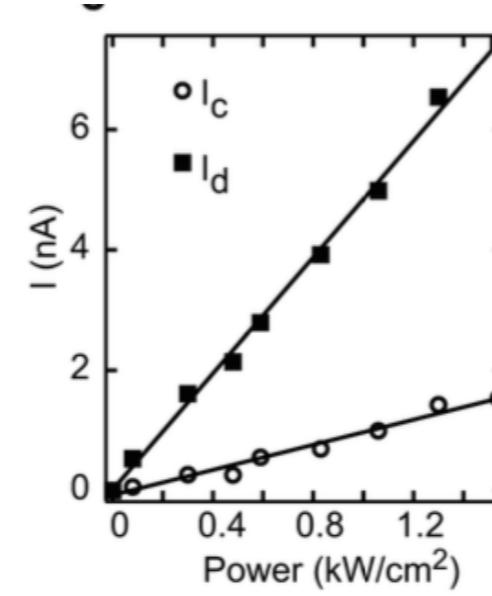
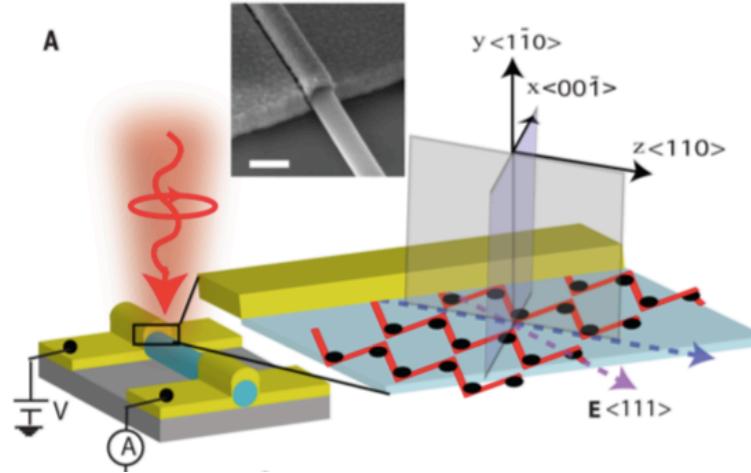
2. For C_{2v} or higher symmetry: The CPGE only exist in the X-Y plane

Main outline:

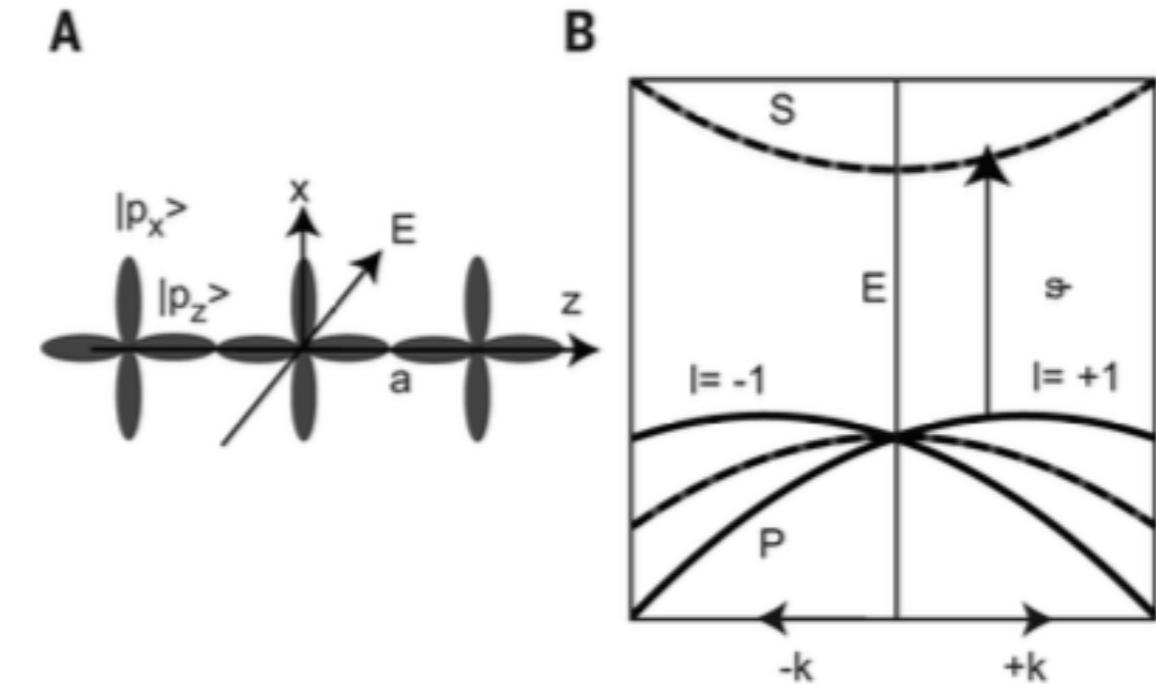
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The CPGE of orbital mechanism

*Si nanowires without breaking spin degeneracies



1. Special direction which contain zigzag atomic chains can generate CPGE



2. sensitive to circular polarization of light, tunable with an external bias.

一维原子链 简并微扰论计算能带非自旋分裂

$$V_s = r E_x \sin\theta \cos\phi \quad (\text{微扰势})$$

微扰前态矢量的构成

$$|\Psi_S(\vec{k}, \vec{r})\rangle = \frac{1}{\sqrt{N}} \sum_j e^{i\vec{k} \cdot \vec{z}_j} \Psi_S(\vec{r} - \vec{z}_j)$$

$$|\Psi_{Px}(\vec{k}, \vec{r})\rangle = \frac{1}{\sqrt{N}} \sum_j e^{i\vec{k} \cdot \vec{z}_j} \Psi_{Px}(\vec{r} - \vec{z}_j)$$

类似地还有 $|\Psi_{Py}\rangle$ $|\Psi_{Pz}\rangle$

由 \vec{E} 的取向 (它处于 x, z 平面) 可知

$$\text{仅有 } \langle \Psi_{Py} | V_x | \Psi_{Pz} \rangle = \langle \Psi_{Pz} | V_x | \Psi_{Py} \rangle \neq 0$$

$$\langle \hat{V} \rangle = \begin{pmatrix} 0 & 0 & irkza \\ 0 & 0 & 0 \\ irkza & 0 & 0 \end{pmatrix}$$

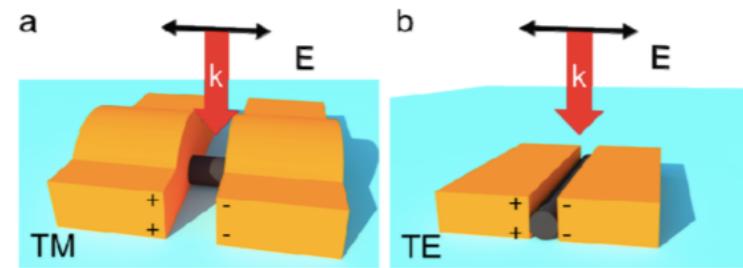
$$\Rightarrow \Psi_{\pm} = \frac{1}{\sqrt{2}} (\Psi_{Px}(k, \vec{r}) \pm i\Psi_{Pz}(k, \vec{r})) \quad (\text{波函数一级近似})$$

$$\Delta E_{\Psi_+, \Psi_-} = 2|k_z|r|a|$$

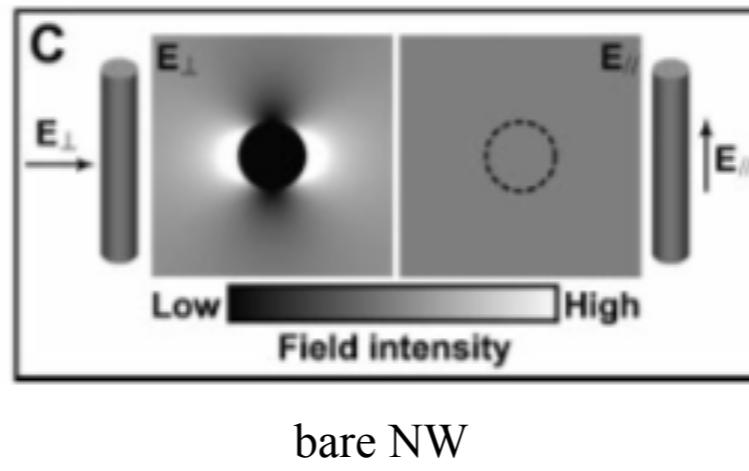
$$\text{电偶极跃迁几率 } P \propto \langle \Psi_S | \vec{\epsilon} \cdot \vec{J} | \Psi_{\pm} \rangle \propto \tilde{E} \times \tilde{\epsilon}^*$$

The CPGE of orbital mechanism

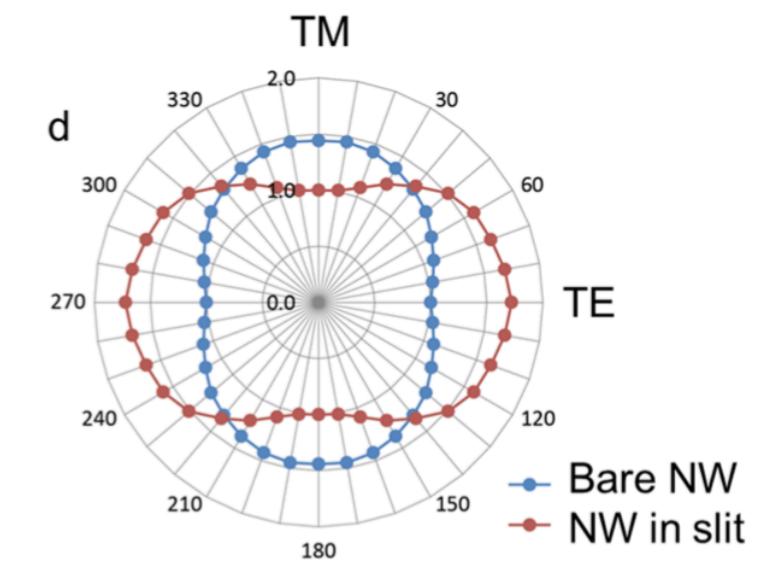
*The mechanism for LPGE



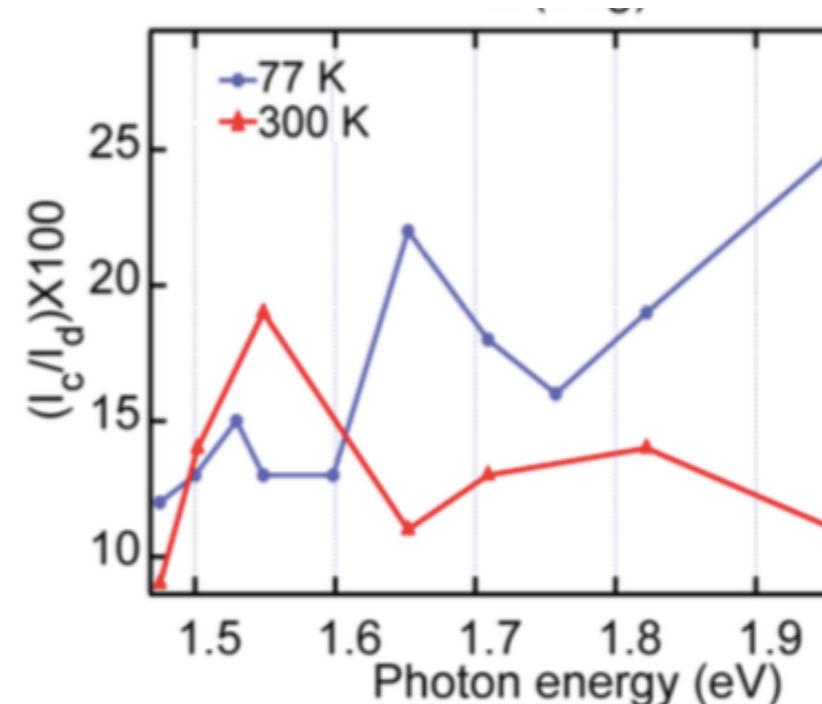
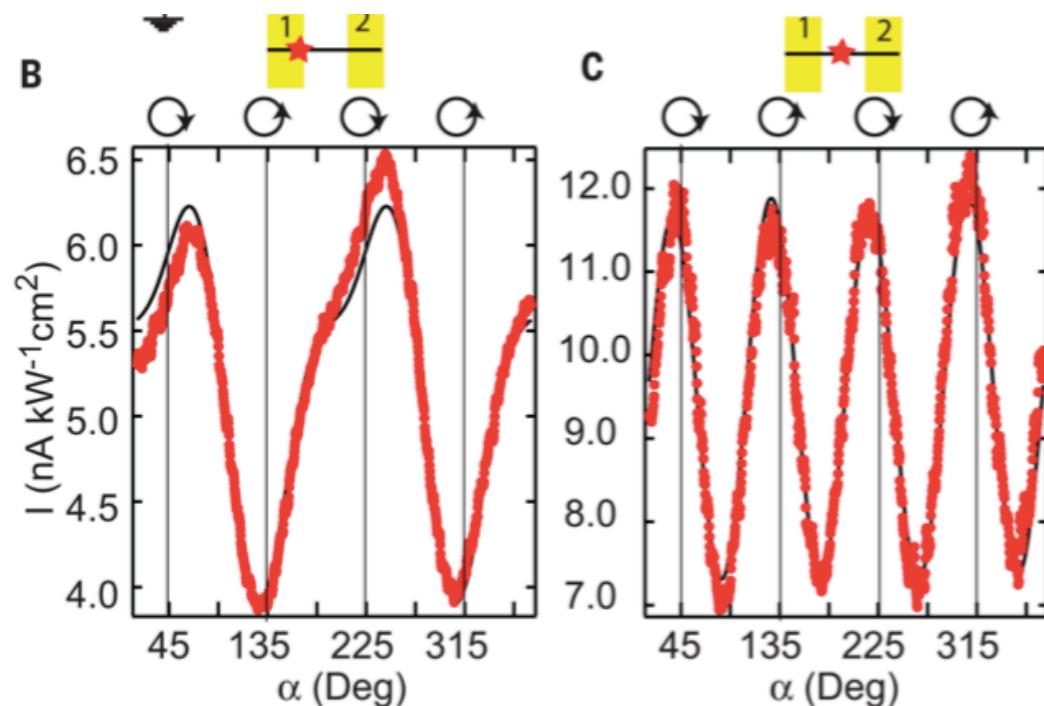
preferential absorption: metal-NW region(TE) ;bare NW(TM)



bare NW



*The difference between metal-NW contact region and the bare NW



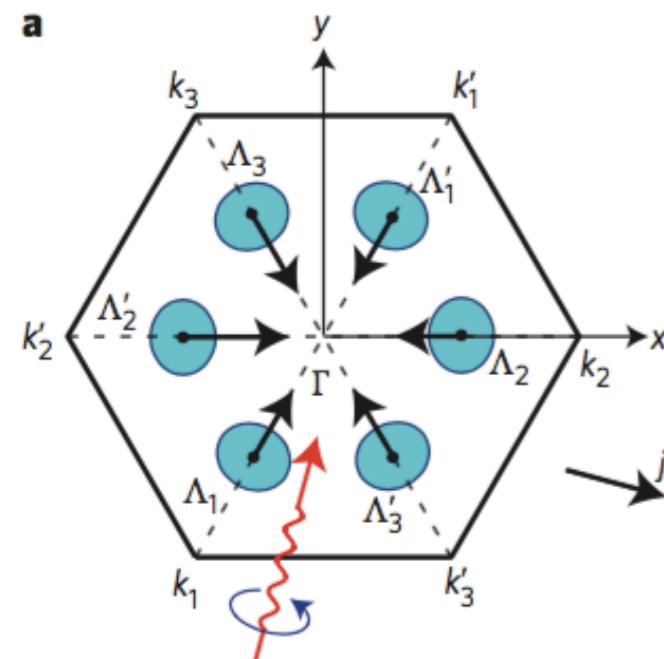
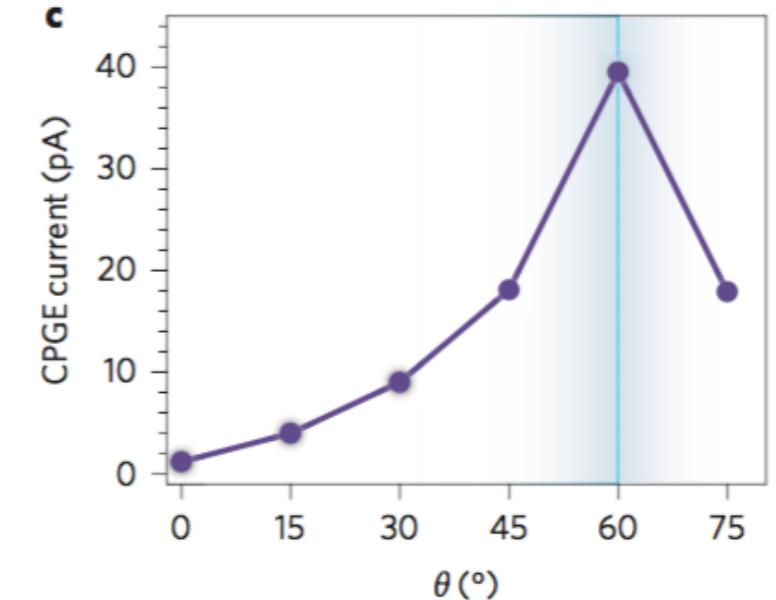
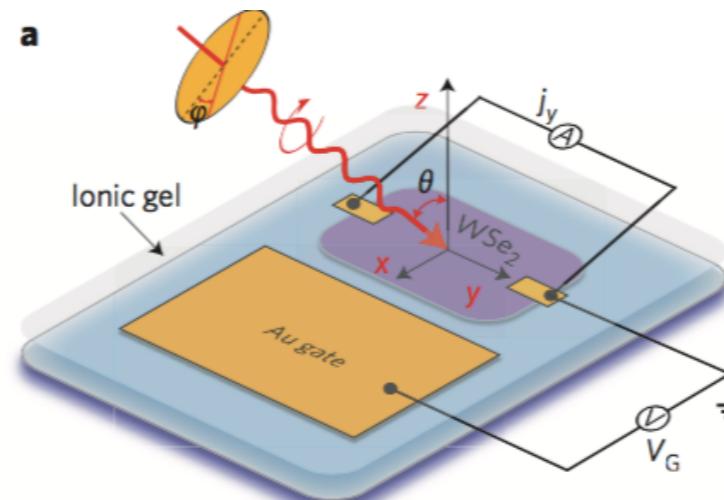
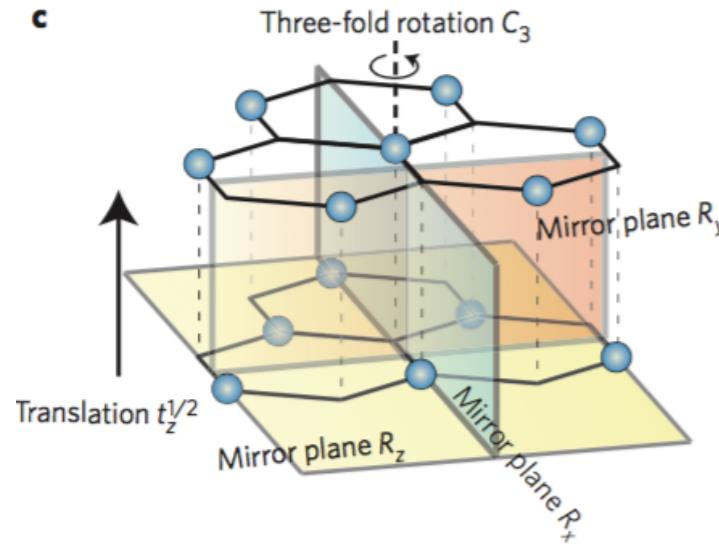
The reason is unknown

Dhara, S(2015). Science
Pengyu Fan(2013),nanonletter
Jianfang Wang (2001).Science

The spin–valley coupled CPGE

*The CPGE in WSe₂(SOC is not necessary)

The external electronic field don't break the symmetry C_{3v}



$$A(\theta, \phi) = A \left[(\mathbf{e}_x \sin \phi - \mathbf{e}_y \cos \phi)(1 + i \cos 2\phi) + i(\mathbf{e}_z \sin \theta - \mathbf{e}_x \cos \theta \cos \phi - \mathbf{e}_y \cos \theta \sin \phi) \sin 2\phi \right]$$

The origination of Helicity dependence

$$H' = \int d\mathbf{r}^3 (ie\hbar / mc) \mathbf{A}(\mathbf{r}) \cdot \nabla$$

$$\mathcal{M}_2(\mathbf{A}) = \mathcal{M}_{2,x} A_x + \mathcal{M}_{2,y} A_y + \mathcal{M}_{2,z} A_z = \mathcal{M}_2 \cdot \mathbf{A}$$

$$\mathcal{M}_{2,u} = (e\hbar / mc) \langle F, \mathbf{k}_{\Lambda_2} | i\partial_u | I, \mathbf{k}_{\Lambda_2} \rangle$$

$$j = \frac{\xi I}{A^2} \sum_{i=1}^3 \mathbf{e}_i \left(\left| \mathcal{M}_2 \cdot \mathbf{A} \left(\theta, \phi - \frac{2(i-2)\pi}{3} \right) \right|^2 - \left| \mathcal{M}_2^* \cdot \mathbf{A} \left(\theta, \phi - \frac{2(i-2)\pi}{3} \right) \right|^2 \right)$$

contain C_3 and time-reversal symmetry

$$\begin{aligned} & |\mathcal{M}_2 \cdot \mathbf{A}(\theta, \phi)|^2 - |\mathcal{M}_2^* \cdot \mathbf{A}(\theta, \phi)|^2 \\ &= (\mathcal{M}_2 \cdot \mathbf{A}(\theta, \phi))(\mathcal{M}_2^* \cdot \mathbf{A}^*(\theta, \phi)) - (\mathcal{M}_2^* \cdot \mathbf{A}(\theta, \phi))(\mathcal{M}_2 \cdot \mathbf{A}^*(\theta, \phi)) \\ &= (\mathbf{A}(\theta, \phi) \times \mathbf{A}^*(\theta, \phi)) \cdot (\mathcal{M}_2 \times \mathcal{M}_2^*). \end{aligned}$$

Non-vanishing current equivalent to $M_2^* \neq C_{phase} M_2$

The spin–valley coupled CPGE

Key point:breaking R_z symmetry

*The symmetry analysis of CPGE in WSe₂

originate from fist principle calculation

$$|I, \mathbf{k}_{\Lambda_2}\rangle = ia_0|d_{xy}^+\rangle + b_0|d_{x^2-y^2}^+\rangle + c_0|d_{z^2}^+\rangle$$

$$|F_1, \mathbf{k}_{\Lambda_2}\rangle = ia_1|d_{xy}^+\rangle + b_1|d_{x^2-y^2}^+\rangle + c_1|d_{3z^2-r^2}^+\rangle$$

time-reversal symmetry T ,
 R_x ($x \rightarrow -x$)

$$|F_2, \mathbf{k}_{\Lambda_2}\rangle = |d_{yz}^+\rangle$$

R_z ($z \rightarrow -z$)

$$|F_3, \mathbf{k}_{\Lambda_2}\rangle = ia_3|d_{xy}^-\rangle + b_3|d_{x^2-y^2}^-\rangle + c_3|d_{3z^2-r^2}^-\rangle$$

$$Y = t_z^{1/2} \otimes R_y(y \rightarrow -y)$$

*Without External field

$$Y|I, \mathbf{k}_{\Lambda_2}\rangle = |I, \mathbf{k}_{\Lambda_2}\rangle$$

$$Y M_2^{I \rightarrow F_1} = M_2^{I \rightarrow F_1}$$

$$R_z|I, \mathbf{k}_{\Lambda_2}\rangle = |I, \mathbf{k}_{\Lambda_2}\rangle$$

$$R_z M_2^{I \rightarrow F_1} = M_2^{I \rightarrow F_1}$$

$$R_z|F_1, \mathbf{k}_{\Lambda_2}\rangle = |F_1, \mathbf{k}_{\Lambda_2}\rangle$$

M is a fist-rank tensor,only $M_x \neq 0$

$$\mathcal{M}_2^{(I \rightarrow F_1)} = \mathcal{M}_{2,x}^{(I \rightarrow F_1)} \mathbf{e}_x = e^{2i\delta} \mathcal{M}_{2,x}^{(I \rightarrow F_1)*} \mathbf{e}_x = e^{2i\delta} \mathcal{M}_2^{(I \rightarrow F_1)*},$$

The spin–valley coupled CPGE

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$$|I, \mathbf{k}_{\Lambda_2}\rangle = ia_0|d_{xy}^+\rangle + b_0|d_{x^2-y^2}^+\rangle + c_0|d_{z^2}^+\rangle$$

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time-reversal symmetry T ,
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$$Y = t_z^{1/2} \otimes R_y (y \rightarrow -y)$$

$$|F'_1, \mathbf{k}_{\Lambda_2}\rangle = |F_1, \mathbf{k}_{\Lambda_2}\rangle + gE_{ex}|F_2, \mathbf{k}_{\Lambda_2}\rangle$$

*With External field

$$|F'_2, \mathbf{k}_{\Lambda_2}\rangle = |F_2, \mathbf{k}_{\Lambda_2}\rangle - gE_{ex}|F_1, \mathbf{k}_{\Lambda_2}\rangle$$

$$Y|F'_1, \mathbf{k}_{\Lambda_2}\rangle = |F'_1, \mathbf{k}_{\Lambda_2}\rangle \quad : \quad \mathcal{M}_{2,y}^{(I \rightarrow F'_1)} = 0$$

$$\mathcal{M}_{2,x}^{(I \rightarrow F'_1)} = \mathcal{M}_{2,x}^{(I \rightarrow F_1)} \neq 0$$

$$TR_x|F_1, \mathbf{k}_{\Lambda_2}\rangle = |F_1, \mathbf{k}_{\Lambda_2}\rangle \quad \mathcal{M}_{2,x}^{(I \rightarrow F'_1)} = \mathcal{M}_{2,x}^{(I \rightarrow F_1)*}$$

$$TR_x|I, \mathbf{k}_{\Lambda_2}\rangle = |I, \mathbf{k}_{\Lambda_2}\rangle$$

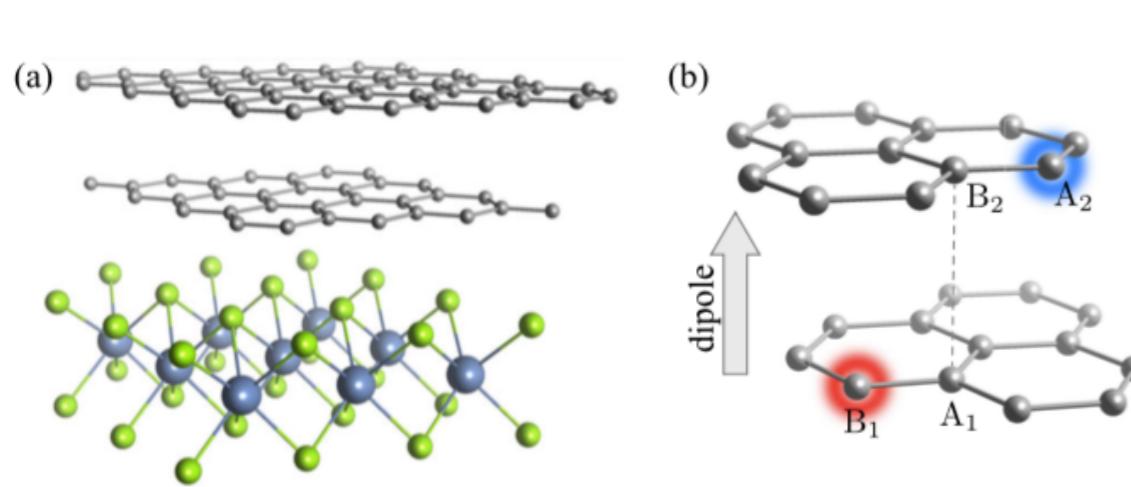
$$\mathcal{M}_{2,z}^{(I \rightarrow F'_1)} = gE\mathcal{M}_{2,z}^{(I \rightarrow F_2)} = m_{2,z}^{(I \rightarrow F'_1)}E_{ex} \neq 0$$

$$TR_x|F_2, \mathbf{k}_{\Lambda_2}\rangle = -|F_2, \mathbf{k}_{\Lambda_2}\rangle \quad \mathcal{M}_{2,z}^{(I \rightarrow F'_1)} = -\mathcal{M}_{2,z}^{(I \rightarrow F_1)*}$$

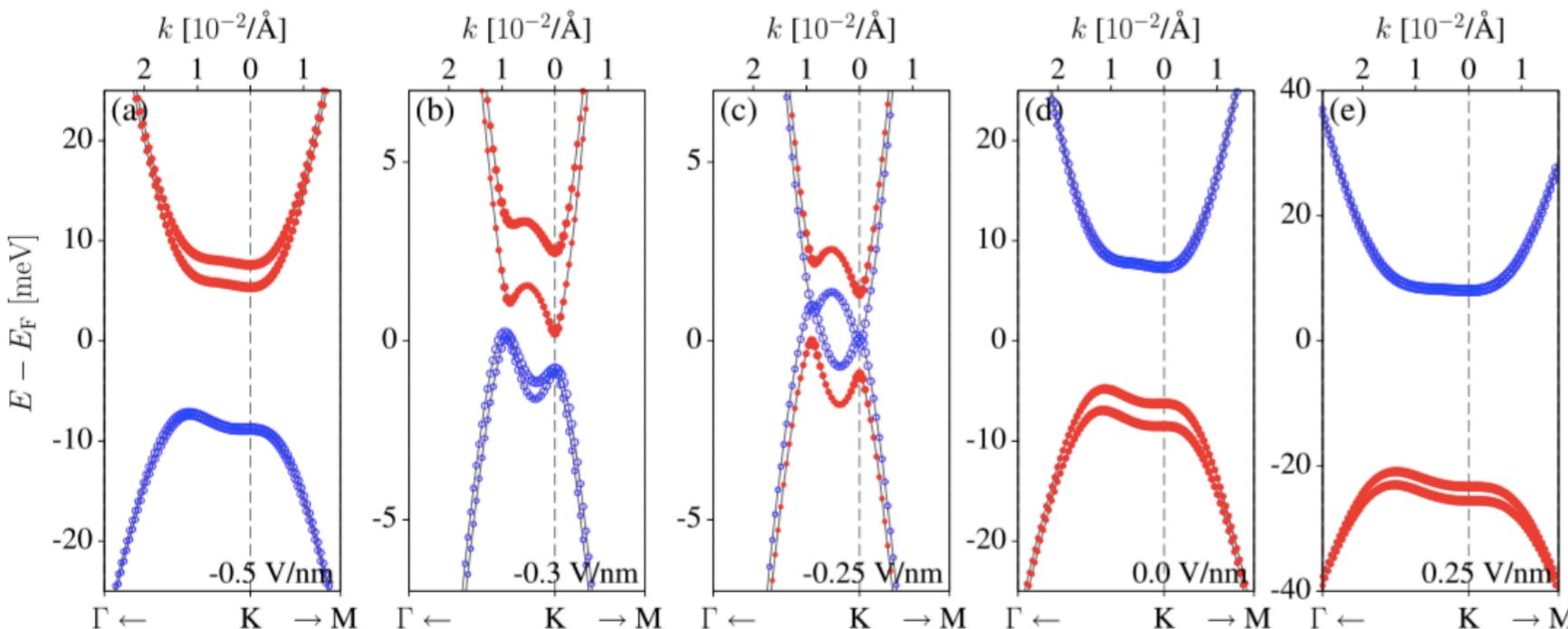
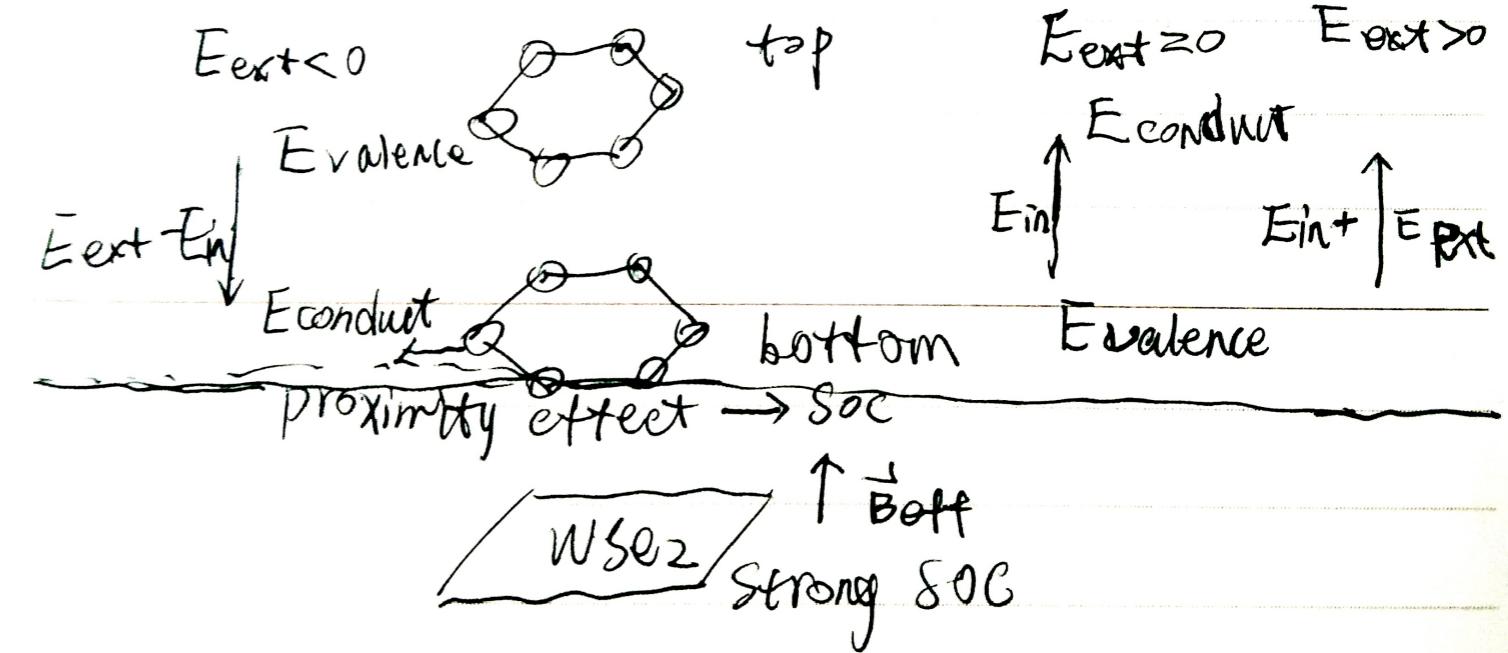
$$\mathcal{M}_2 \times \mathcal{M}_2^* = 2\mathcal{M}_{2,x}^{(I \rightarrow F'_1)}\mathcal{M}_{2,z}^{(I \rightarrow F'_1)}\mathbf{e}_y \neq 0$$

Spin orbit valve

*Bilayer Graphene on Monolayer WSe₂



Spontaneous polarization creates built-in transverse electric

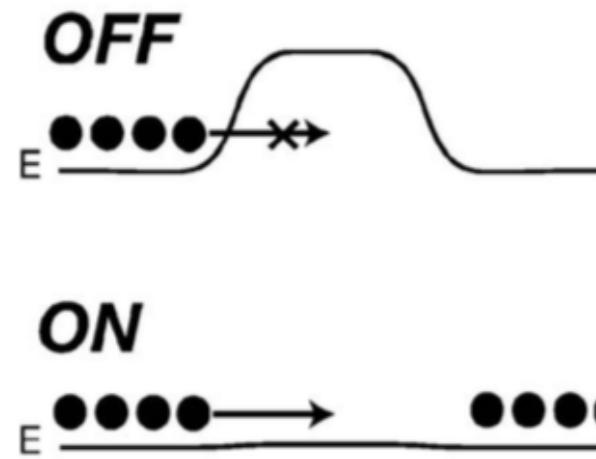


$$E_{soc}^{on}/E_{soc}^{off} = 100$$

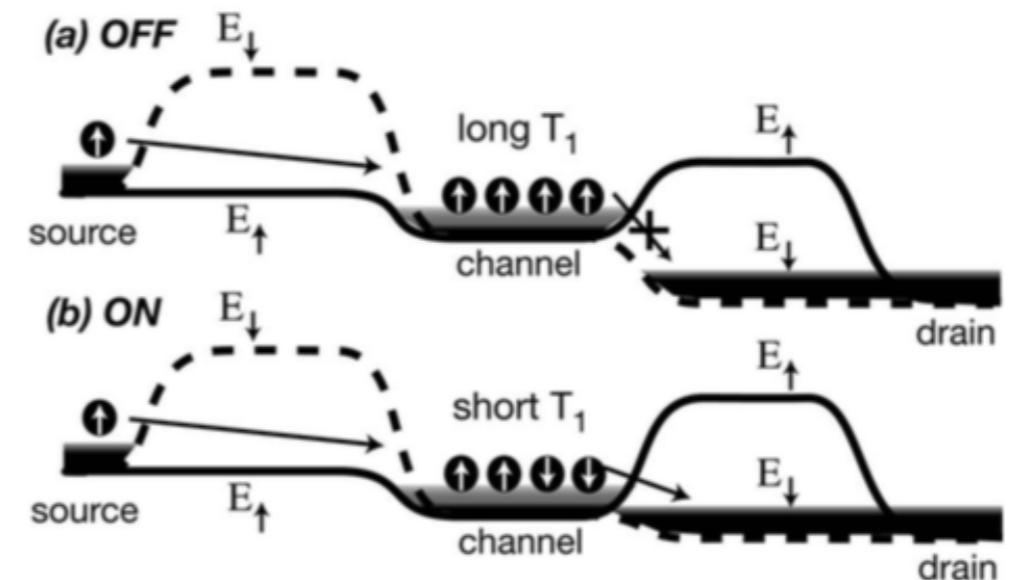
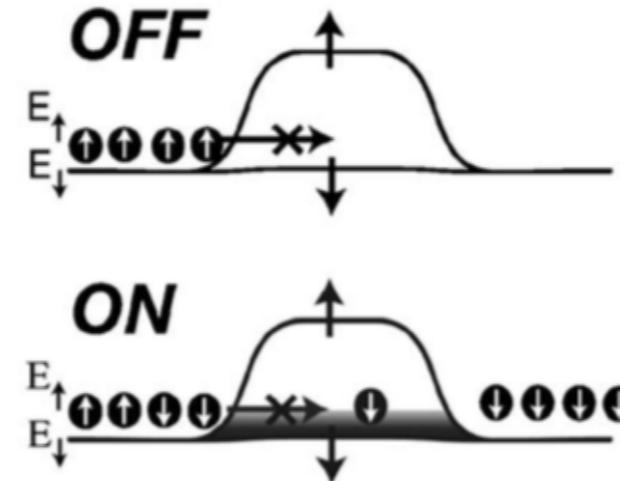
Spin orbit valve

*Bilayer Graphene on Monolayer WSe₂ construct spin FET

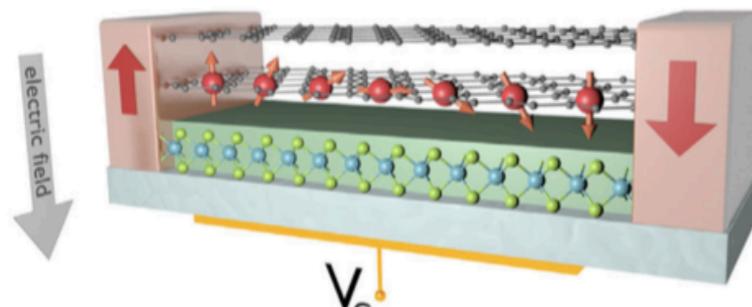
(a) charge-based current gating



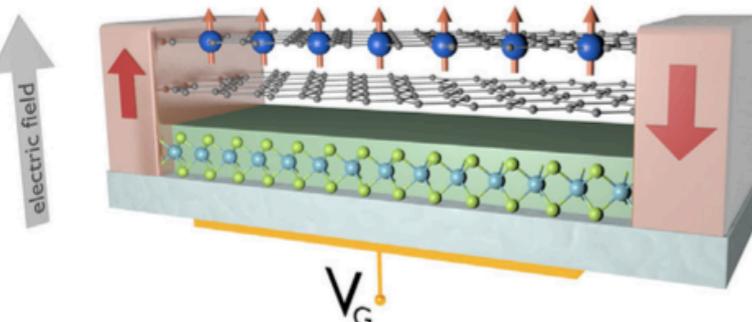
(b) spin-based current gating



(a)



(b)



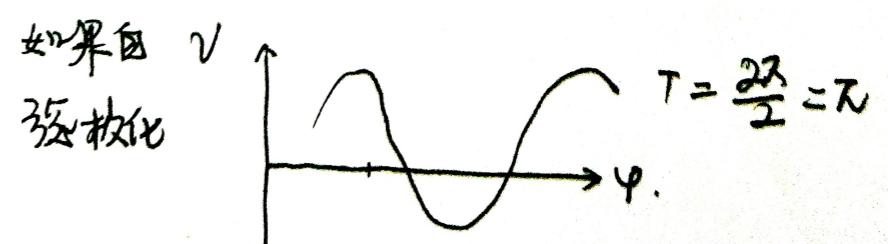
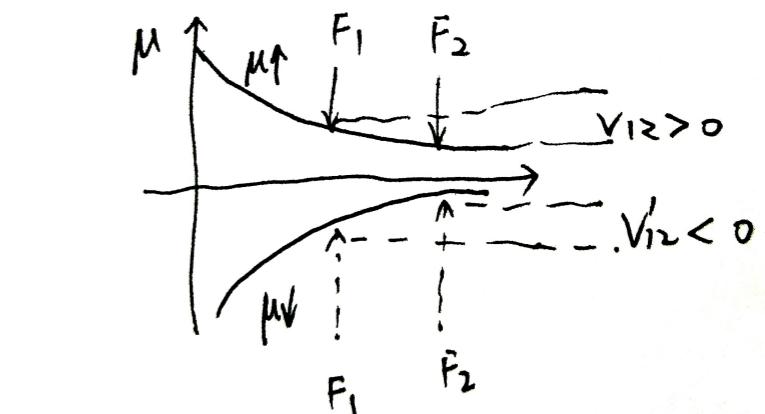
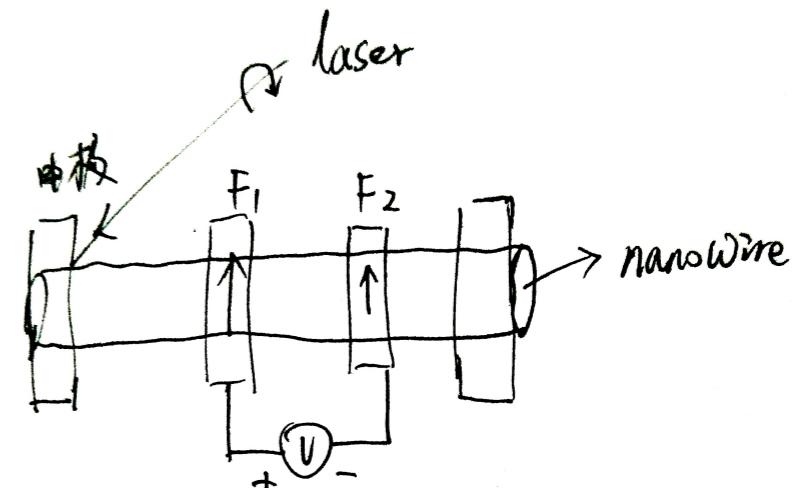
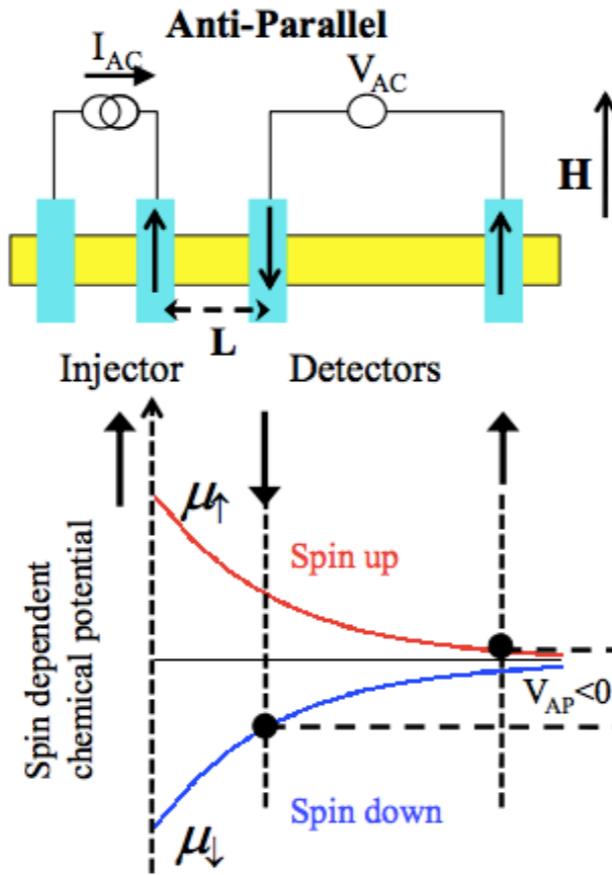
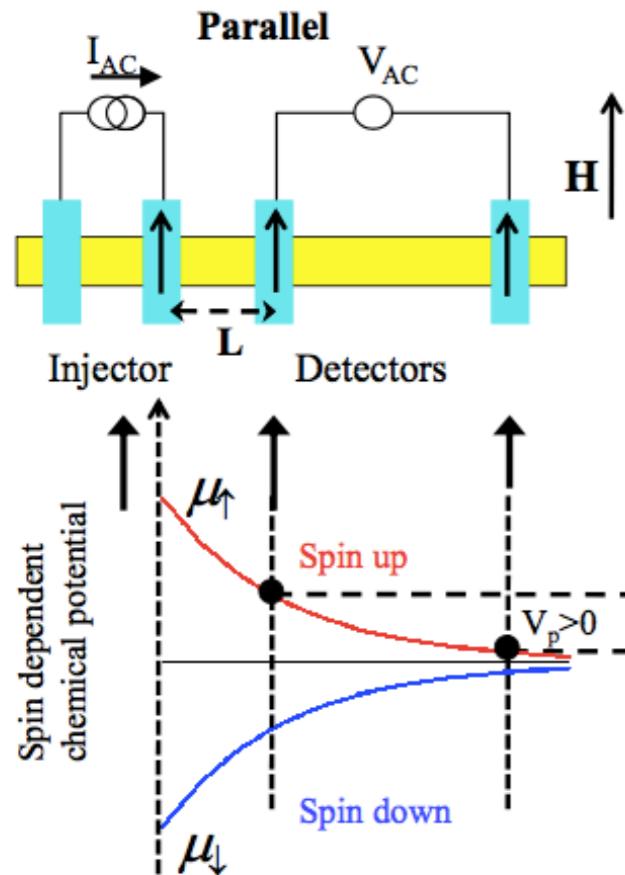
For D-P spin relaxation mechanism:

$$\frac{1}{\tau_s} = \Omega^2 \tau_p, \tau^{on}/\tau^{off} = 1/10000$$

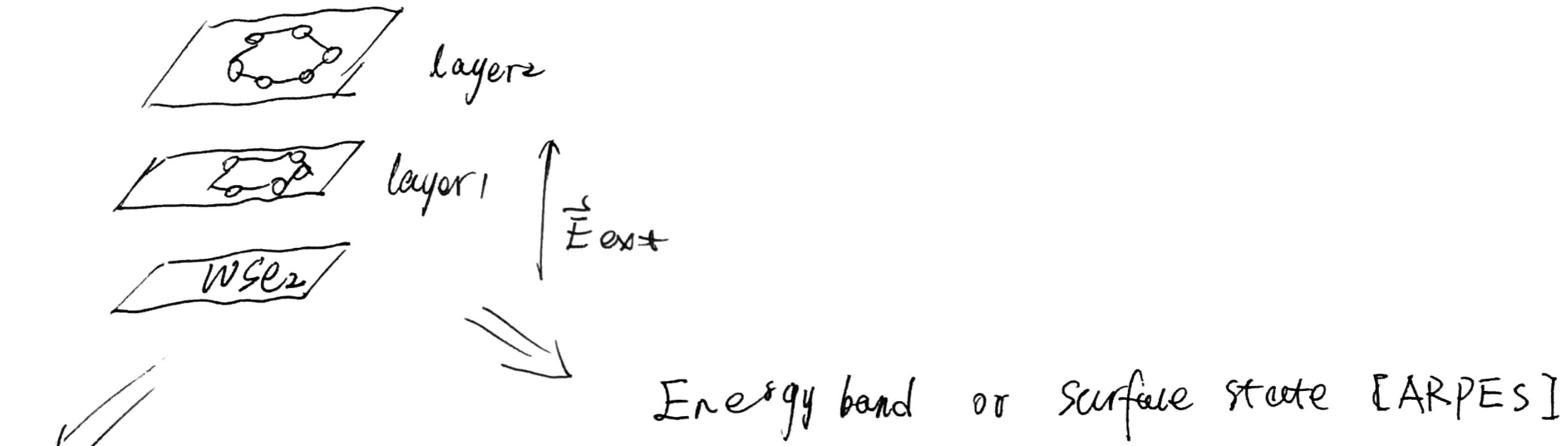
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Identify whether the “CPGE” is spin polarized



Bilayer Graphene on Monolayer WSe₂



CPGE measuring

Kerr rotation. directly measuring T_s

① p-type . n-type

② gate voltage dependence

③ Saturation phenomenon (p-type)

Thanks for your listening!