Electronic and Optical Properties induced by Out-of-Plane Mirror Symmetry Breaking in Janus Transition Metal Dichalcogenides

The 67th Fullerenes-Nanotubes-Graphene General Symposium
Kochi University of Technology, Eikokuji, September 1-3, 2024

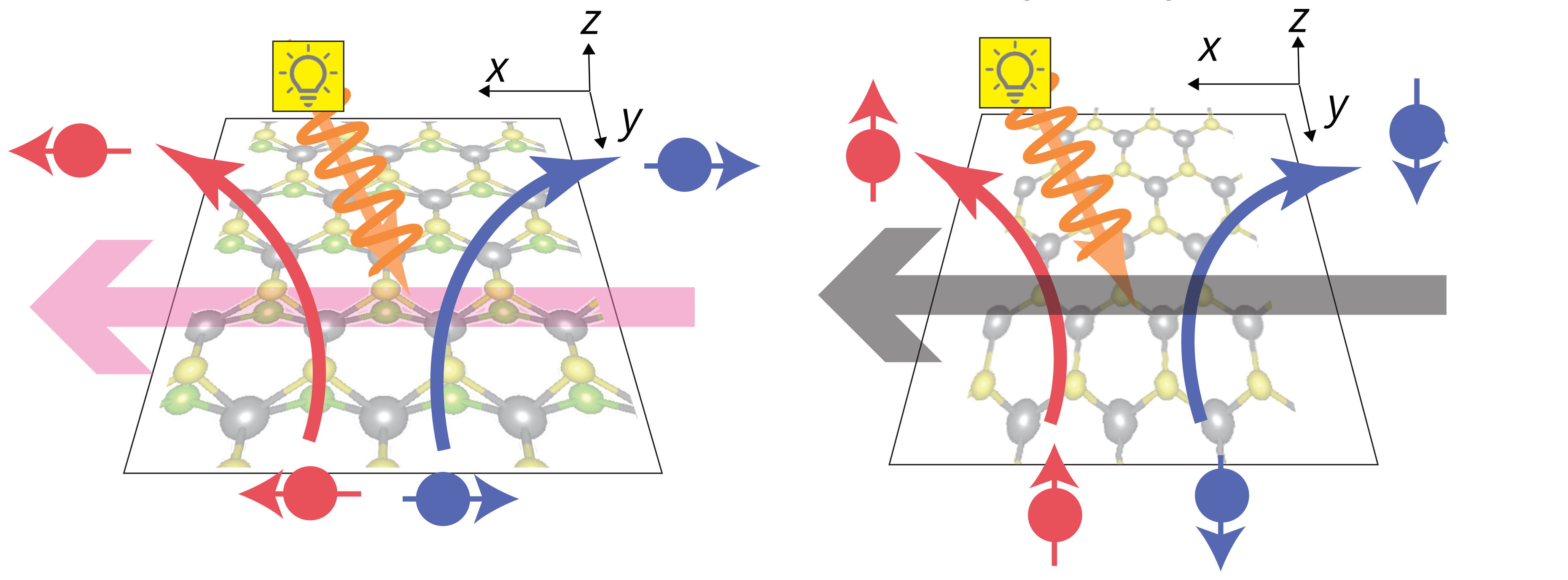
3P-28

Homepage

Tomoaki Kameda, Katsunori Wakabayashi
Department of Nanotechnology for Sustainable Energy, School of Science and Technology,
Kwansei Gakuin University, Sanda, Hyogo, Japan

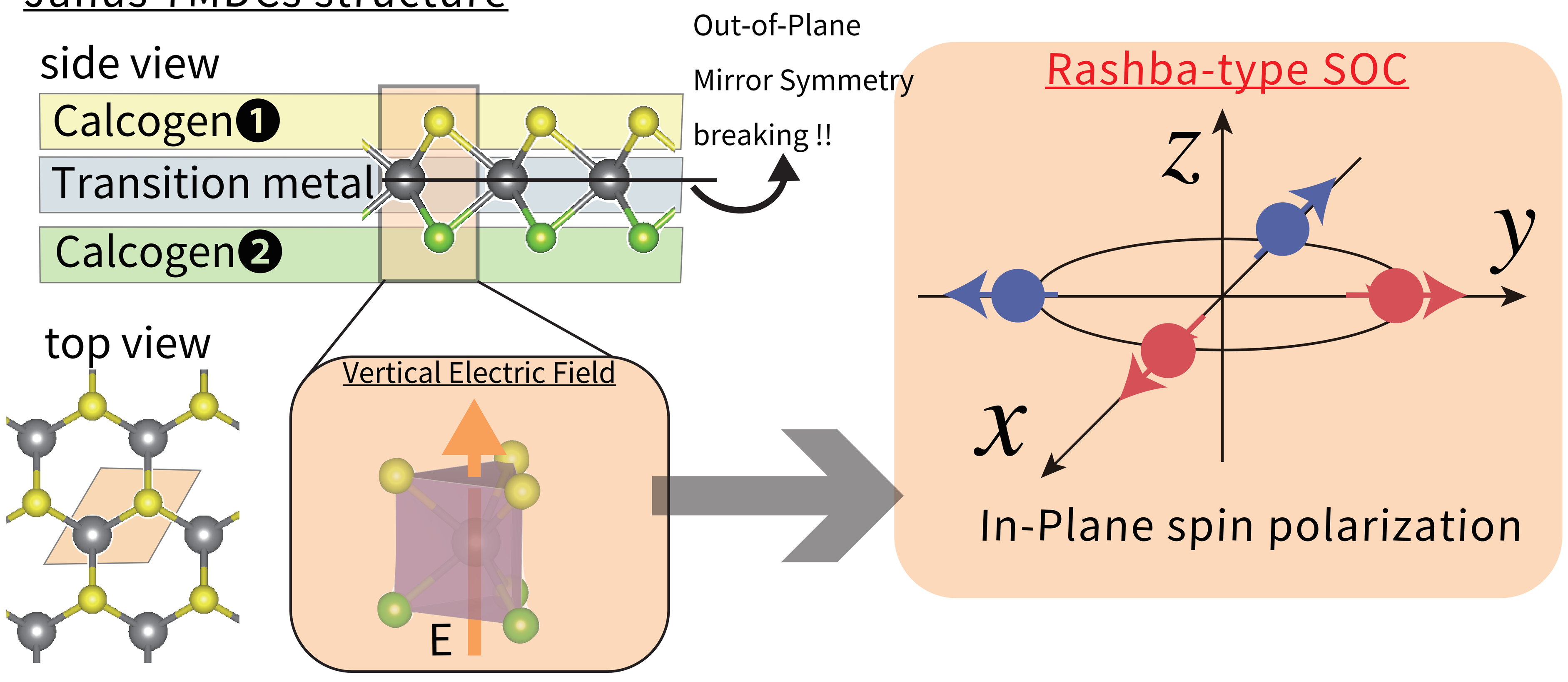
ABSTRACT

Janus TMDCs generate in-plane spin current by light irradiation



Out-of-Plane Mirror Symmetry breaking and Rashba-type spin orbit coupling (SOC)

Janus TMDCs structure

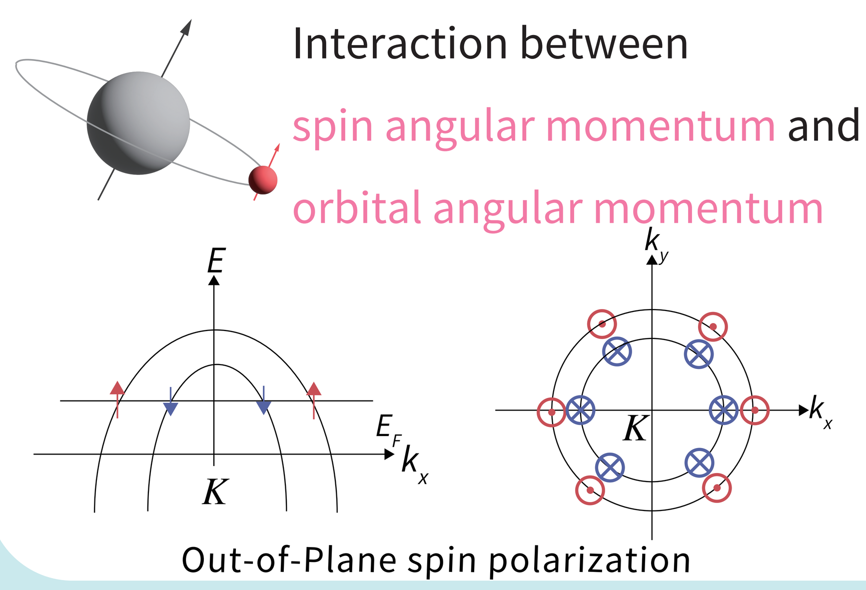


Janus TMDCs generate In-plane spin current by light irradiation because Out-of-Plane mirror symmetry breaking leads Rashba-type SOC

RASHBA SPIN ORBIT COUPLING

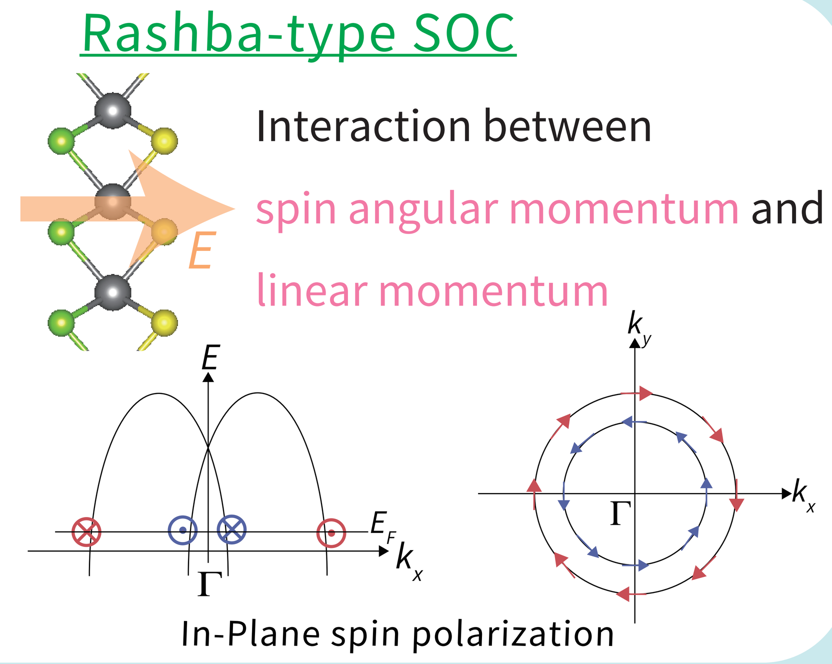
Ising-type SOC

Interaction between spin angular momentum and orbital angular momentum



Rashba-type SOC

Interaction between spin angular momentum and linear momentum



KUBO FORMULA

Kubo formula is used to calculate the electrical and optical conductivity of a material based on quantum mechanical linear response theory.

In particular, it is used to describe the response of a system to an external electric field.

Optical spin current conductivity

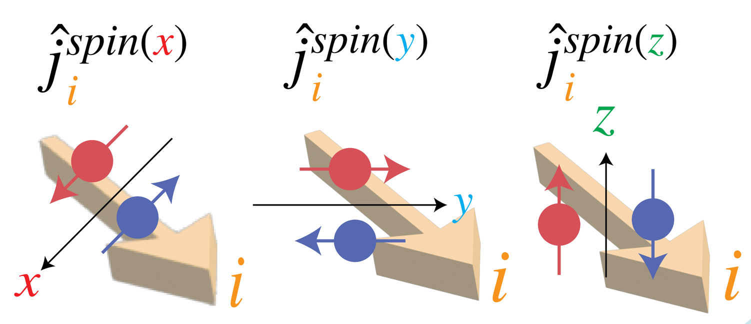
$$\sigma_{ij}^{spin(z)}(\omega) = \frac{i\hbar e}{(2\pi)^2}\int_{BZ} d^2\mathbf{k}\Sigma_{n\neq m}\frac{f(E_n(\mathbf{k}))-f(E_m(\mathbf{k}))}{E_m(\mathbf{k})-E_n(\mathbf{k})}\times\frac{\langle u_n(\mathbf{k})|\hat{j}_i^{spin(z)}|u_m(\mathbf{k})\rangle\langle u_m(\mathbf{k})|\hat{v}_j|u_n(\mathbf{k})\rangle}{E_m(\mathbf{k})-E_n(\mathbf{k})-\hbar\omega-i\eta}$$

$f(E_n(\mathbf{k}))$: Fermi dispersion function

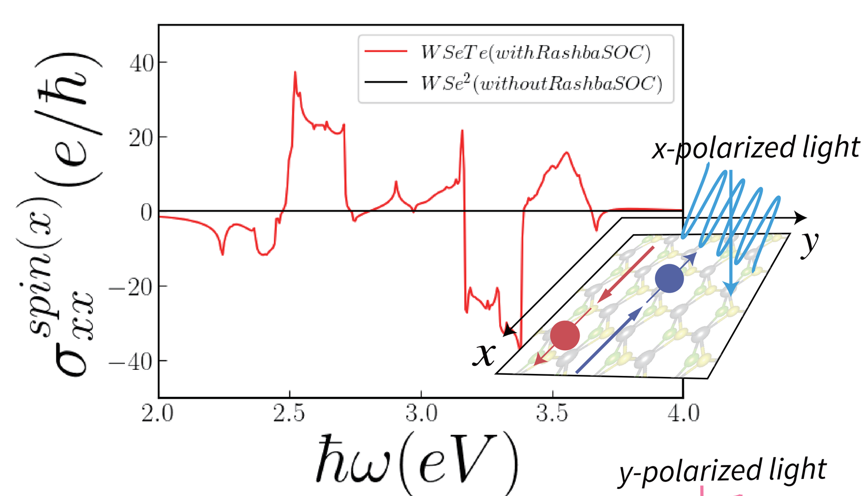
$\hat{v}_i = \frac{1}{\hbar}\frac{\partial \hat{H}(\mathbf{k})}{\partial k_i}$: Velocity operator

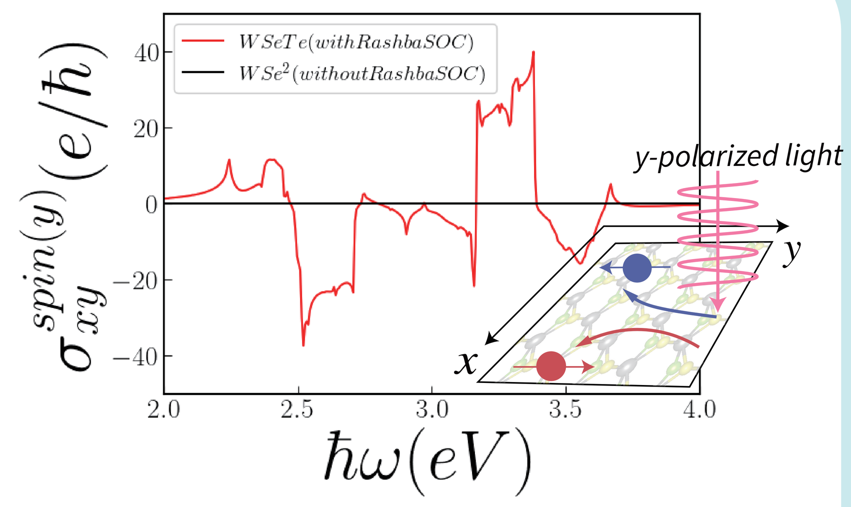
$\hat{j}_i^{spin(z)} = \frac{1}{2}\{\hat{\sigma}_z, \hat{v}_i\}$: Spin current operator

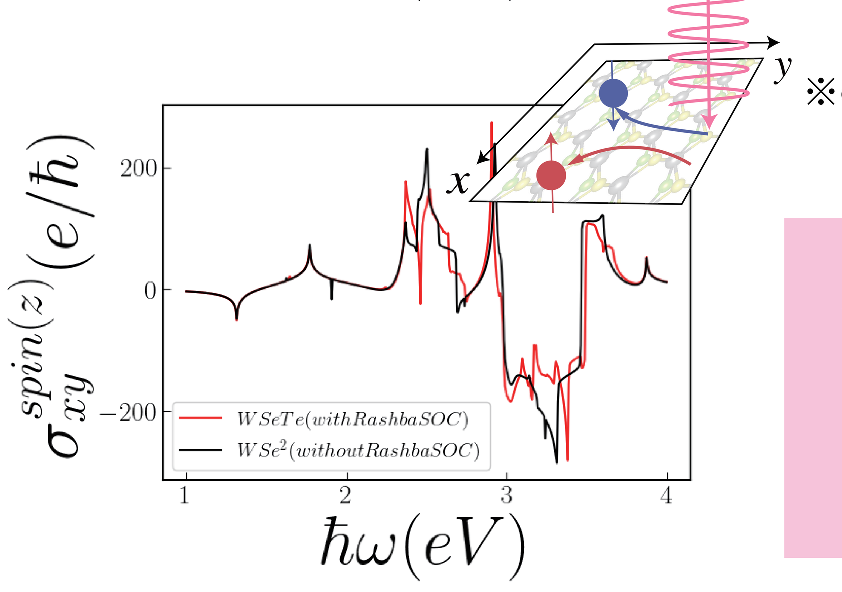
Spin polarization direction



OPTICAL SPIN CURRENT CONDUCTIVITY



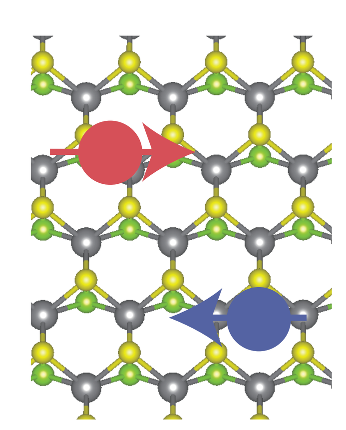




※other conductivities $\sigma_{xy}^{spin(x)}, \sigma_{xx}^{spin(y)}, \sigma_{xx}^{spin(z)}$ is all 0.

Janus TMDCs exhibit unique spin transport properties not found in conventional TMDCs.

spin polarized direction		Janus TMDCs	Conventional TMDCs
in plane spin	x, y	○	—
out of plane spin	z	○	○



EFFECTIVE TIGHT BINDING MODEL

Hamiltonian

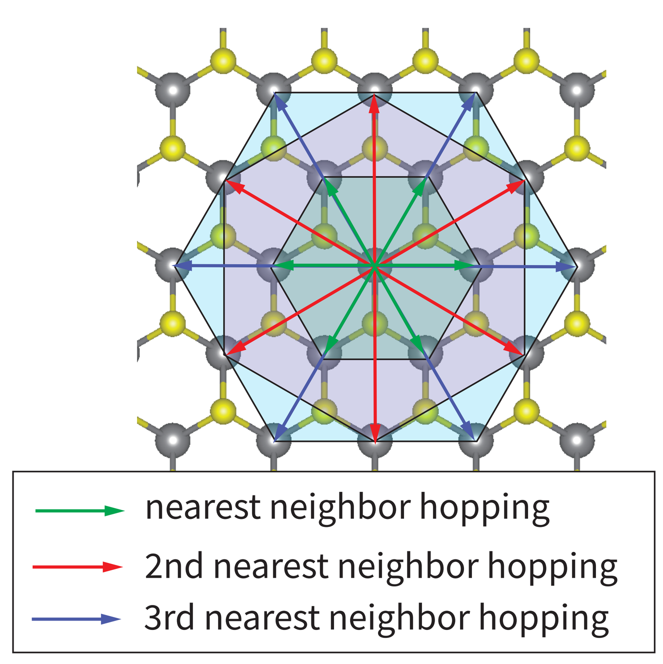
three orbitals of Transition metal atom $d_{z^2}, d_{xy}, d_{x^2-y^2}$

$$H_{total}(\mathbf{k}) = H_{hopping}(\mathbf{k}) + H_I(\mathbf{k}) + H_R(\mathbf{k})$$

$H_{hopping}(\mathbf{k}) = H_{nearest} + H_{2nd} + H_{3rd}$ hopping hamiltonian

$H_I(\mathbf{k}) = \frac{1}{2}\lambda\hat{L}_z\otimes\sigma_0$ Ising type SOC hamiltonian

$H_R(\mathbf{k})$ Rashba type SOC hamiltonian



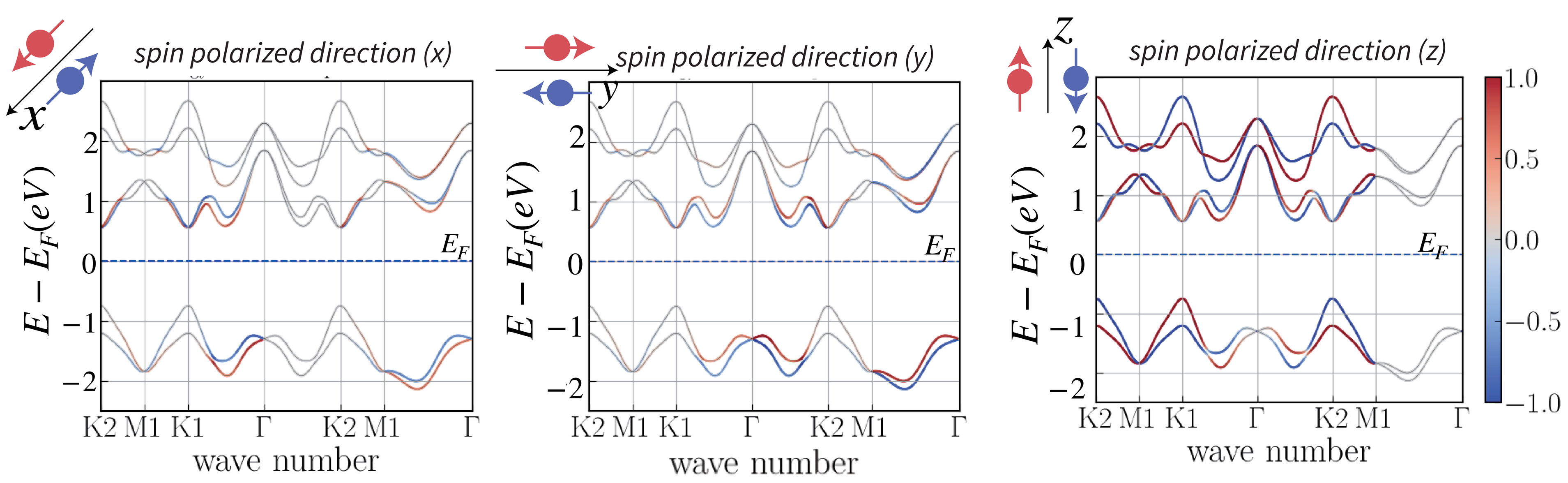
Janus TMDCs and TMDCs model

Model	SOC type	Hamiltonian
TMDCs model (WSe²)	Ising type SOC	$H_{total}(\mathbf{k}) = H_{hopping}(\mathbf{k}) + H_I(\mathbf{k})$
Janus TMDCs model (WSeTe)	Ising type SOC Rashba type SOC	$H_{total}(\mathbf{k}) = H_{hopping}(\mathbf{k}) + H_I(\mathbf{k}) + H_R(\mathbf{k})$

WSe₂ as a model for TMDCs in order to comparing Janus TMDCs model.

WSeTe as a model for Janus TMDCs because the Rashba-type SOC effect is particularly strong in WSeTe.

Energy band structre (WSeTe)



※ In TMDCs model, spin polarized direction (x),(y) are not exist.

Janus TMDCs have in-plane spin polarized (x), (y) near Γ point.

SUMMARY

suggesting new possibilities for spintronics devices

Janus TMDCs have a variety of spin polarization directions that are not found in conventional TMDCs.

providing a guideline for new material design for In-plane spin currents

In-plane spin currents can be introduced by introducing asymmetry into materials.

References
[1] Zhang, J. et al. ACS Nano 11, 8192–8198 (2017).
[2] Du, L. et al. Nat. Rev. Phys. 3, 193–206 (2021).
[3] Liu, G.et al. Phys. Rev. B 88, 085433 (2013).