応用物理学会2025年春季大会 @ 東京理科大学 野田キャンパス
2025/3/14 (金)

講演番号：14p-K301-17

単層ヤヌス遷移金属ダイカルコゲナイドにおける光誘起スピン流に関する理論研究

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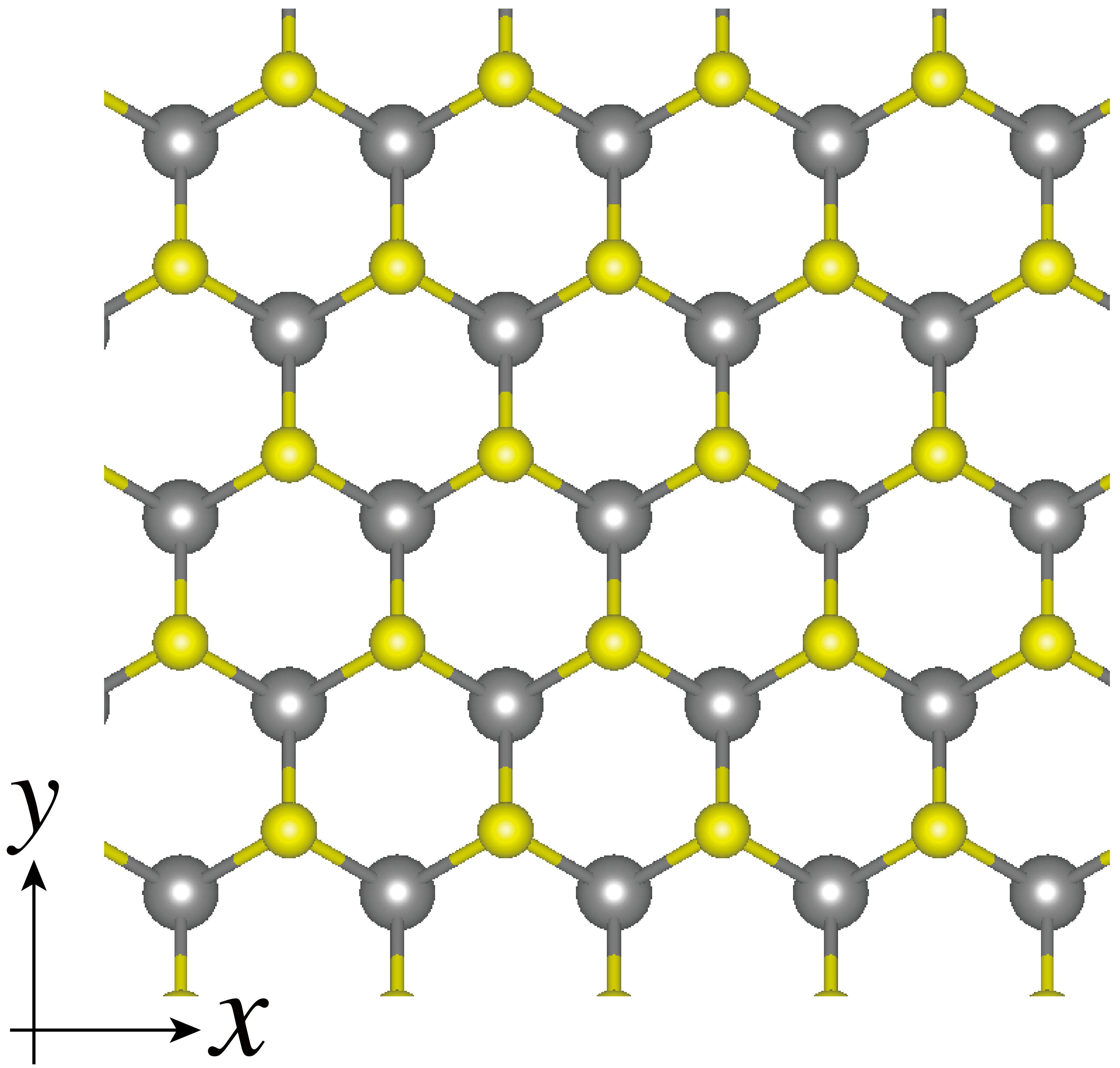
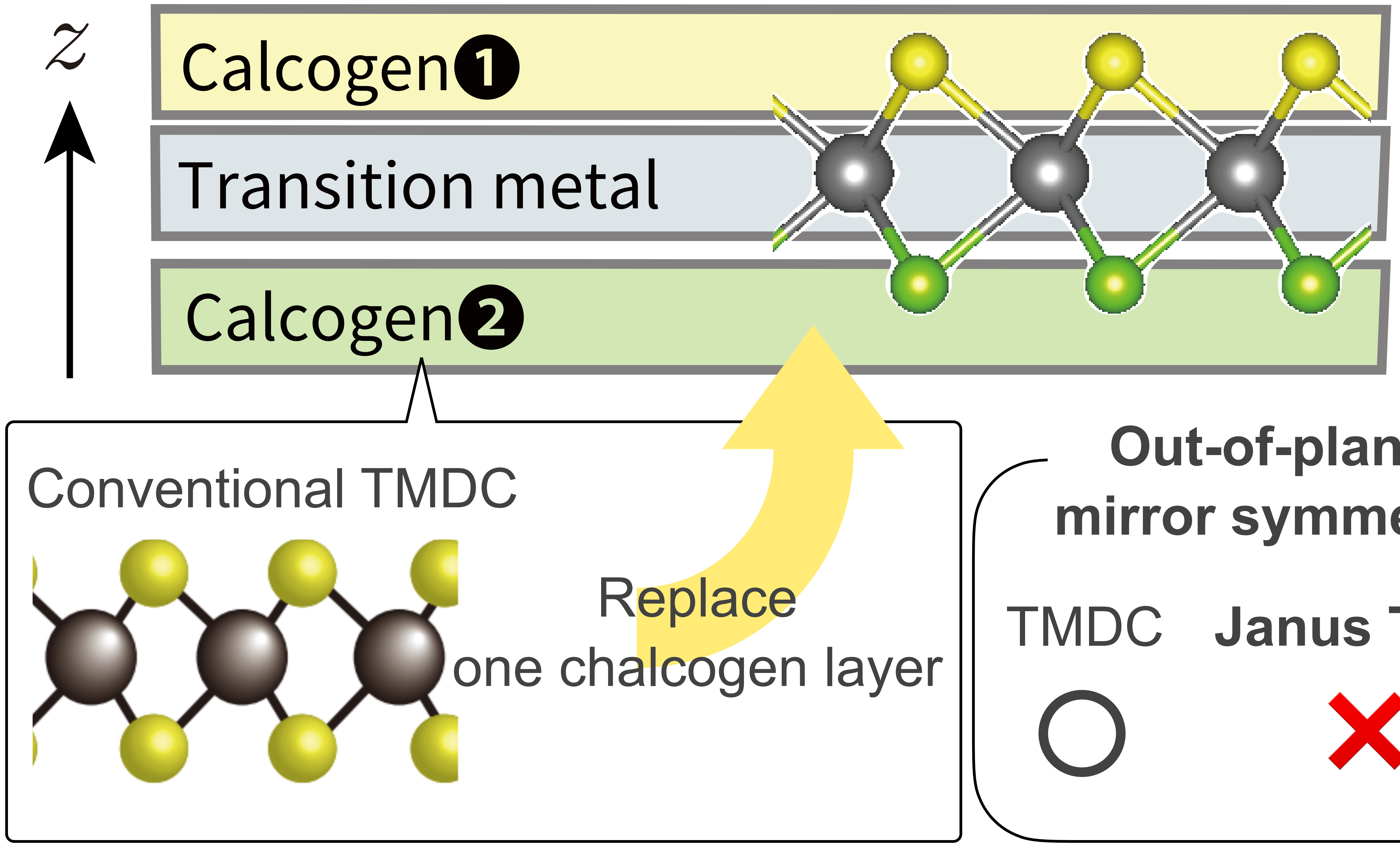
Monolayer Janus transition metal dichalcogenide (Janus TMDC)

Top view



Side view



Out-of-plane mirror symmetry

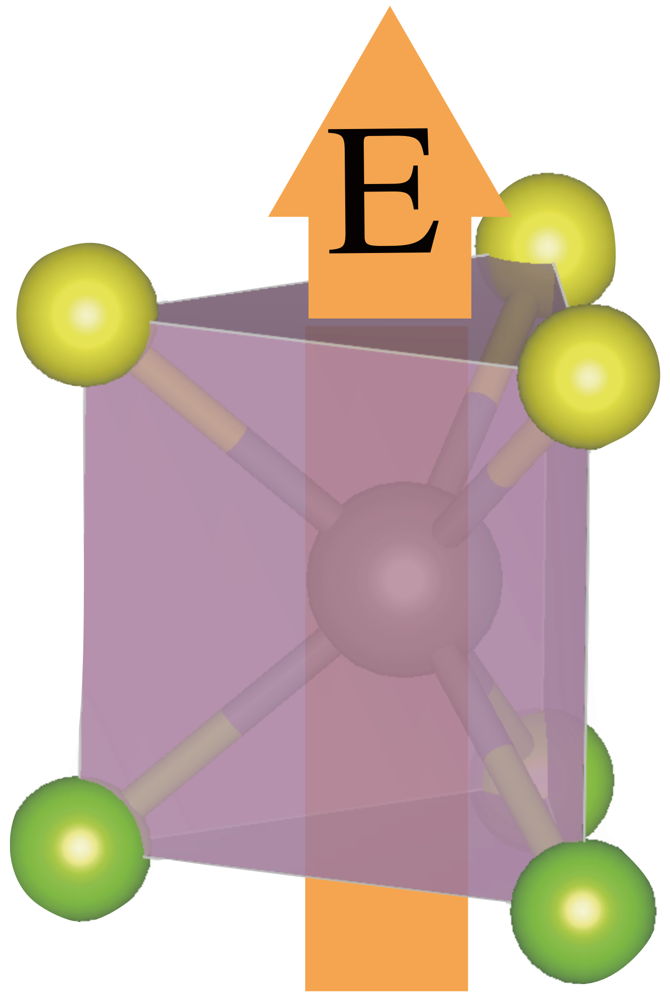
TMDC	**Janus TMDC**
○	✕

・**Honeycomb lattice** type two-dimensional thin film crystal

・Composed of **transition metal atoms** (1 species) and **chalcogens** (2 species)

1.Zhang, J. et al. ACS Nano 11, 8192–8198 (2017). 2. Liu, Z., Tee, S., Guan, G. & Han, M. NANO-MICRO LETTERS 16, (2024).

Rashba-type spin-orbit coupling (Rashba SOC) in Janus TMDCs



- Out-of-plane mirror symmetry breaking
- Internal electric field

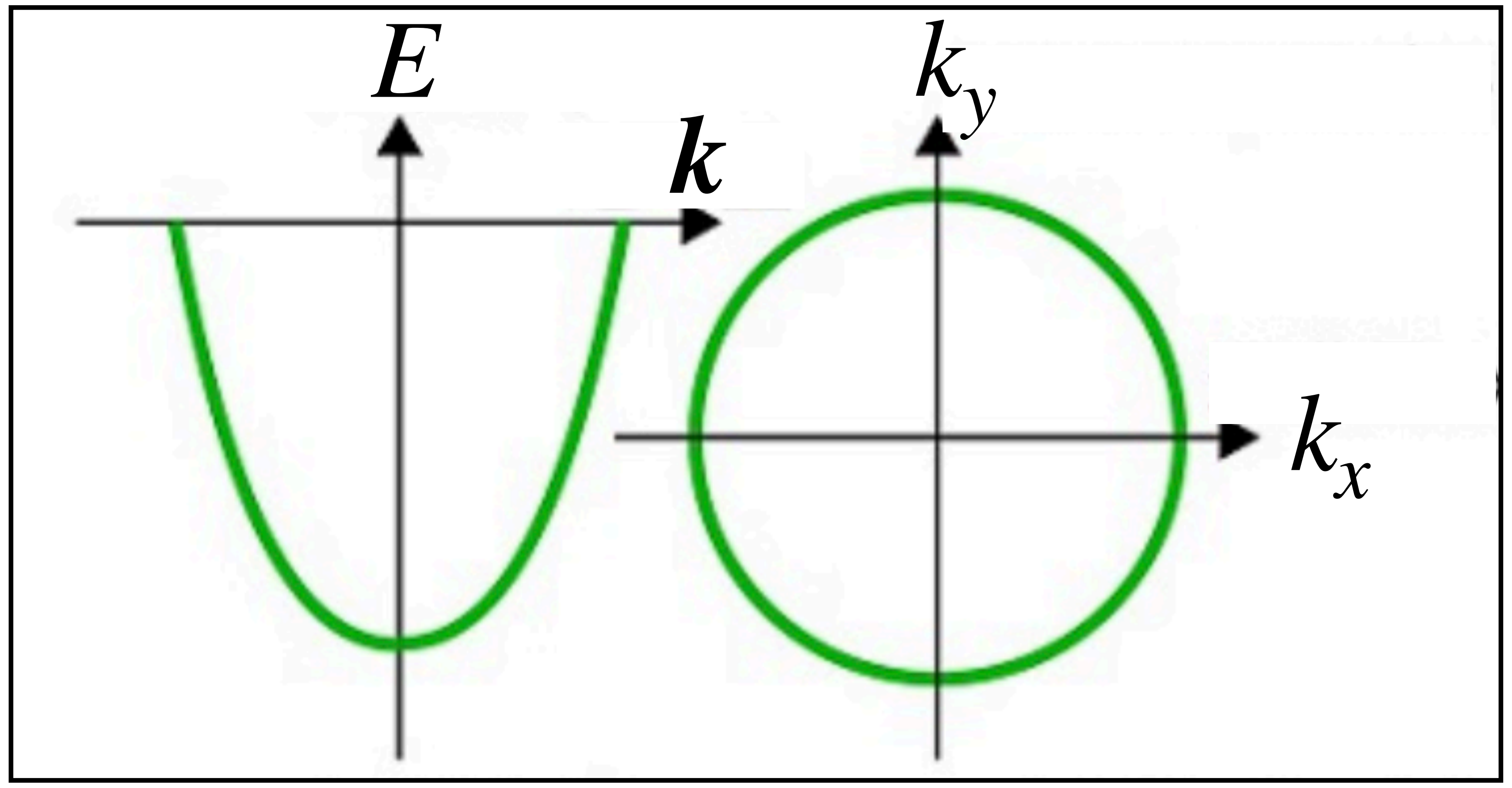
Janus TMDCs have
Rashba-type spin-orbit coupling
without external electric field

Topic of study

Investigation of
the contribution of **Rashba SOC**
to **spin current generation**
in **Janus TMDCs**

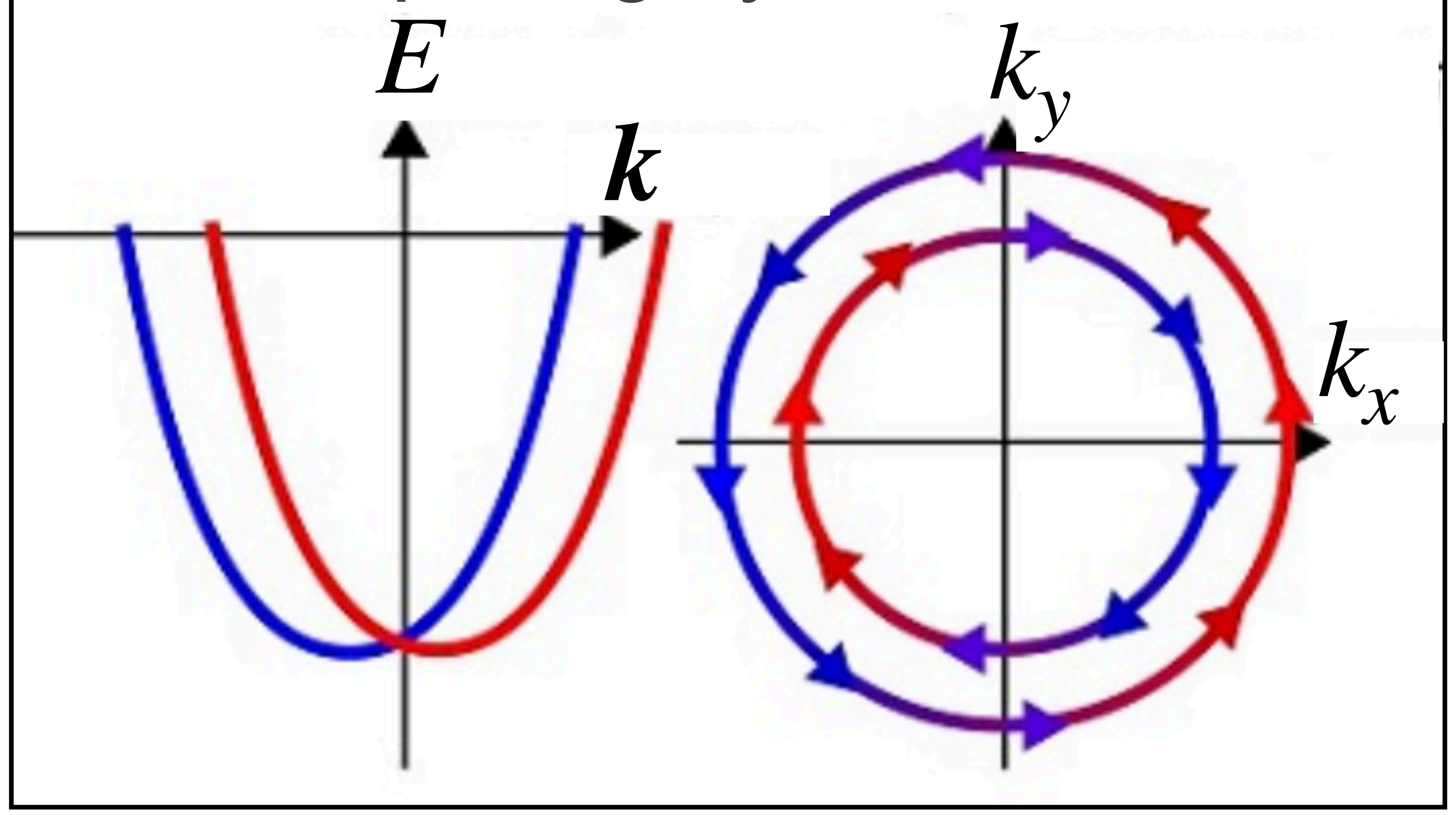
Spin polarized **perpendicular in the plane of the electron momentum direction**

Example: Free electron systems



Rashba SOC

Band splitting by **Rashba SOC**

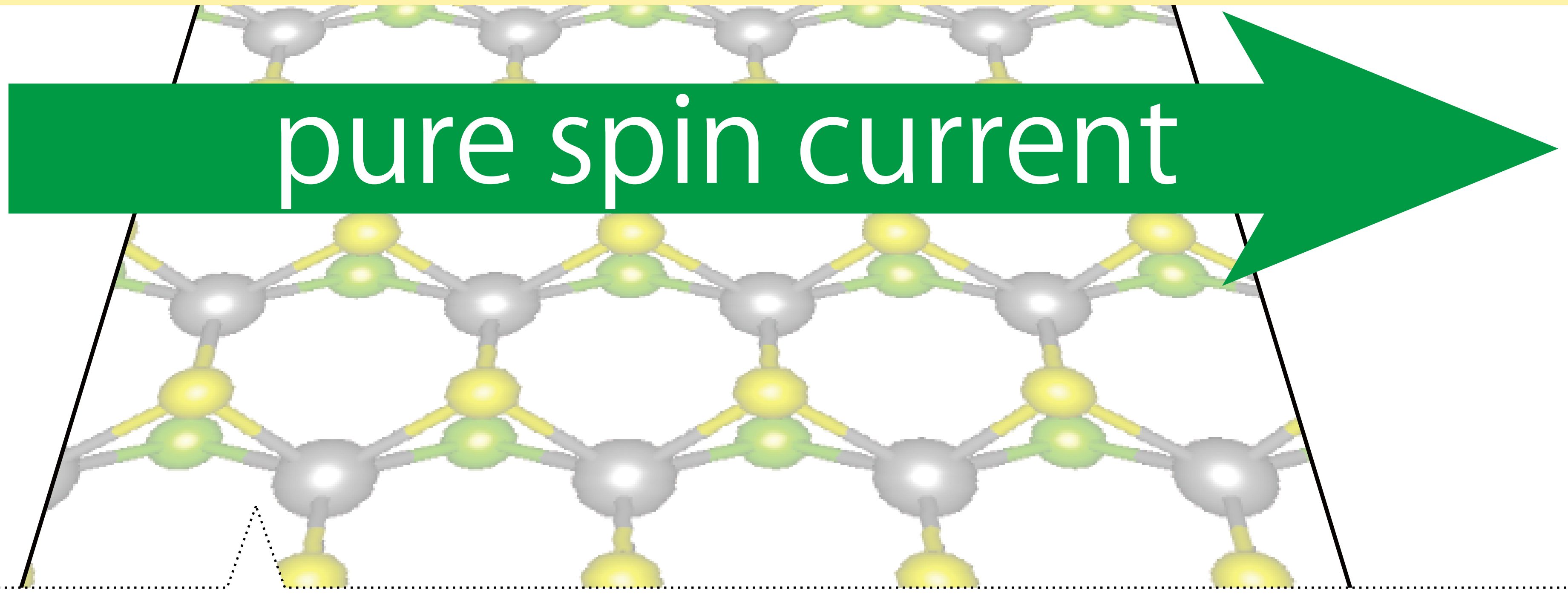


Key findings

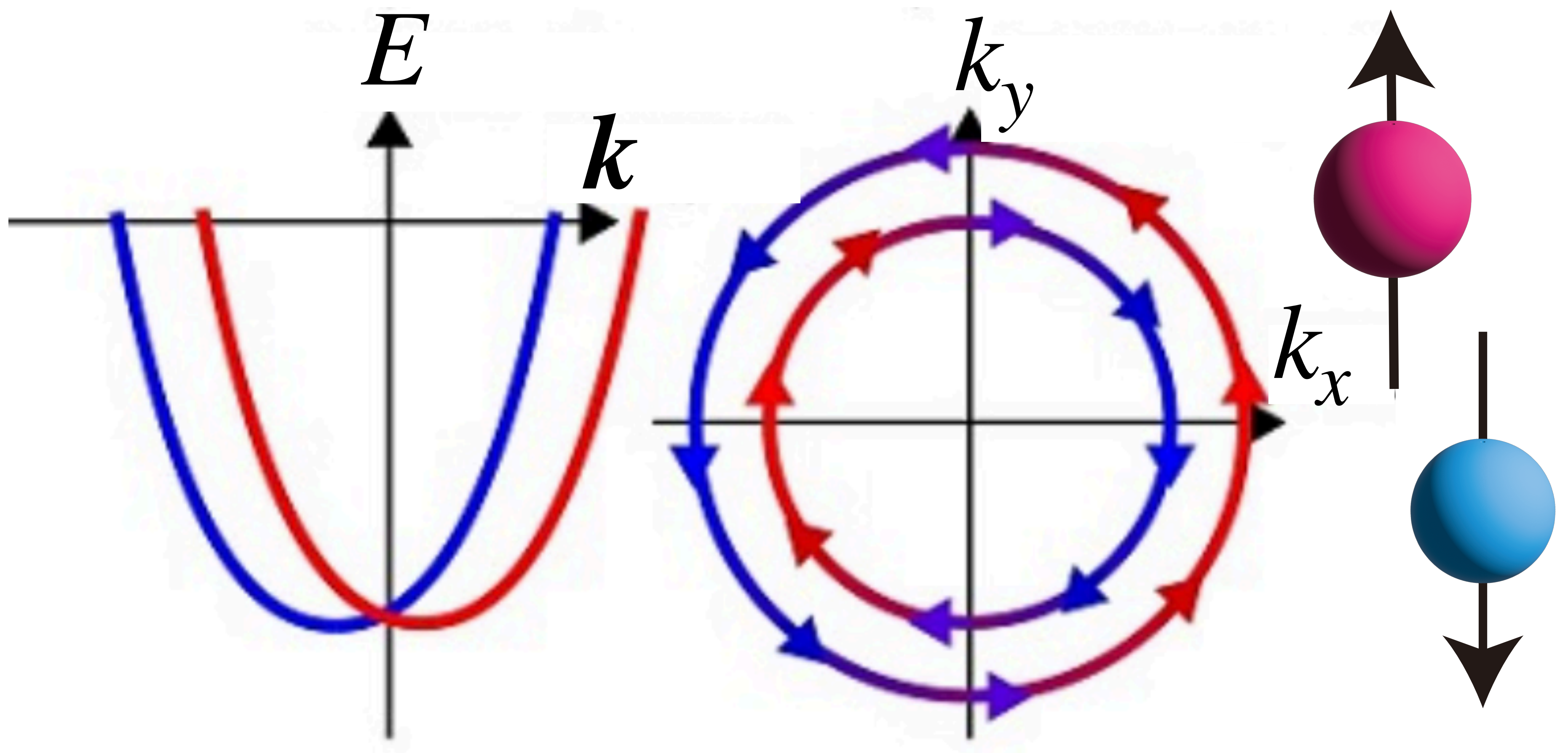
There is a **optically-induced** **pure spin current** in the Janus TMDC that is induced by the **Rashba SOC**

Thesis of study

Janus TMDC is a candidate for **optospintronics devices**

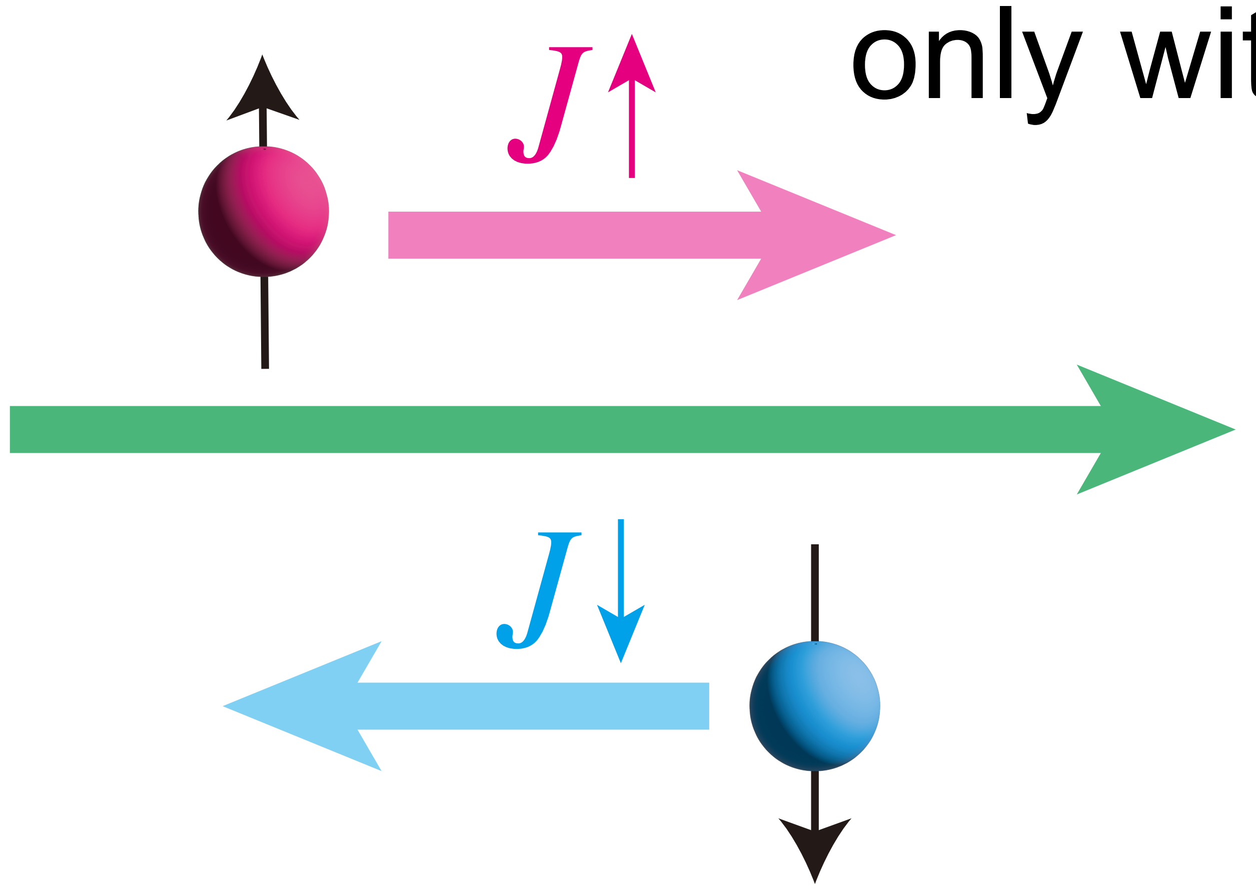


Band splitting by **Rashba SOC**



pure spin current

Flow of the spin angular momentum only without flow of the charge



$$J^{spin} = J\uparrow - J\downarrow \neq 0$$

$$J = J\uparrow + J\downarrow = 0$$

optically-induced

・Electric field induced by light

Methods

Step① **Tight-binding model**

・Rashba SOC parameter

・Energy band structure

・Spin polarization

Step② **Spin dependent optical hall conductivity**

・Kubo formula

・Evaluation

Spin dependent optical hall conductivity

Spin current generation efficiency

(**spin Hall angle**)

Multi-orbital TB model and Rashba SOC parameter

Considering $d_{z^2}, d_{xy}, d_{x^2-y^2}$ orbitals of transition metal atom

Common to TMDC

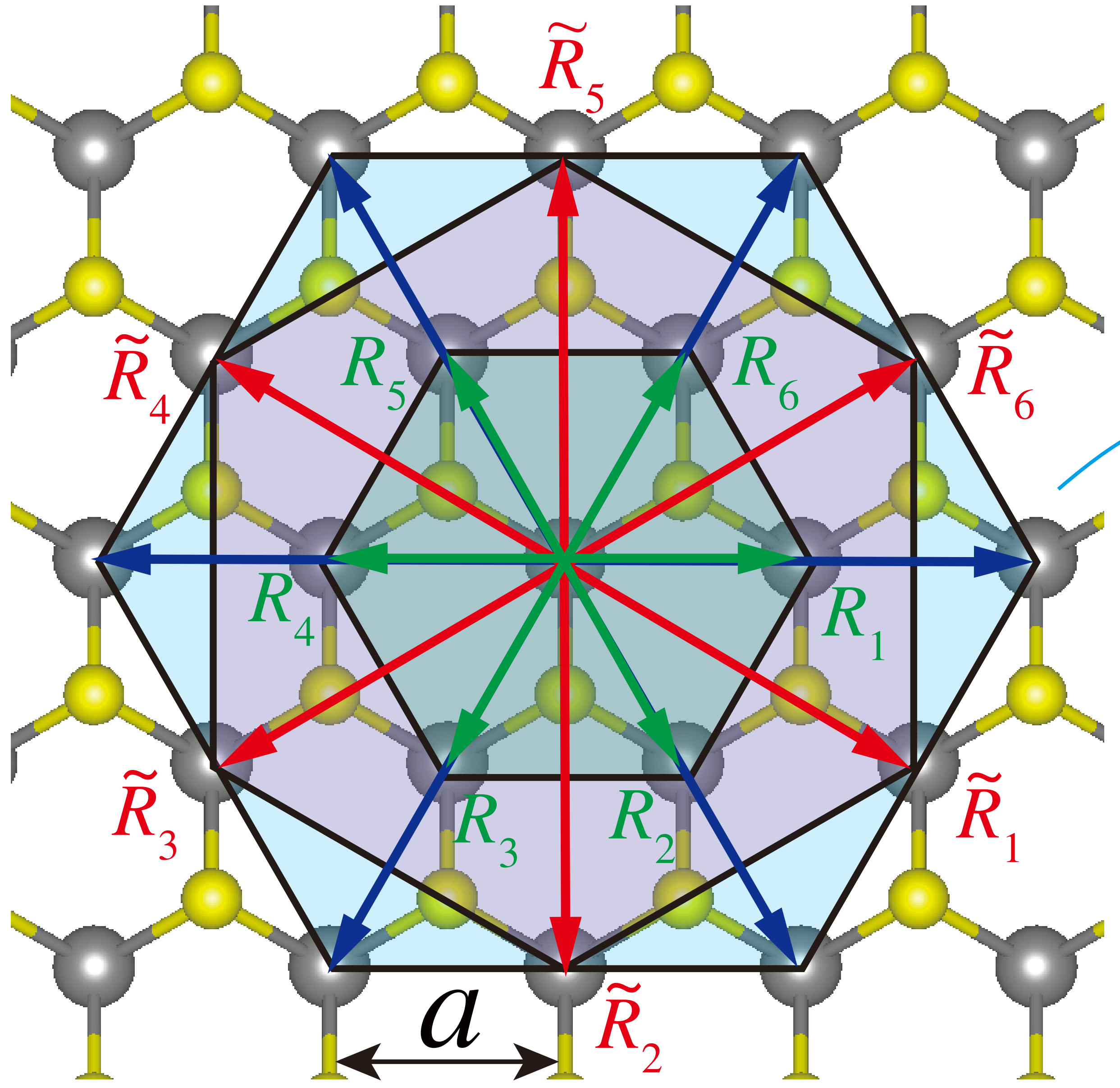
$$\hat{H}(\boldsymbol{k}) = \boxed{\underbrace{\hat{\sigma}_0 \otimes \hat{H}_{TNN}(\boldsymbol{k})}_{\text{Non-SOC term}} + \underbrace{\hat{\sigma}_z \otimes \frac{1}{2}\lambda \hat{L}_z}_{\text{Ising SOC term}}} + \underbrace{\boxed{\hat{H}_R(\boldsymbol{k})}}_{\text{Rashba SOC term}}$$

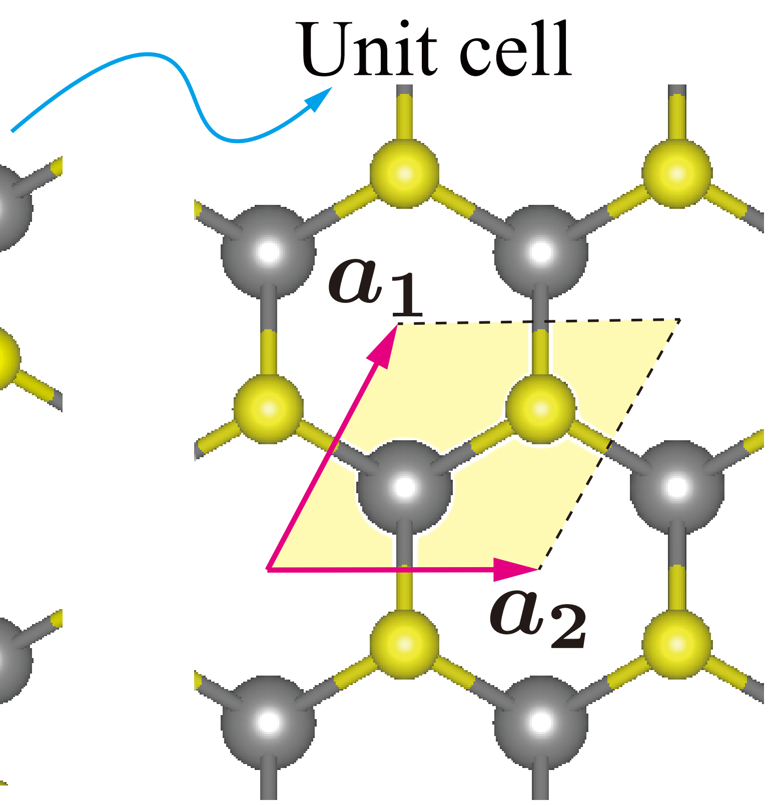
※ $\hat{H}_R = (f_x(\boldsymbol{k})\hat{\sigma}_y - f_y(\boldsymbol{k})\hat{\sigma}_x) \otimes diag(2\alpha_0, 0, 0)$

$$f_x(\boldsymbol{k}) = \sin(2\alpha) + \sin(\alpha)\cos(\beta),$$

$$f_y(\boldsymbol{k}) = \sqrt{3}\sin(\beta)\cos(\alpha).$$

$$(\alpha, \beta) = (\tfrac{1}{2}k_x a, \tfrac{\sqrt{3}}{2}k_y a)$$





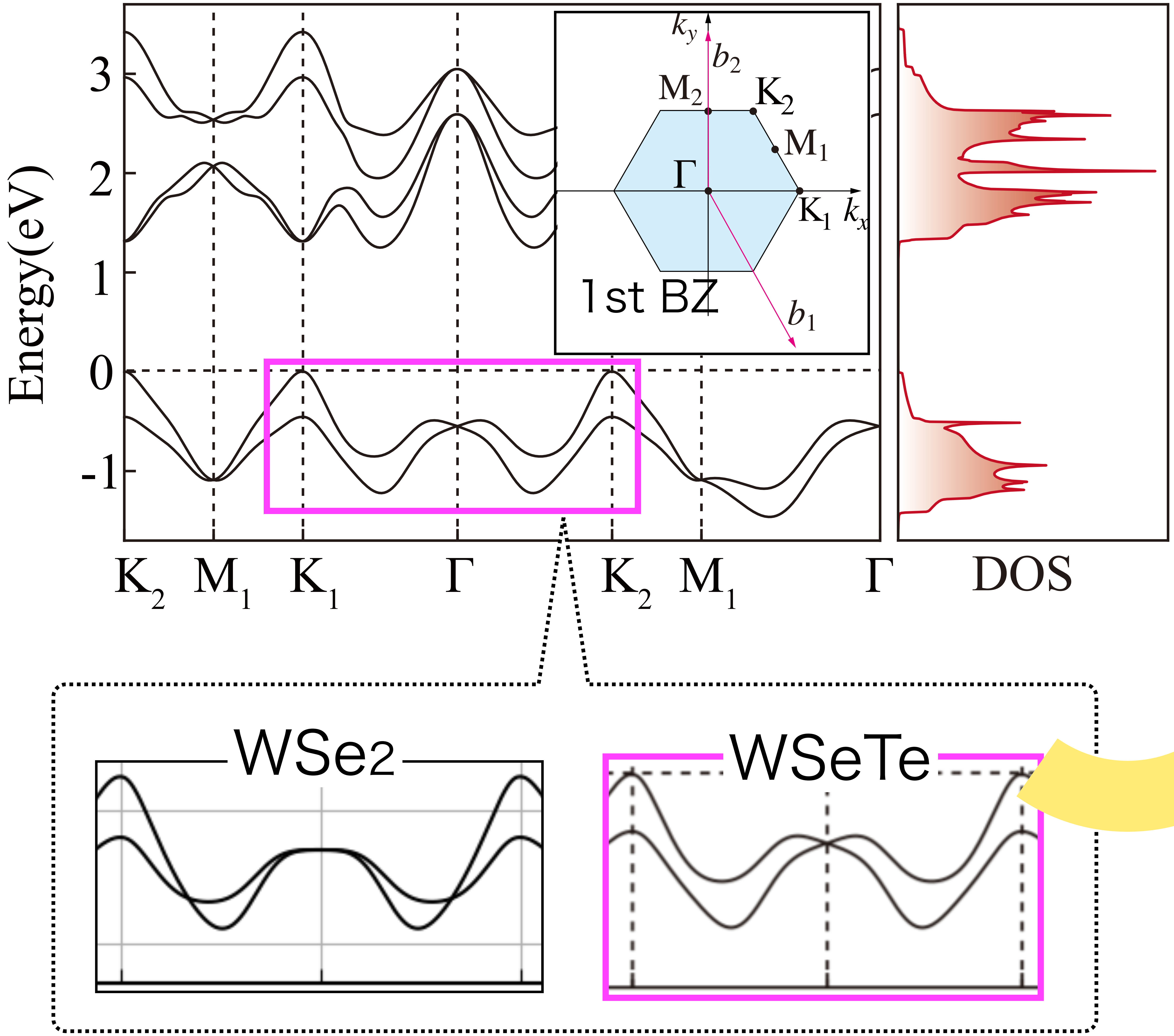
Nearest neighbor　Second　Third

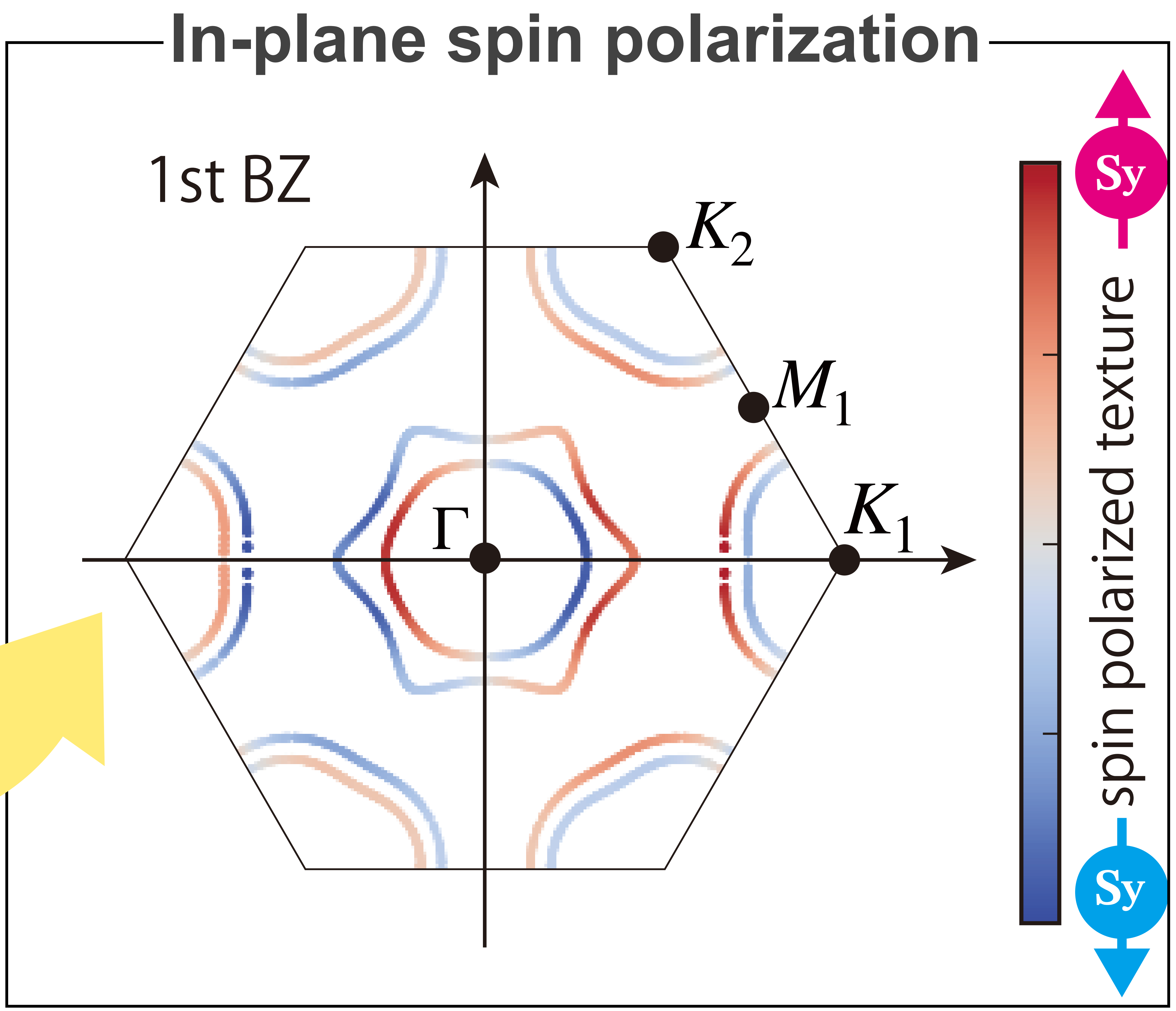
- Rashba SOC parameter α_0
  - Determining the intensity of band splitting
  - Setting $\alpha_0 = 0.045$ eV

  , which is corresponds to **WSeTe**

1.Yao, Q.-F. *et al*. *Phys. Rev. B* **95**, 165401 (2017).

Energy band structure and spin polarization of WSeTe





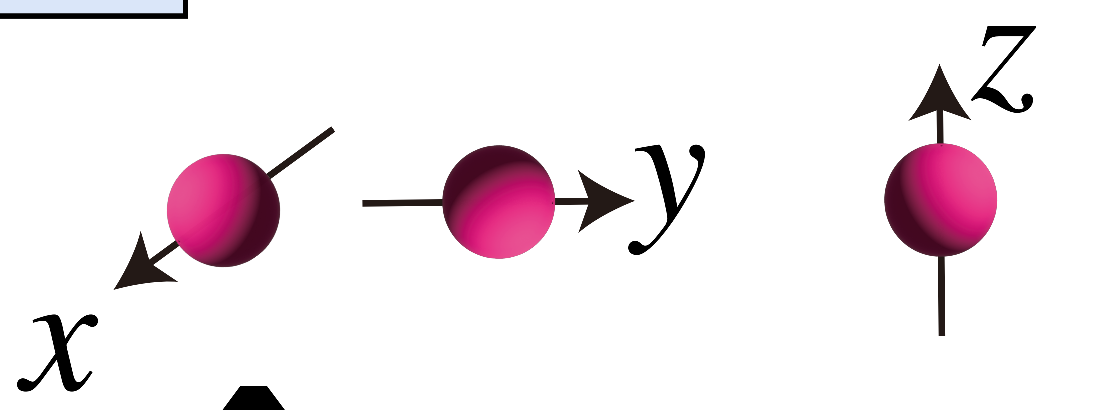
- **Rashba SOC-derived band splitting** occurs near the Γ point

Spin dependent optical hall conductivity

$$\sigma_{ij}^{spin(k)}(\omega) = \frac{i\hbar e}{(2\pi)^2}\int_{BZ} d^2\boldsymbol{k}\Sigma_{n\neq m}\frac{f(E_n(\boldsymbol{k})) - f(E_m(\boldsymbol{k}))}{E_m(\boldsymbol{k}) - E_n(\boldsymbol{k})} \times \frac{\langle u_n(\boldsymbol{k})\,|\,\hat{j}_i^{spin(k)}\,|\,u_m(\boldsymbol{k})\langle u_m(\boldsymbol{k})\,|\,\hat{v}_j\,|\,u_n(\boldsymbol{k})\rangle}{E_m(\boldsymbol{k}) - E_n(\boldsymbol{k}) - \hbar\omega - i\eta}$$

Spin Hall Angle

$$\theta^{\text{spin}} = \frac{2e}{\hbar}\frac{\sigma_{xy}^{\text{spin}}}{\sigma_{xx}}$$



$$\hat{\sigma}_{ij}^{spin(k)}$$

Calculated from TBM

$E_n(\boldsymbol{k})$: **Energy eigenvalue** n**-band**

$|\,u_n(\boldsymbol{k})\rangle$: **Energy eigenstate** n**-band**

$\hat{v}_i = \dfrac{1}{\hbar}\dfrac{\partial \hat{H}(\boldsymbol{k})}{\partial k_i}$: **Velocity operator**

$\hat{j}_i^{spin(z)} = \dfrac{1}{2}\{\hat{\sigma}_z, \hat{v}_i\}$: **Spin current density operator**

variable value

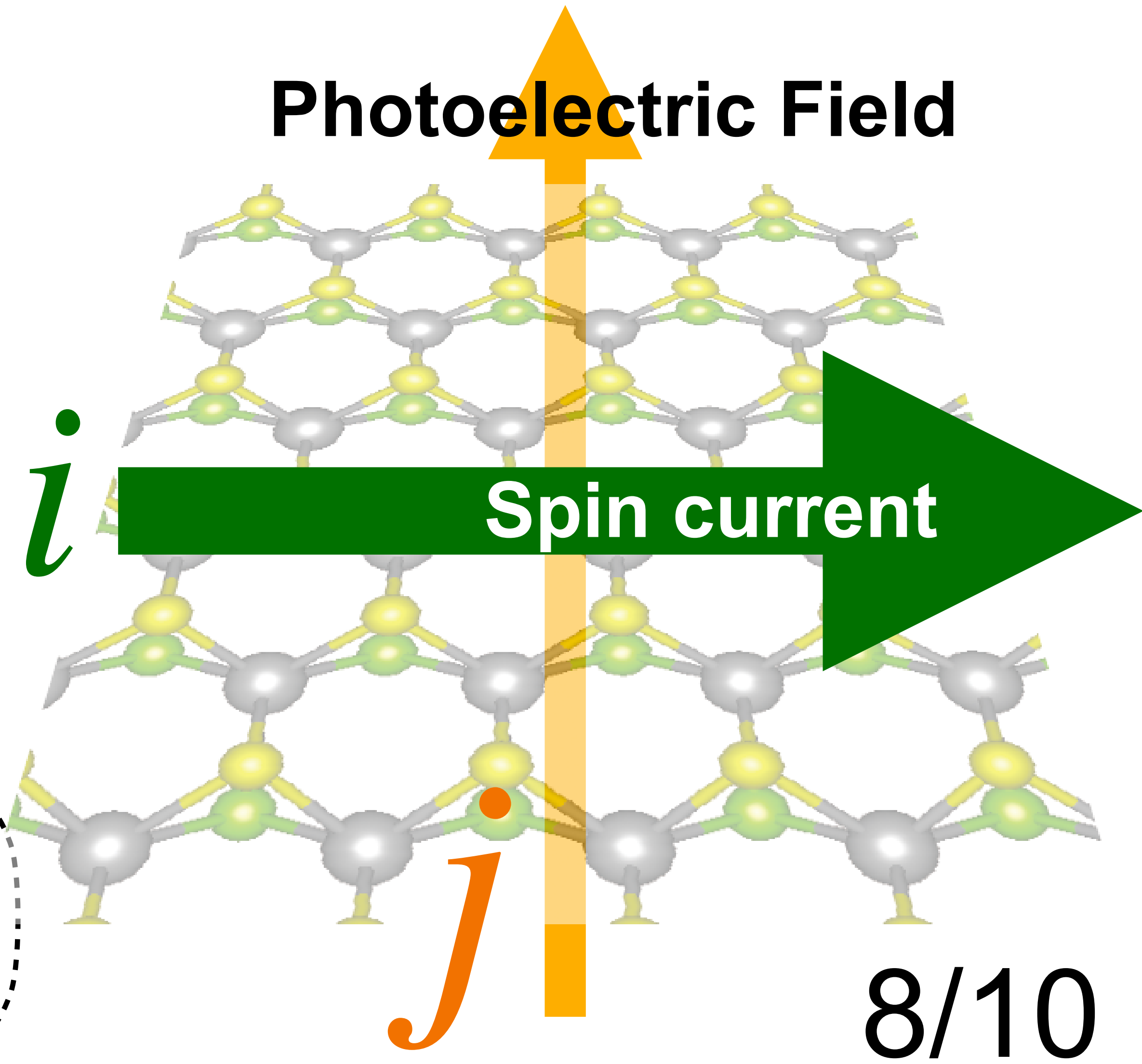
ω : **optical angular frequency**

i : **Spin current conduction direction**

j : **Photoelectric field oscillation direction**

$spin(k)$: **Spin polarization direction**

Experimental conditions and external parameters



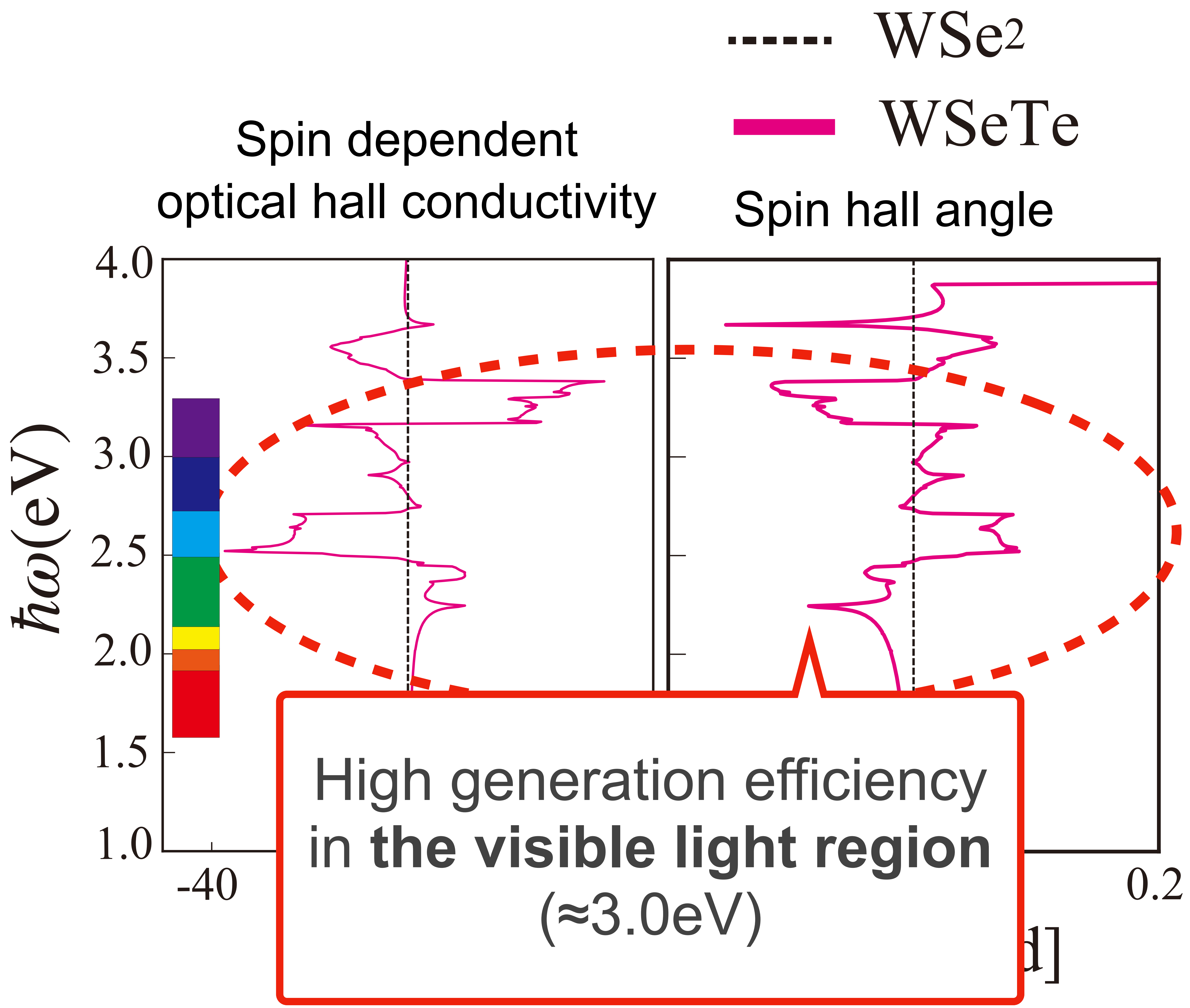
Other symbols

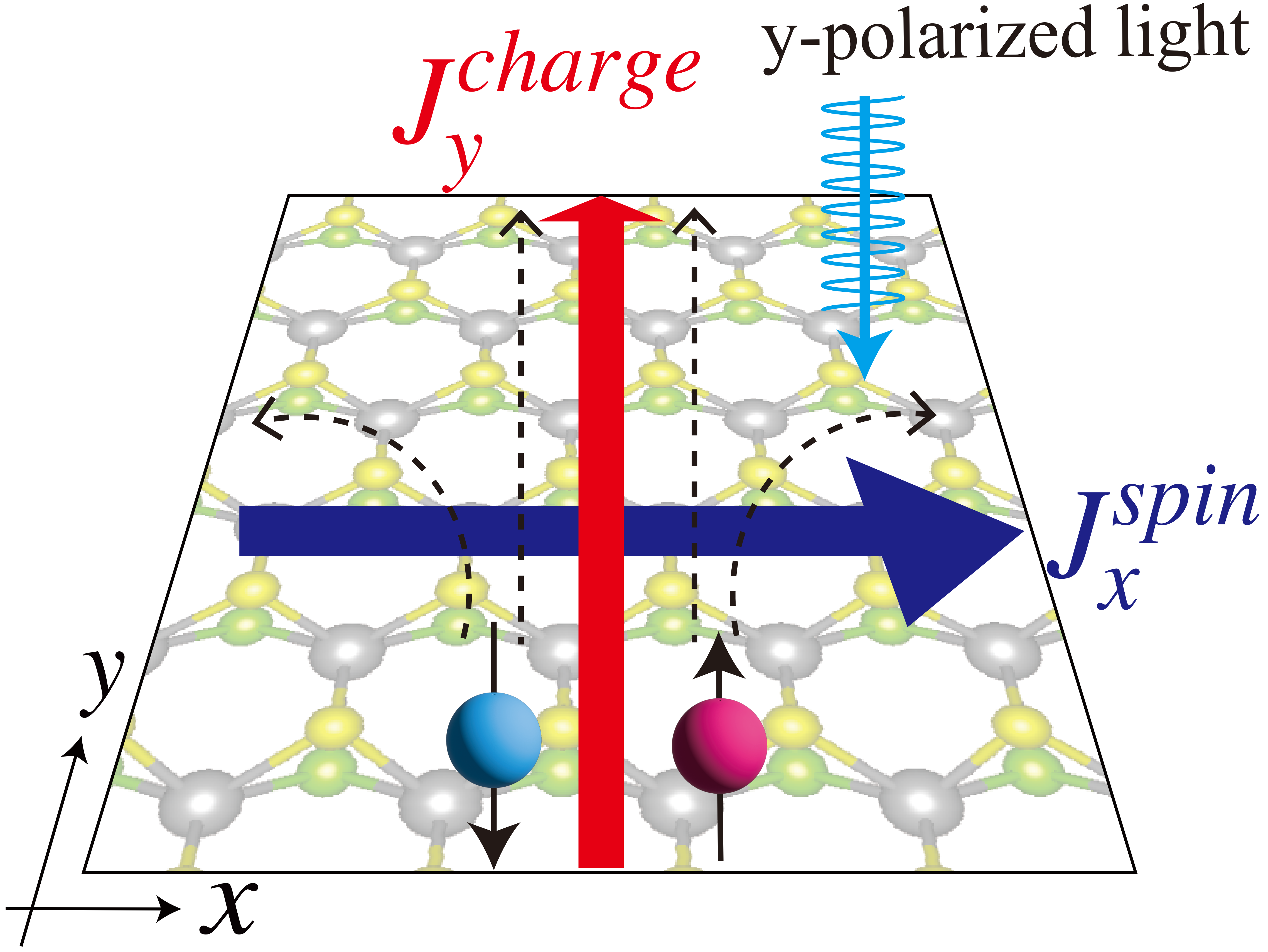
η : an infinitesimally small real number

$\hat{\sigma}_z$: Pauli matrix (z-component)

$f(E_n(\boldsymbol{k}))$: Fermi distribution function

Optically induced pure spin current





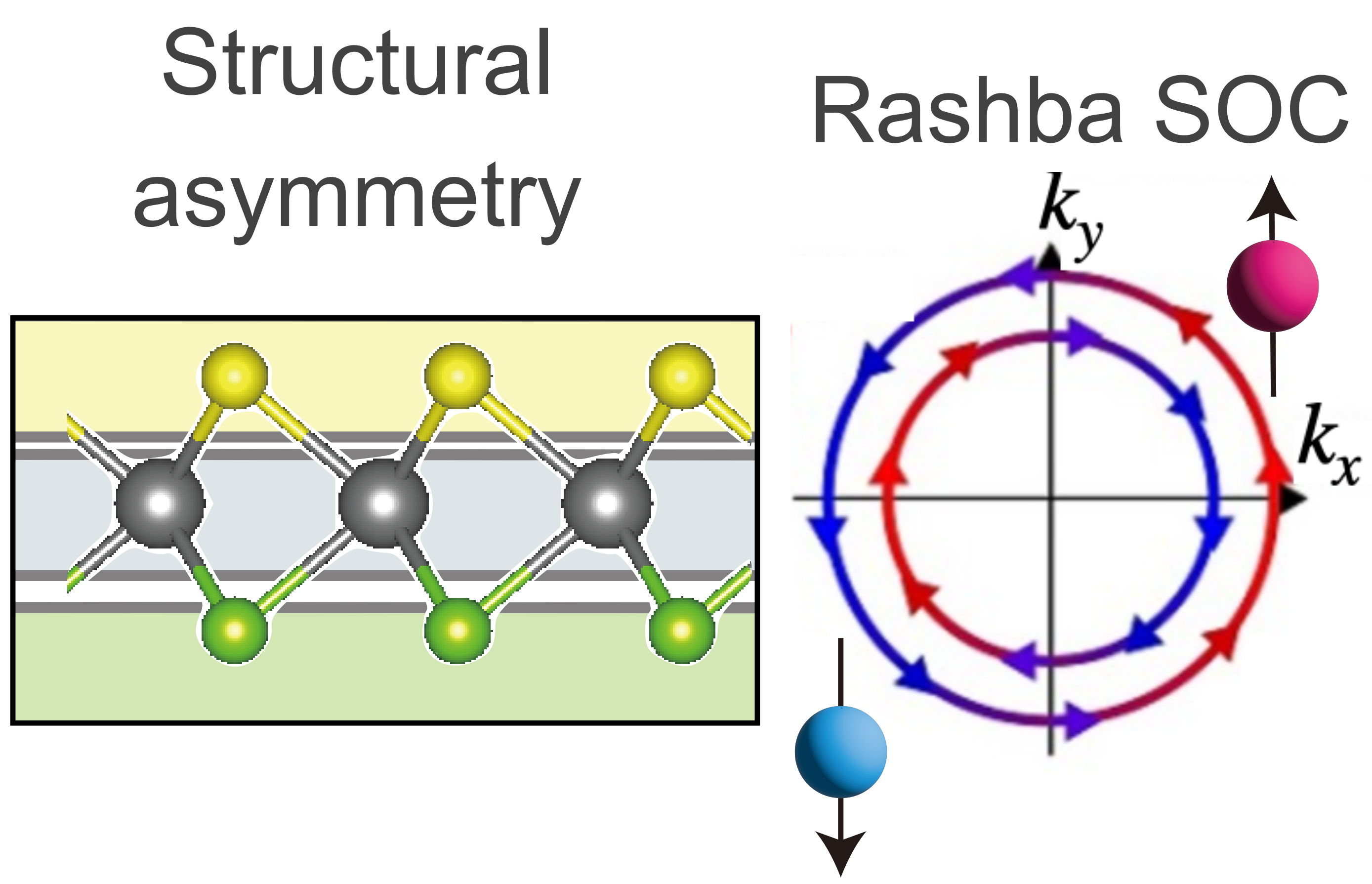
- **Pure spin currents are generated**

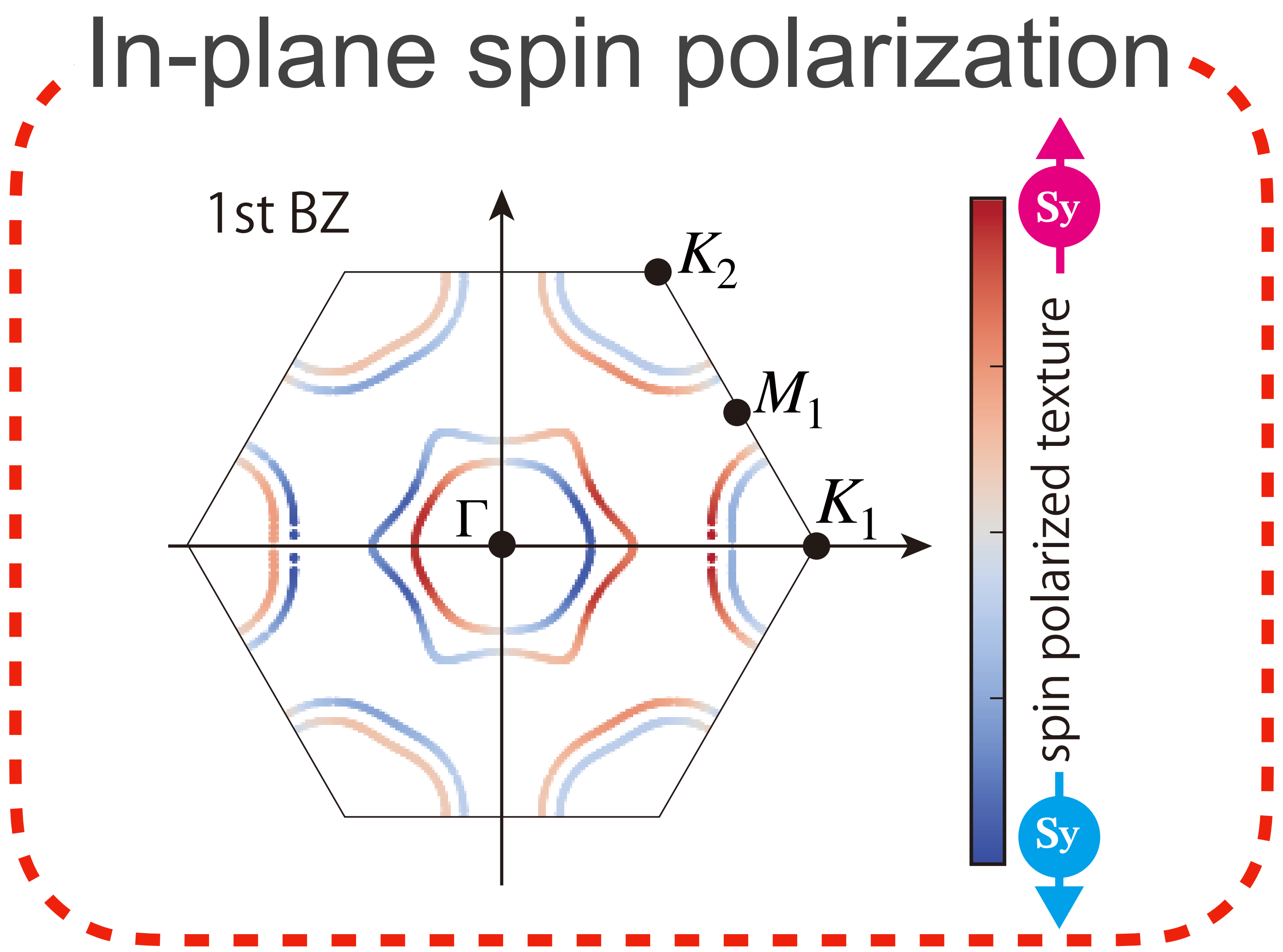
T. Kameda and K. Wakabayashi, "Optically induced spin current in Janus transition-metal dichalcogenides," **submitted to Phys. Rev. B** (2025).

Summary

Optically induced pure spin current in Janus TMDC

Factors





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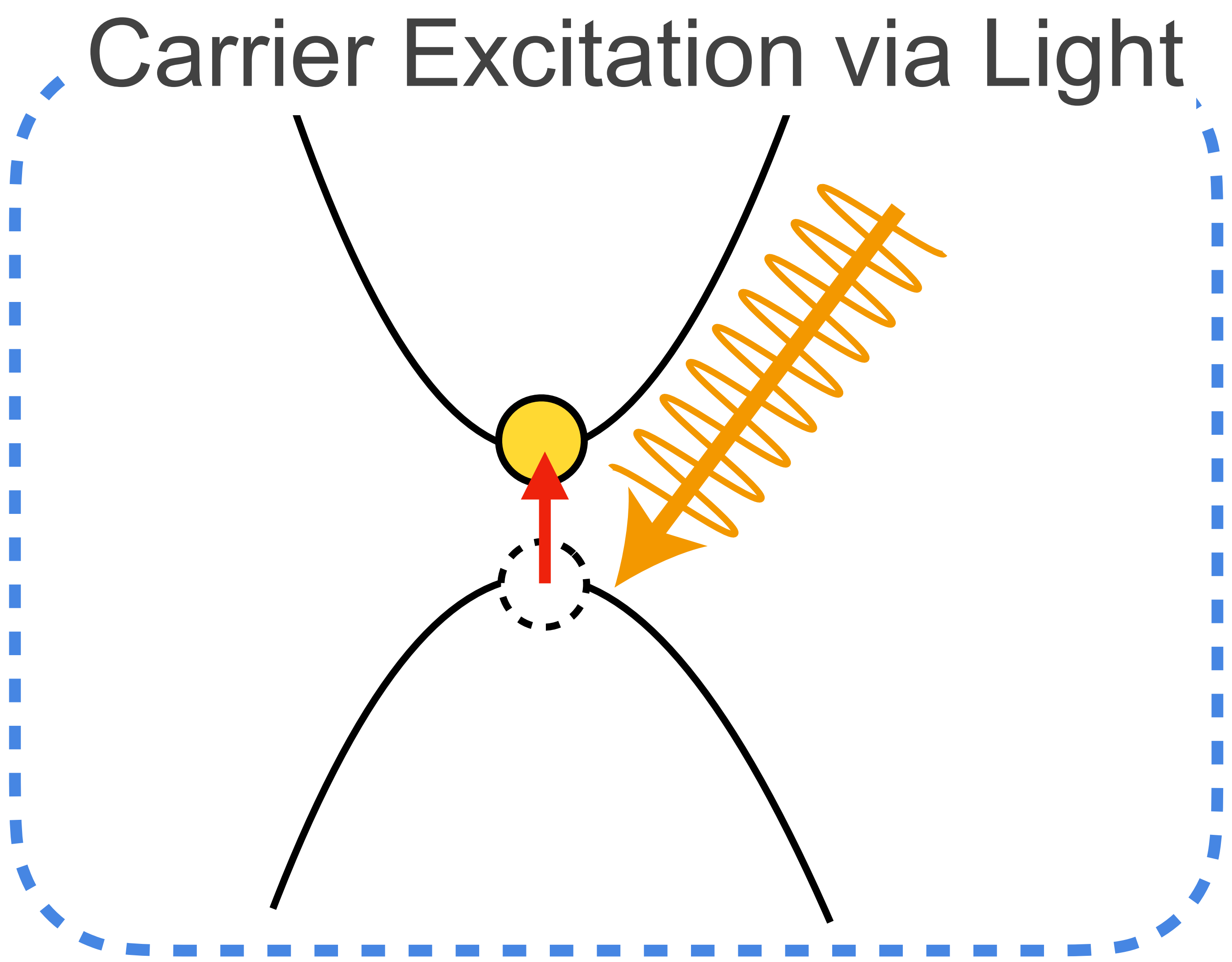
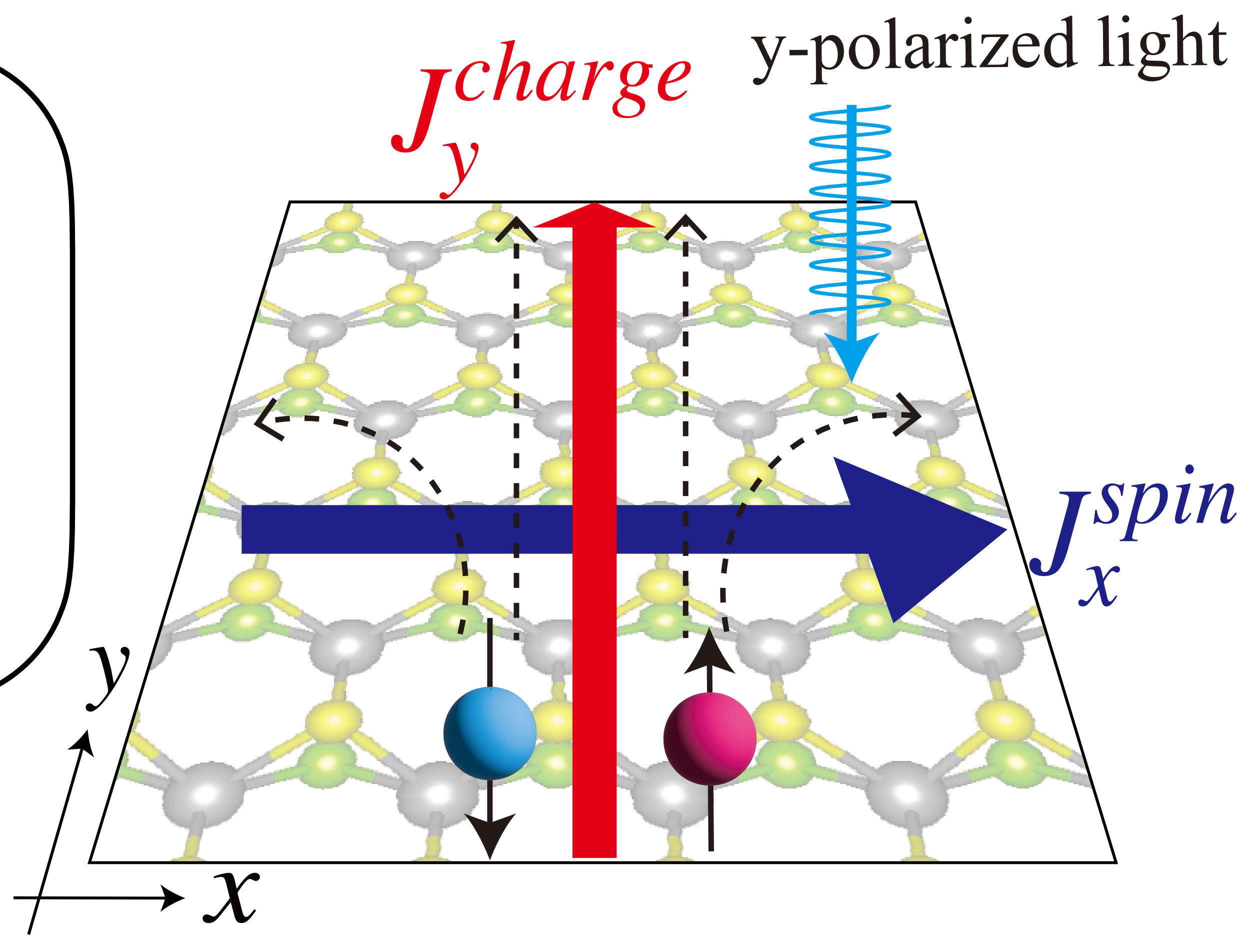
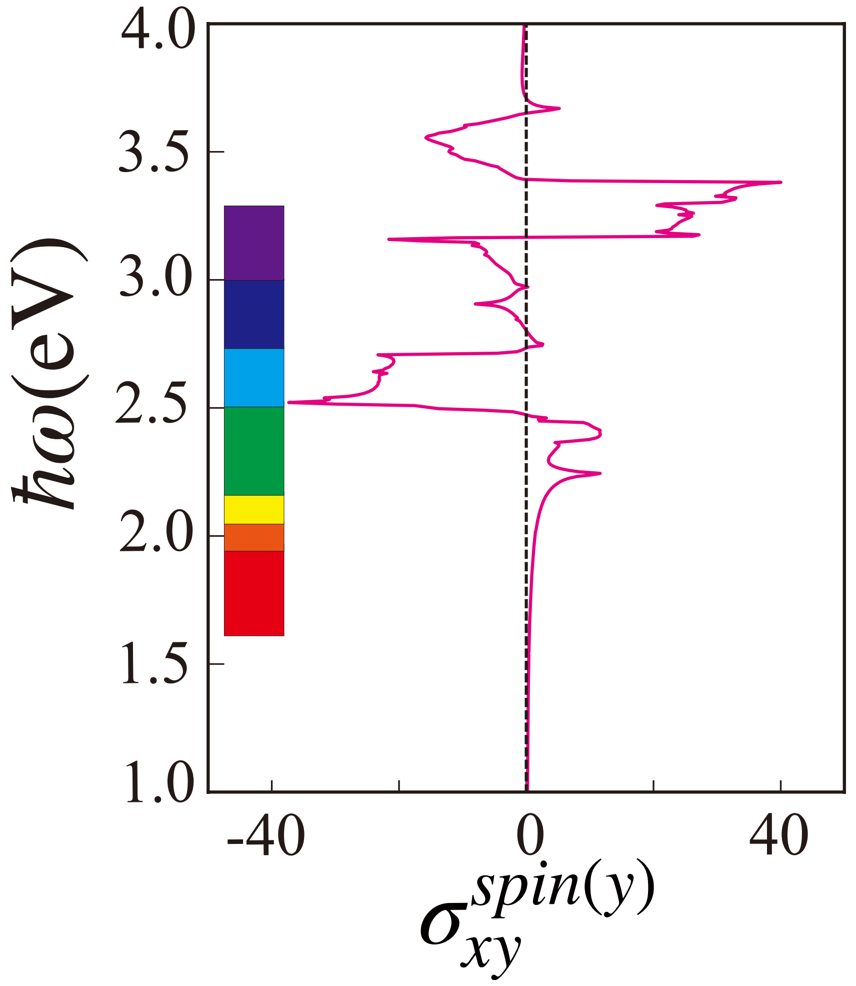


Methods

Step① Tight-binding model

Step② Spin dependent optical hall conductivity





Our results offer a new degree of freedom

for designing optospintronic devices, such as **spin current harvesting** via light irradiation in 2D materials

T. Kameda and K. Wakabayashi, "Optically induced spin current in Janus transition-metal dichalcogenides," **submitted to Phys. Rev. B** (2025).

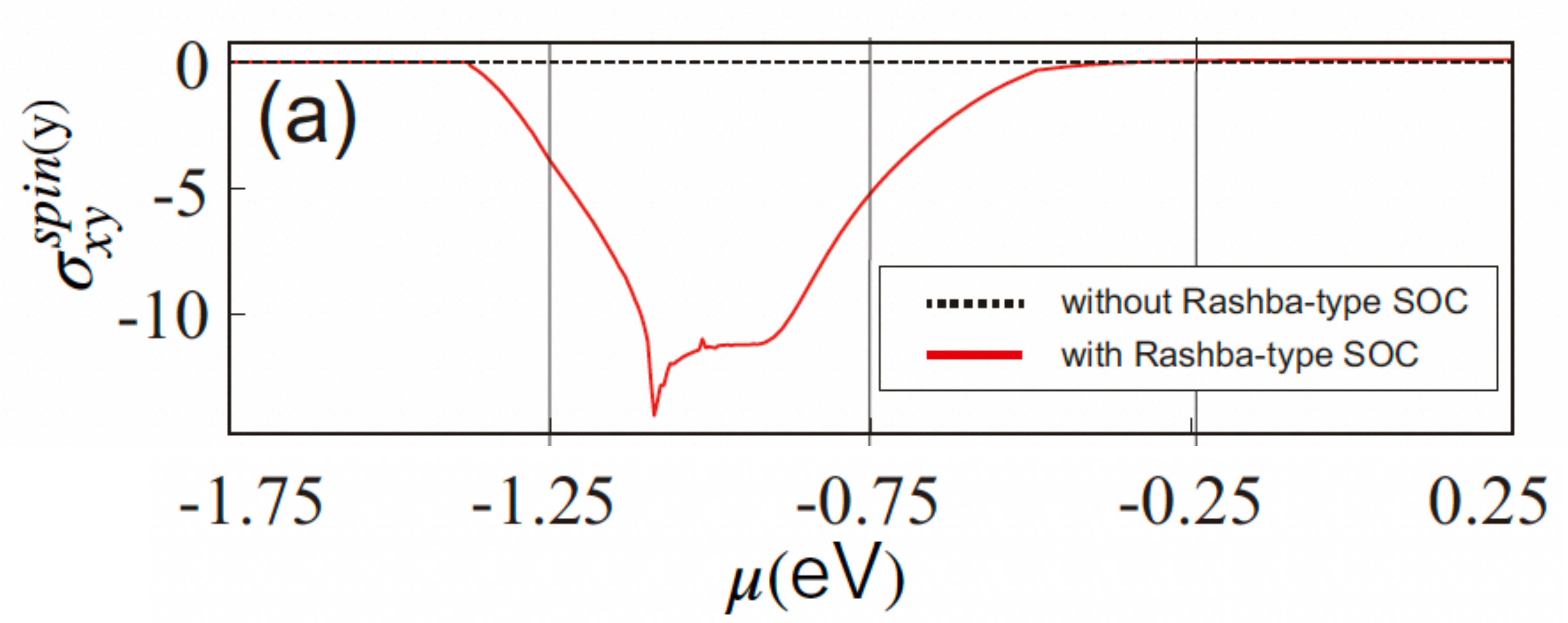
Appendix Direct current limit

$$\sigma_{ij}^{\mathrm{spin}(k)}(\omega) = \frac{e}{(2\pi)^2} \int_{\mathrm{BZ}} \boxed{\Omega_{ij}^{\mathrm{spin}(k)}(\omega, \boldsymbol{k})} d^2\boldsymbol{k}$$

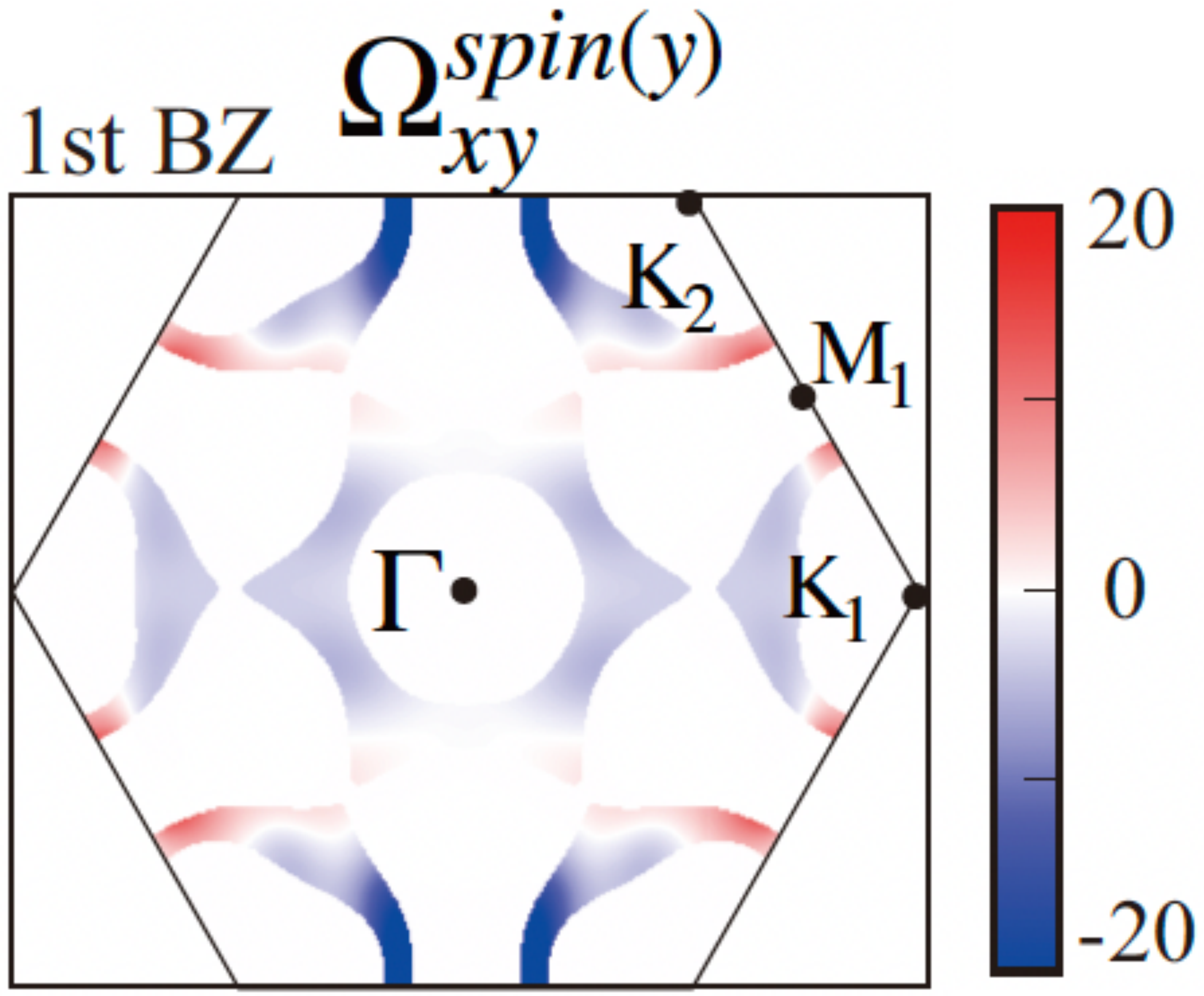
$\omega = 0$

Spin Berry curvature

$$\Omega_{i\perp j}^{\mathrm{spin}(k)}(\boldsymbol{k}) = \hbar \sum_n f(E_n(\boldsymbol{k})) \sum_{m(\neq n)} \frac{-2\mathrm{Im}\langle u_n(\boldsymbol{k})|\hat{j}_i^{\mathrm{spin}(k)}|u_m(\boldsymbol{k})\rangle\langle u_m(\boldsymbol{k})|\hat{v}_j|u_n(\boldsymbol{k})\rangle}{(E_m(\boldsymbol{k}) - E_n(\boldsymbol{k}))^2}$$



Spin dependent conductivity (DC limit)

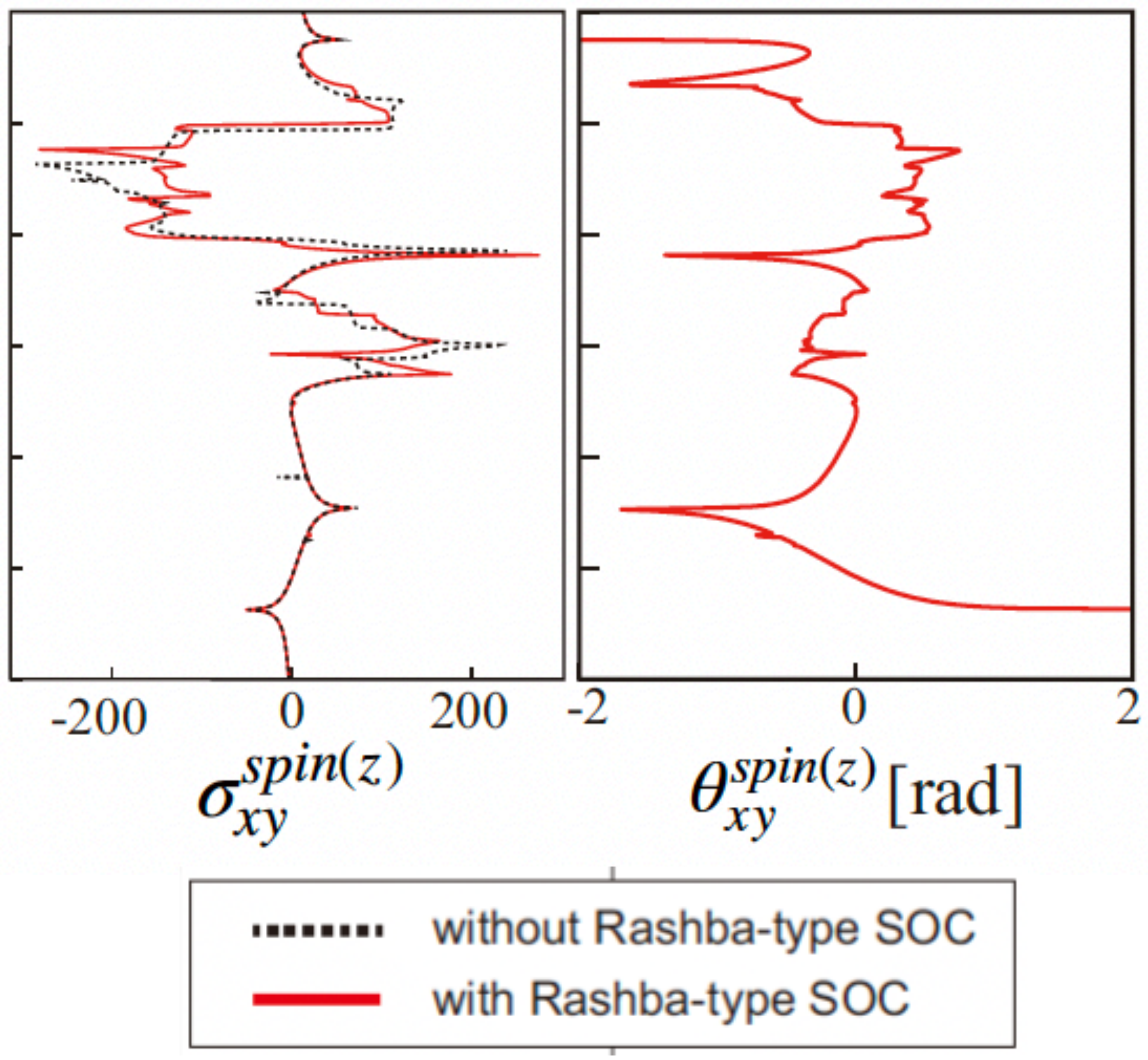


Spin Berry curvature

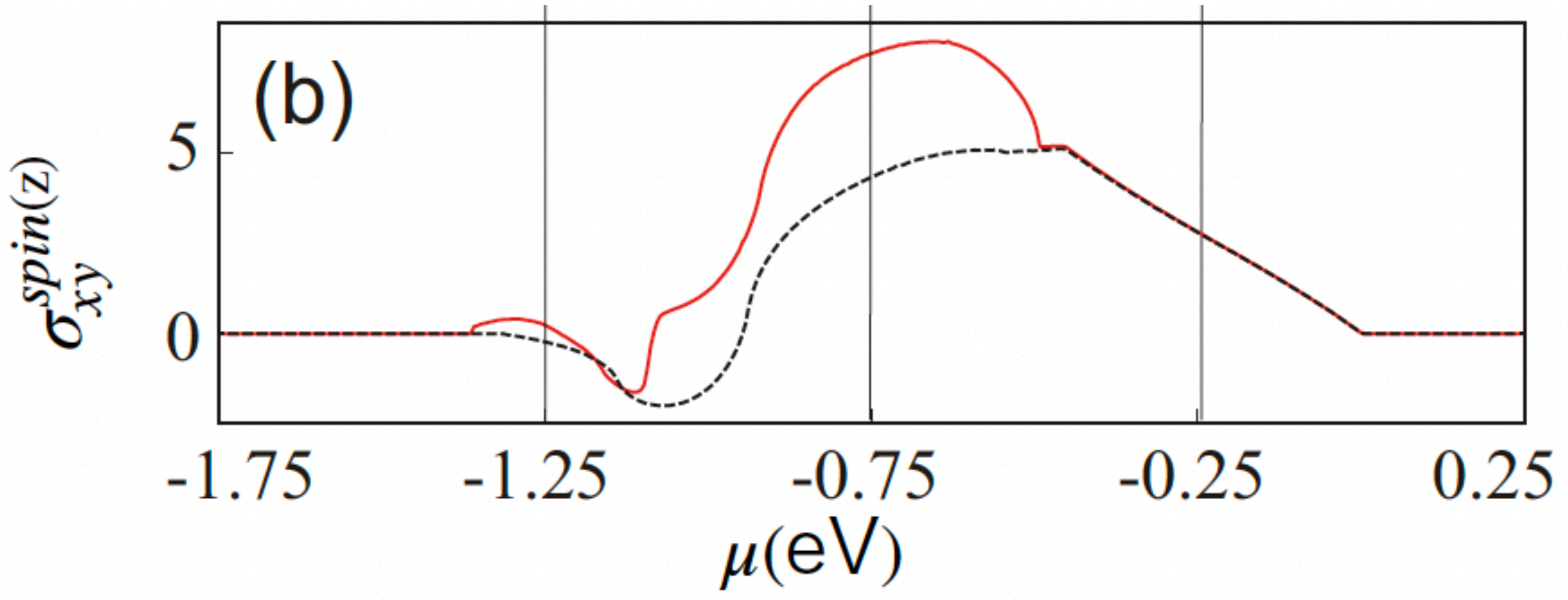
Appendix Ising SOC derived pure spin current

Spin dependent optical conductivity

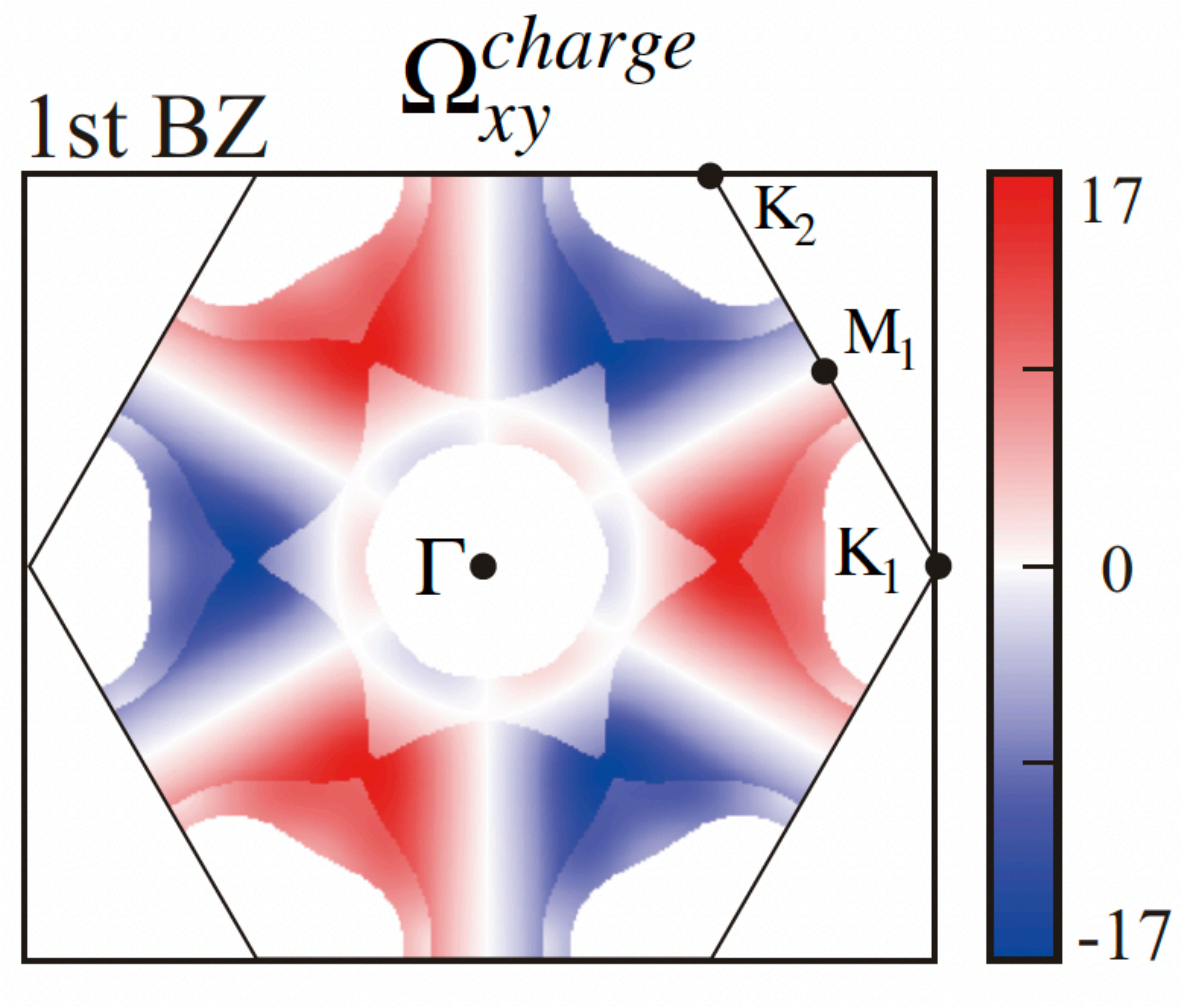
Spin Hall angle



Spin dependent conductivity (DC limit)



Appendix Charge Hall current



Appendix Neumann's principle

Methods

Step① Tight-binding model

- Rashba SOC parameter
- Energy band structure
- Spin polarization

Step② Spin dependent optical hall conductivity

- Kubo formula
- Evaluation

  Spin dependent optical hall conductivity

  Spin current generation efficiency (**spin Hall angle**)

Energy eigenvalues, eigenstates

Step③ Symmetry analysis

- Neumann's principle

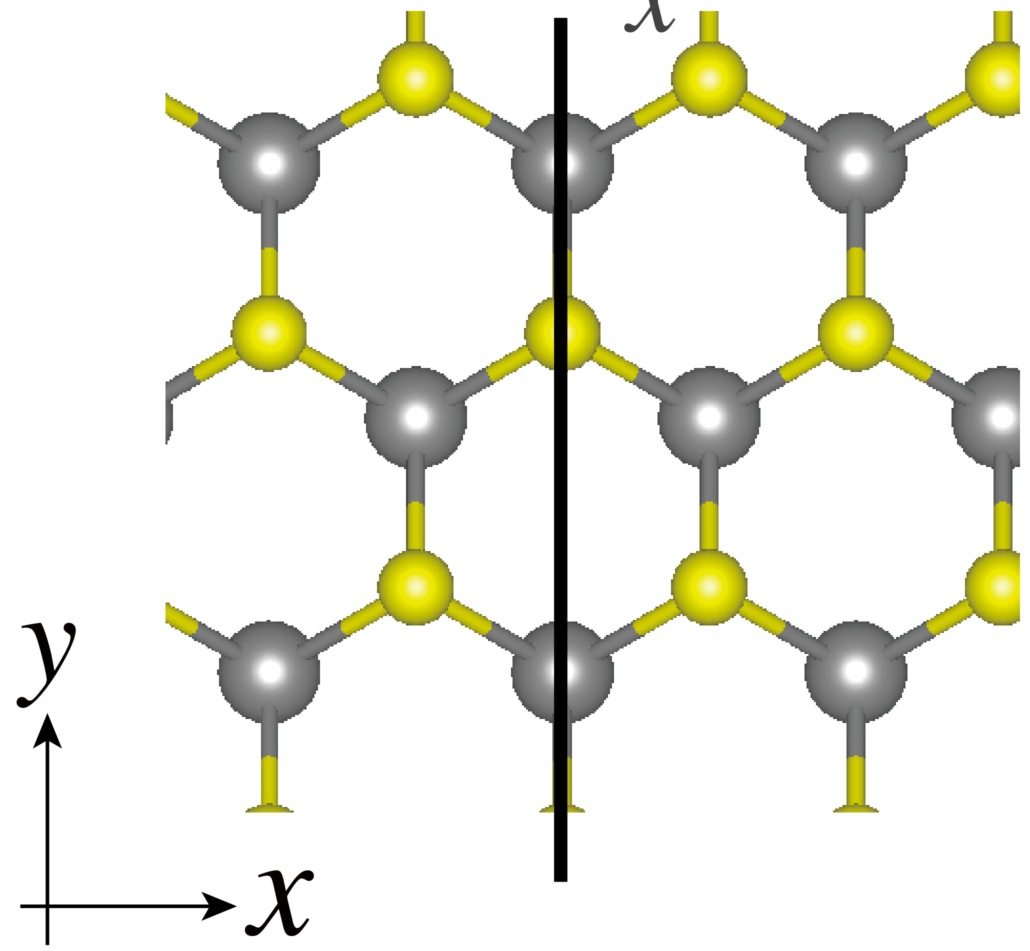
Step3 Symmetry analysis

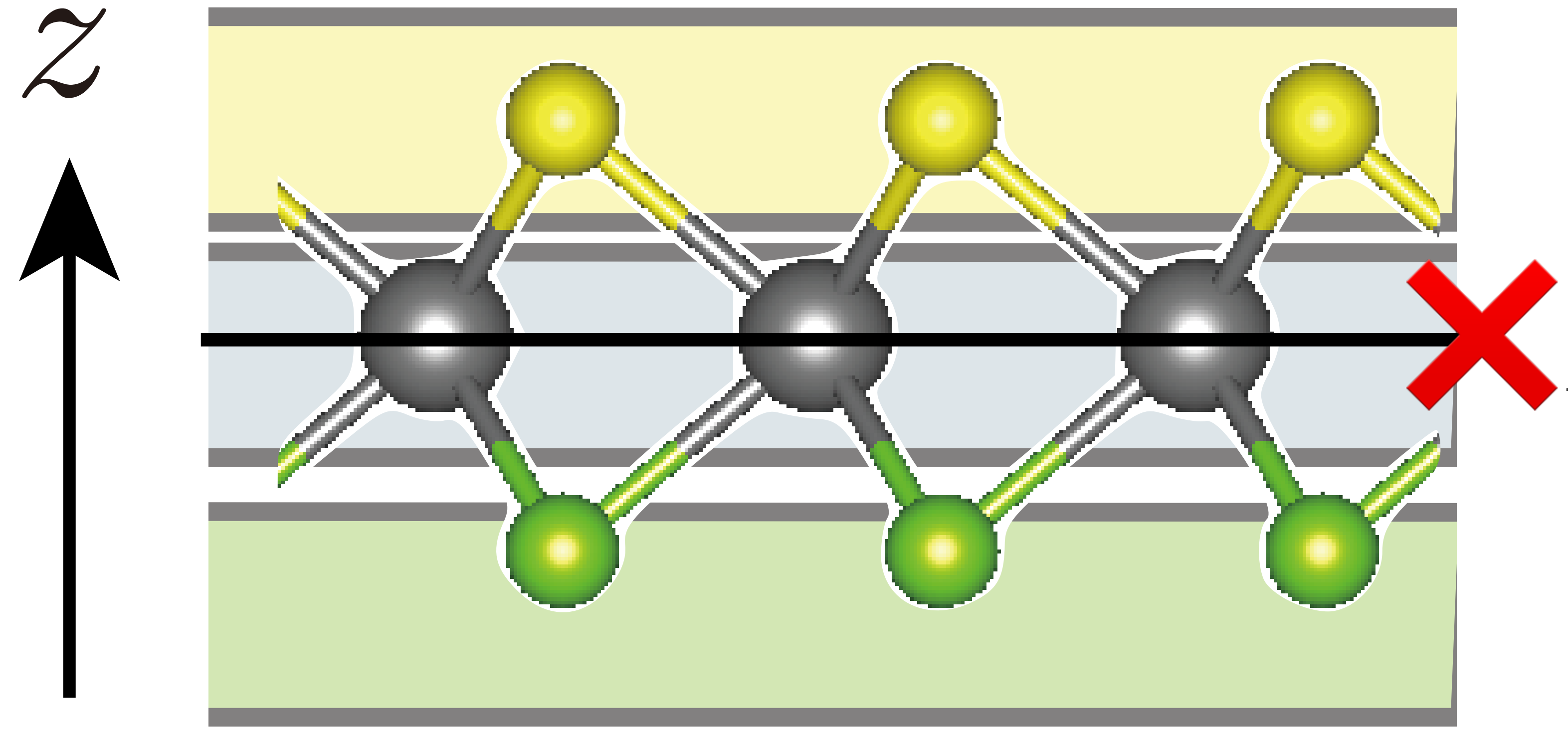
Neumann's principle

The physical properties of a crystal must obey **the symmetry of its structure**

Symmetry

$\hat{M}_x$



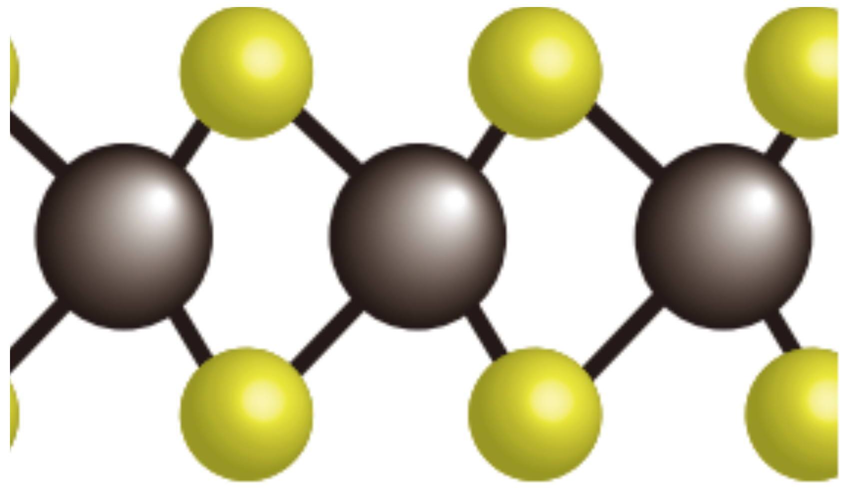


✗ $\hat{M}_z$

$$\sigma^{\alpha}_{\beta\gamma} = \mathbf{det}(R) R_{\alpha\alpha'} R_{\beta\beta'} R_{\gamma\gamma'} \sigma^{\alpha'}_{\beta'\gamma'}$$

$\hat{R}$ Symmetry operator $\quad \mathbf{det}(R) = \pm 1$

Conventional TMDC $\hat{M}_x \ \hat{M}_z$



$$\sigma^{spin(y)} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$$

Symmetry operator $\hat{M}_x$

$$\hat{M}_x = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \longrightarrow \sigma^{spin(y)} = \begin{pmatrix} 0 & \sigma^{y}_{xy} \\ \sigma^{y}_{yx} & 0 \end{pmatrix}$$

可視光のエネルギーと色は、波長によって異なります。

- 紫：エネルギーが高い（380～450nm、2.755～3.26eV）
- 青：エネルギーが高い（430～490nm）
- 緑：エネルギーが低い（495～570nm、2.175～2.50eV）
- 黄：エネルギーが低い（570～590nm、2.10～2.175eV）
- 橙：エネルギーが低い（590～620nm、1.99～2.10eV）
- 赤：エネルギーが最も低い（620～750nm、1.65～1.99eV）