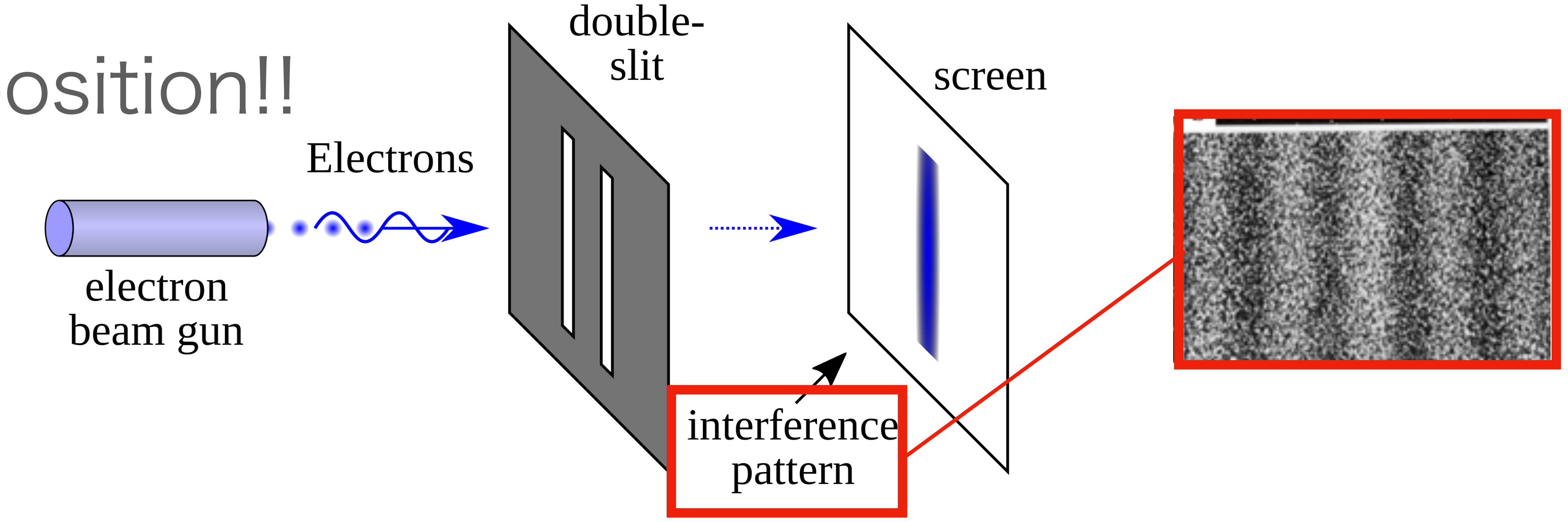
Derivation and Characteristics of Geometric Phases in Quantum Mechanics

Introduction to Berry Phase

Tomoaki Kameda 16 May 2024

Review of previous seminar ①

phase of wave function(WF), gauge transformation, vector potential…



- Phase of WF is observable in case of superposition!!

- Local gauge transformation

$$\psi(\vec{r}) \rightarrow \psi'(\vec{r}) = \psi(\vec{r})e^{i\theta(\vec{r})}$$

➡ ψ, ψ' are same mean in physics

Problem

Momentum is not a gauge invariant…

$$\langle\psi'|\hat{p}_i|\psi'\rangle = \langle\psi|\hat{p}_i|\psi\rangle + \hbar\langle\psi|\frac{\partial\theta}{\partial r_i}|\psi\rangle$$

Solution→introduce vector potential

$$\nabla \times \boldsymbol{A} = \boldsymbol{B}$$

$\boldsymbol{A}$: in electro-magnetism it is called vector potential

$\boldsymbol{B}$: in electro-magnetism it is called magnetic field

Review of previous seminar ②

Connection, Curvature, and their gauge properties

Gauge invariance

$$\begin{cases} \boldsymbol{A}' = \boldsymbol{A} - \frac{\hbar}{e}\nabla\theta \\ \boldsymbol{B}' = \boldsymbol{B} \end{cases}$$

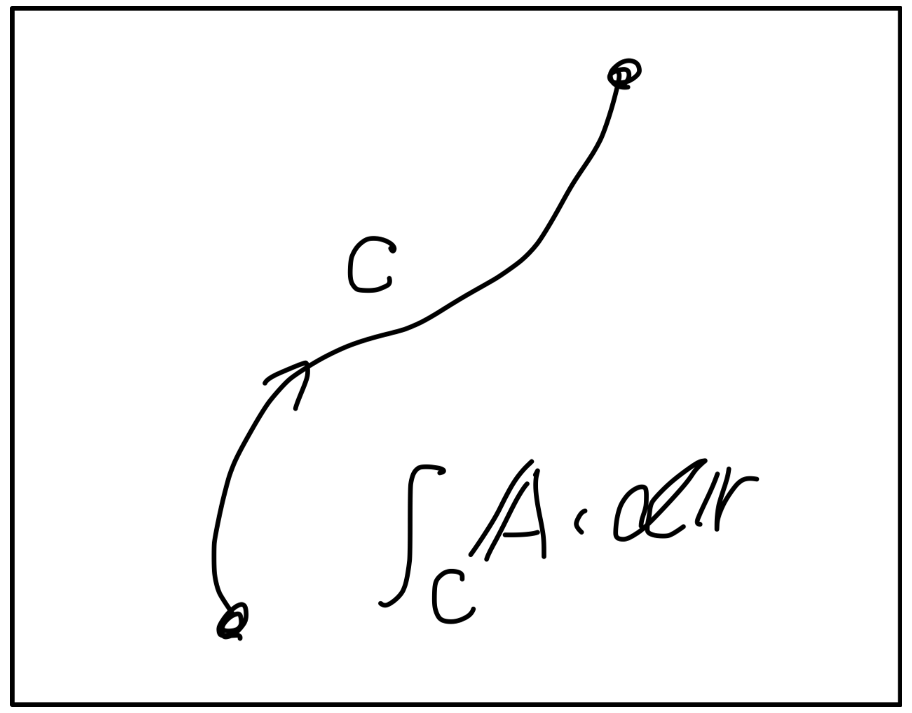
$\boldsymbol{A}' = \boldsymbol{A} - \frac{\hbar}{e}\nabla\theta$ → Not observable

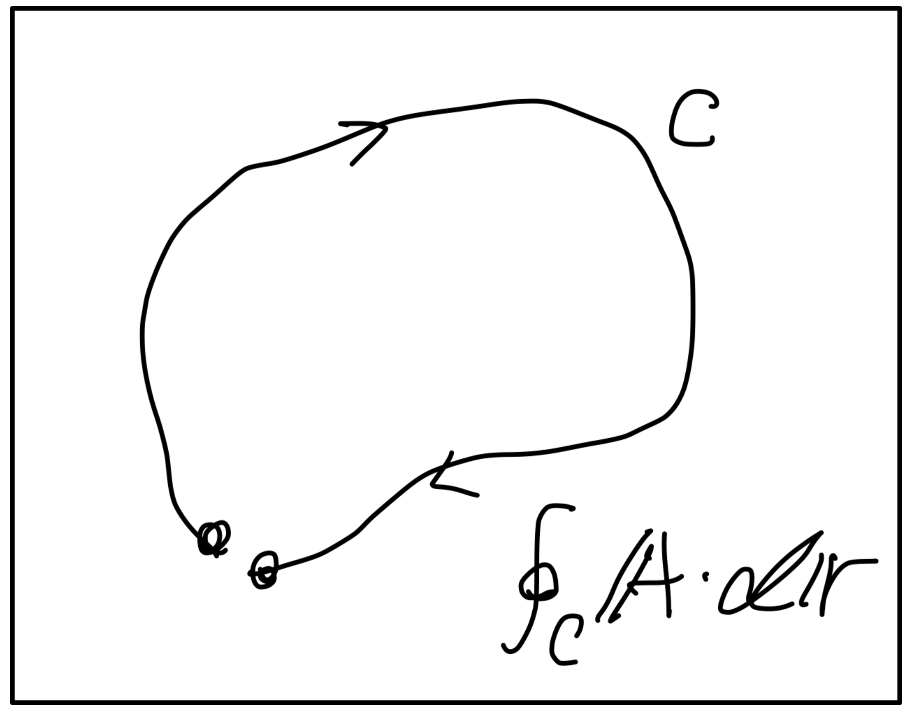
$\boldsymbol{B}' = \boldsymbol{B}$ → observable!

Consider the line integral of a closed curve

$\oint_C \boldsymbol{A}\cdot d\boldsymbol{r}$ → observable!

$$\oint_C \boldsymbol{A}\cdot d\boldsymbol{r} = \int_S \nabla\times\boldsymbol{A}\cdot d\boldsymbol{S} = \int_S \boldsymbol{B}\cdot d\boldsymbol{S}$$



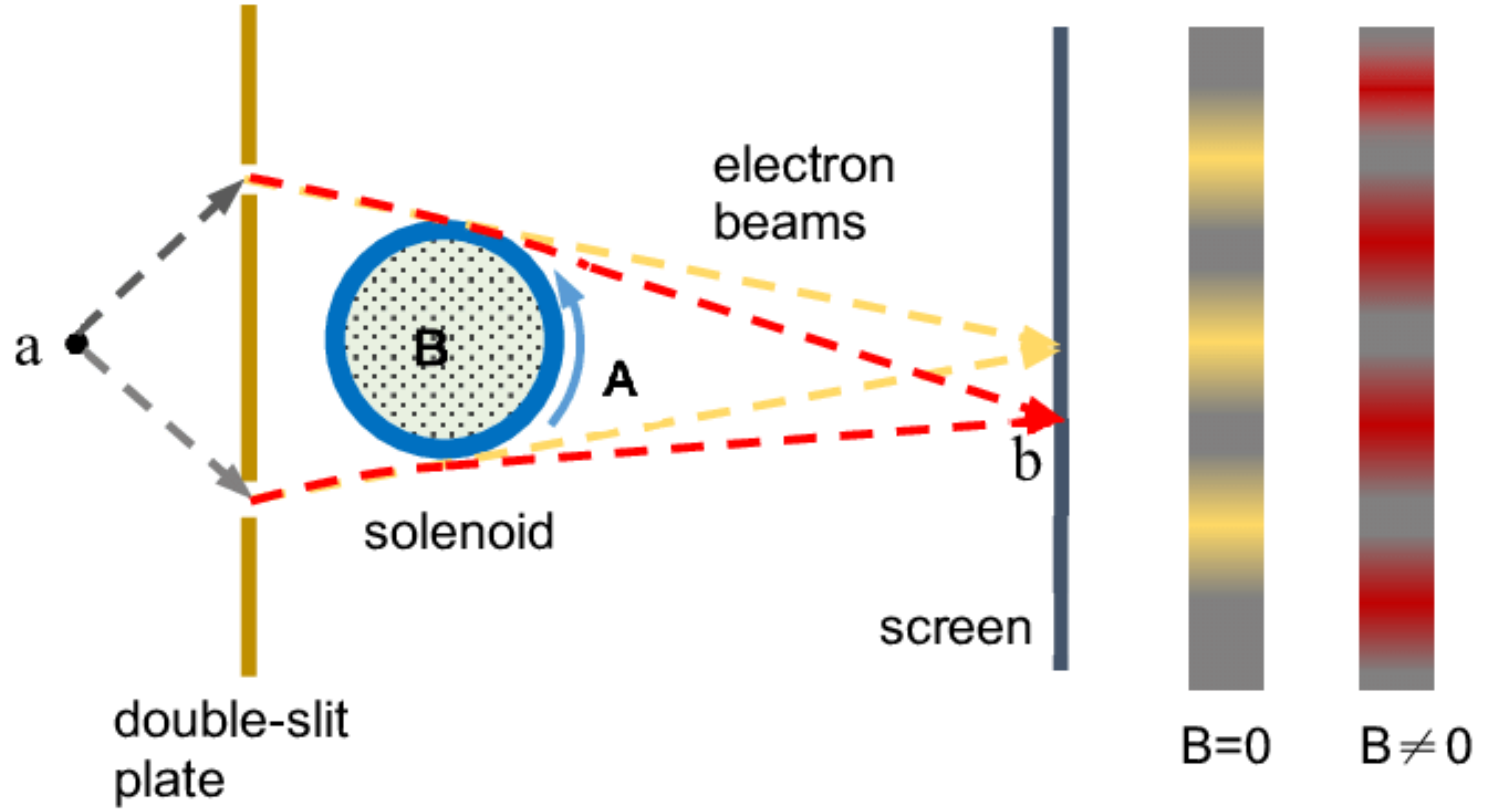


What were these checked for?

→ Because a similar structure appears when considering the Berry phase！！

Aharonov-Bohm effect

Vector potential appears in physics phenomena



Even when **the magnetic field is zero,**

the phase difference changes due to the vector potential.

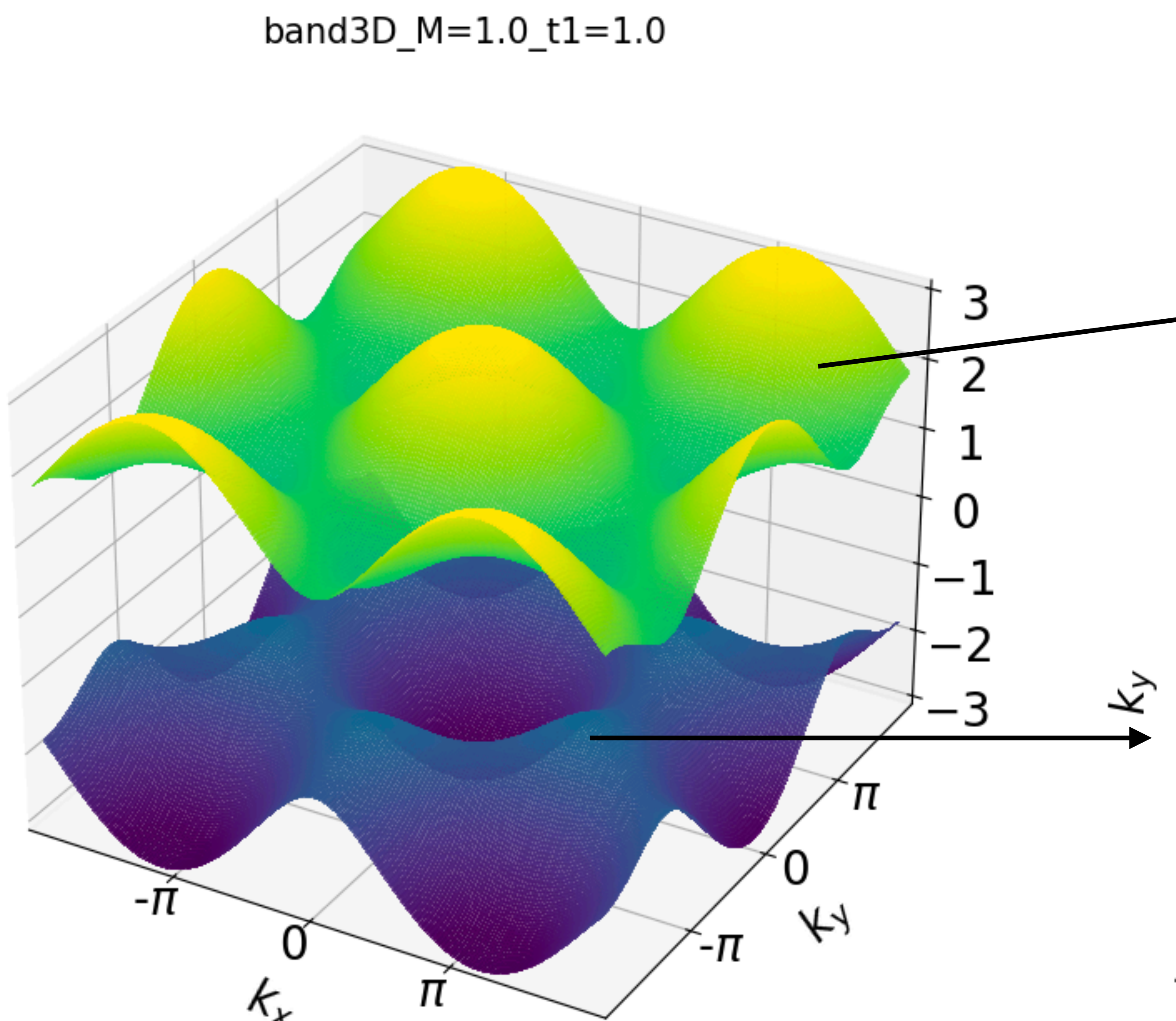
An interpretation for Aharonov-Bohm effect with classical electromagnetic theory

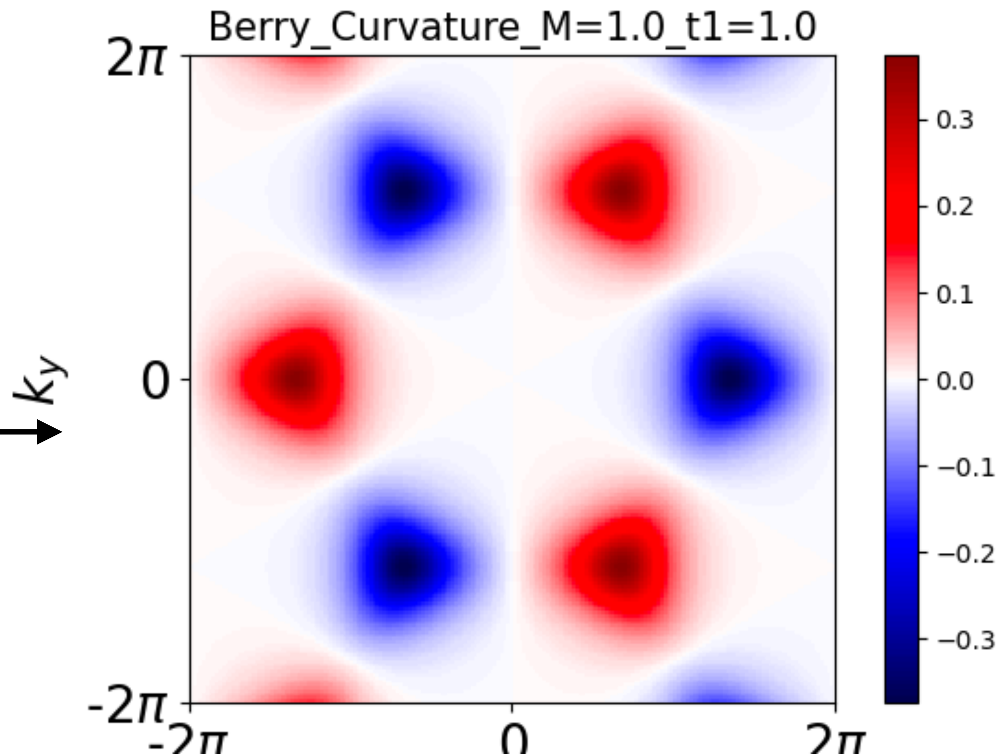
Todays seminar topics

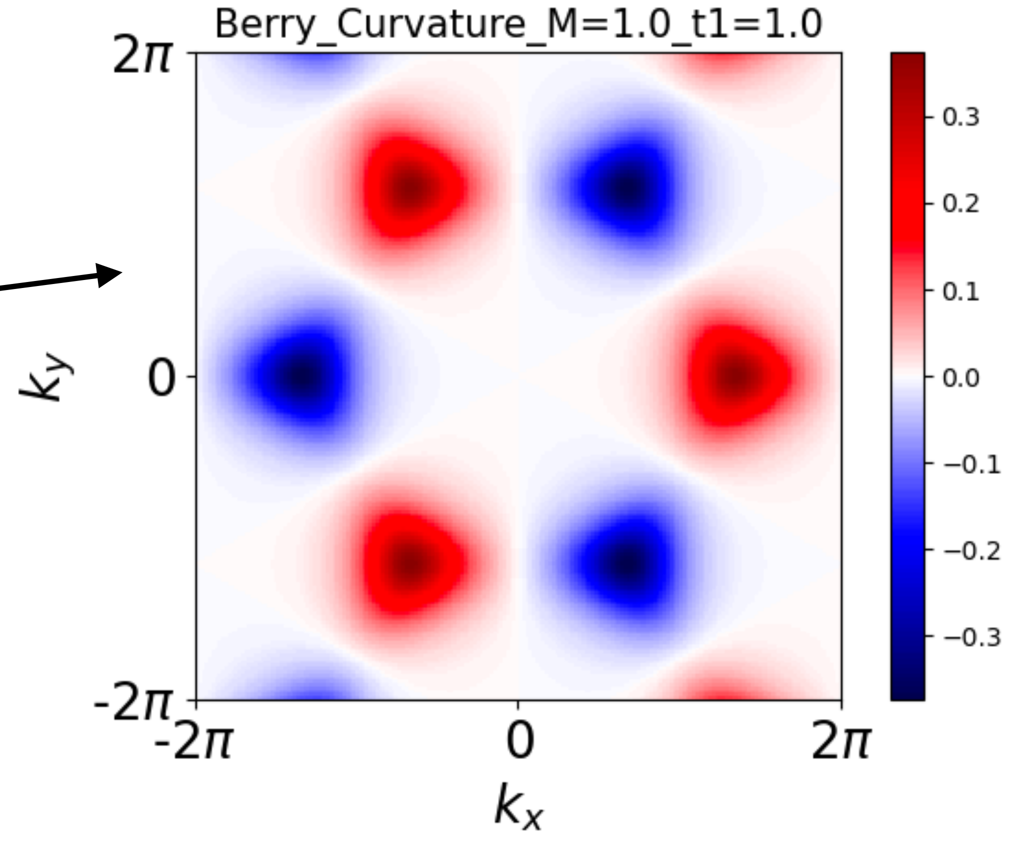
Derivation berry phase in general space

- Derivation berry phase in general space
- Properties of berry phase, curvature and connection
- Expression transformation for numerical calculations

After this seminar, you can calculate berry pahse, curvature, connection







These are berry curvature in h-BN(hexagonal-BN)

Derivation of the Berry phase

Parameter-dependent Hamiltonian①

Definition

The "Berry phase" is the phase acquired by a quantum system moving along a circuit **C** *on a given adiabatic surface.*

"Solid State Physics," Grosso, G.,Parravicini, G.P.

System

Hamiltonian is dependent on some parameter $\boldsymbol{R}$.
$\boldsymbol{R}$ *changes in a time-dependent manner.*

$$\hat{H} = \hat{H}(\boldsymbol{R}) \quad \boldsymbol{R} = (R_1, R_2, \dots)$$

$$\hat{H}(\boldsymbol{R}) \left|\phi_n(\boldsymbol{R})\right\rangle = E_n(\boldsymbol{R}) \left|\phi_n(\boldsymbol{R})\right\rangle$$

Problem

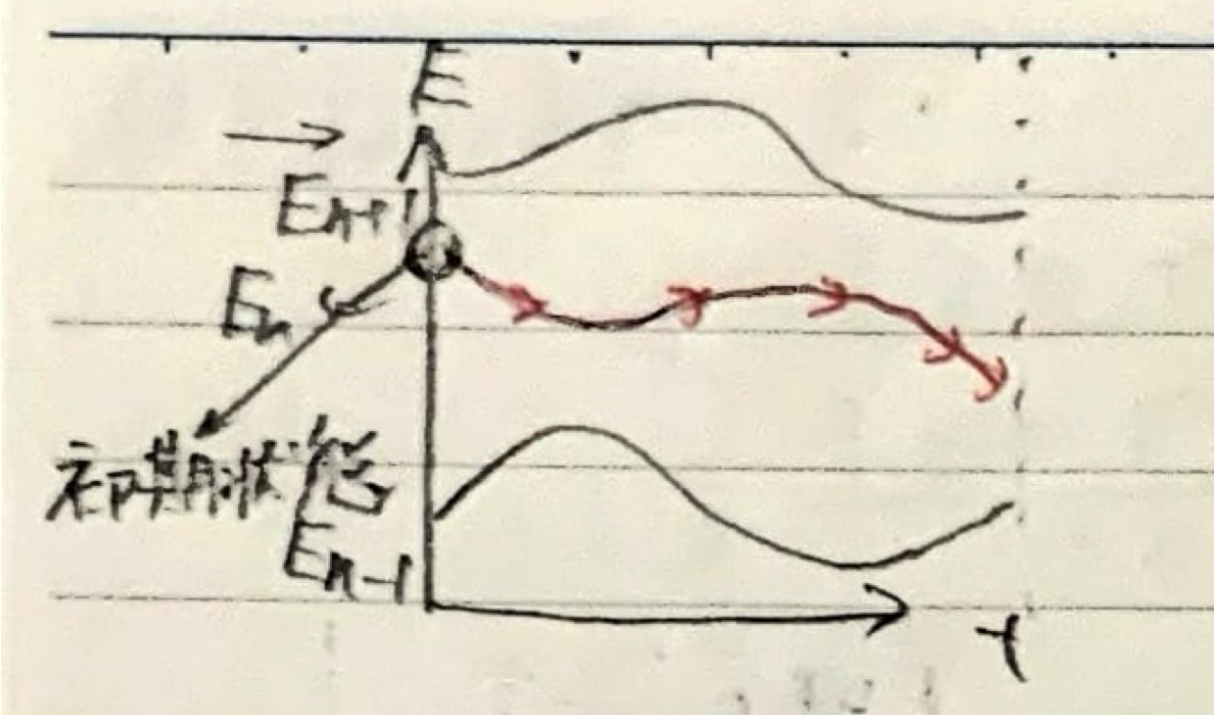
How can we solve time-dependent Schrödinger equation?

$$\left|\psi_{(t=0)}\right\rangle = \left|\phi_n(\boldsymbol{R}_{(t=0)})\right\rangle$$ Initial state eigen state(t=0)

$$i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle = \hat{H}(\boldsymbol{R}(t))\left|\psi(t)\right\rangle$$

Assumptions for solving

- *there is non-degeneracy in the eigen energy*
- *the system is adiabatic*



縮退しておらず、時間経過してもn番目の固有状態に居続ける
断熱近似→一種の近似　摂動論より荒い

Derivation of the Berry phase

Parameter-dependent Hamiltonian②

Wave functions get some phase over time.

$$|\psi(t)\rangle = e^{i\theta(t)}|\phi_n(\boldsymbol{R}(t))\rangle \quad (1)$$

We want to calculate!

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}(\boldsymbol{R}(t))|\psi(t)\rangle \quad (2)$$

(1)→(2)

$$\theta(t) = -\frac{1}{\hbar}\int_0^t E_n(\boldsymbol{R}(t'))dt' + i\int_0^t \langle\phi_n(\boldsymbol{R}(t'))|\frac{\partial}{\partial t'}|\phi_n(\boldsymbol{R}(t'))\rangle dt' \quad (3)$$

Dinamic phase

Berry phase!!

Berry phase

$$\gamma(t) = i\int_0^t \langle\phi_n(\boldsymbol{R}(t'))|\frac{\partial}{\partial t'}|\phi_n(\boldsymbol{R}(t'))\rangle dt' = i\int_C \langle\phi_n(\boldsymbol{R})|\frac{\partial}{\partial \boldsymbol{R}}|\phi_n(\boldsymbol{R})\rangle \cdot d\boldsymbol{R} = \int_C A_n(\boldsymbol{R})\cdot d\boldsymbol{R} \quad (4)$$

$$A_n(\boldsymbol{R}) = i\langle\phi_n(\boldsymbol{R})|\frac{\partial}{\partial \boldsymbol{R}}|\phi_n(\boldsymbol{R})\rangle$$

Berry connection(in this case, vector field in R space)

Derivation of the Berry phase

Berry connection properties and berry curvature

Gauge transformation

$$\hat{H}(\boldsymbol{R})\left|\phi_n(\boldsymbol{R})\right\rangle = E_n(\boldsymbol{R})\left|\phi_n(\boldsymbol{R})\right\rangle \quad (1)$$

$$\left|\phi_n'(\boldsymbol{R})\right\rangle = e^{i\theta_n(\boldsymbol{R})}\left|\phi_n(\boldsymbol{R})\right\rangle \quad (2)$$

$$A_n(\boldsymbol{R}) = i\left\langle\phi_n(\boldsymbol{R})\right|\frac{\partial}{\partial \boldsymbol{R}}\left|\phi_n(\boldsymbol{R})\right\rangle \quad (3)$$

$$\Rightarrow \quad A_n'(\boldsymbol{R}) = i\left\langle\phi_n'(\boldsymbol{R})\right|\frac{\partial}{\partial \boldsymbol{R}}\left|\phi_n'(\boldsymbol{R})\right\rangle = \boldsymbol{A}^n - \frac{\partial \theta^n}{\partial \boldsymbol{R}}$$

$$\Rightarrow \quad \boldsymbol{A}_n' = \boldsymbol{A}_n - \nabla_{\boldsymbol{R}}\theta_n \quad (4)$$

Look like!!

In last seminar→vector potential gauge transformation

$$\begin{cases} \boldsymbol{A}' = \boldsymbol{A} - \frac{\hbar}{e}\nabla\theta \\ \boldsymbol{B}' = \boldsymbol{B} \end{cases}$$

$\boldsymbol{A}' = \boldsymbol{A} - \frac{\hbar}{e}\nabla\theta$ → Not observable

$\boldsymbol{B}' = \boldsymbol{B}$ → observable!

Berry curvature

$$\boldsymbol{B}_n(\boldsymbol{R}) = \nabla_{\boldsymbol{R}} \times \boldsymbol{A}_n(\boldsymbol{R}) \quad \Rightarrow \quad \boldsymbol{B}_n' = \boldsymbol{B}_n$$

Gauge invariant!

Gauge invariance of berry phase

You can check it !!

Other form of Berry curvature

Expression transformation for numerical calculations

Motivation $\boldsymbol{B}_n(\boldsymbol{R}) = \nabla_{\boldsymbol{R}} \times \boldsymbol{A}_n(\boldsymbol{R})$

① Physical meaning is difficult to understand. → gauge invariance, divergence during degeneracy.

② Expression unsuitable for numerical calculations.→ Indeterminacy of the phase of the wave function.

Result

$$B_{n,z}(\boldsymbol{R}) = -2Im \sum_{(m\neq n)} \frac{\langle \phi_n(\boldsymbol{R})| \frac{\partial \hat{H}(\boldsymbol{R})}{\partial R_x} |\phi_m(\boldsymbol{R})\rangle \langle \phi_m(\boldsymbol{R})| \frac{\partial \hat{H}(\boldsymbol{R})}{\partial R_y} |\phi_n(\boldsymbol{R})\rangle}{(E_n - E_m)^2}$$

check it!

References

・スピン流とトポロジカル絶縁体

・Wu, T. T. & Yang, C. N. Concept of nonintegrable phase factors and global formulation of gauge fields. Phys. Rev. D **12**, 3845–3857 (1975).

・Dirac, P. A. M. Quantised singularities in the electromagnetic field,. Proc. R. Soc. Lond. Ser. A, Contain. Pap. a Math. Phys. Character **133**, 60–72 (1931).

・“Solid State Physics,” Grosso, G.,Parravicini, G.P.

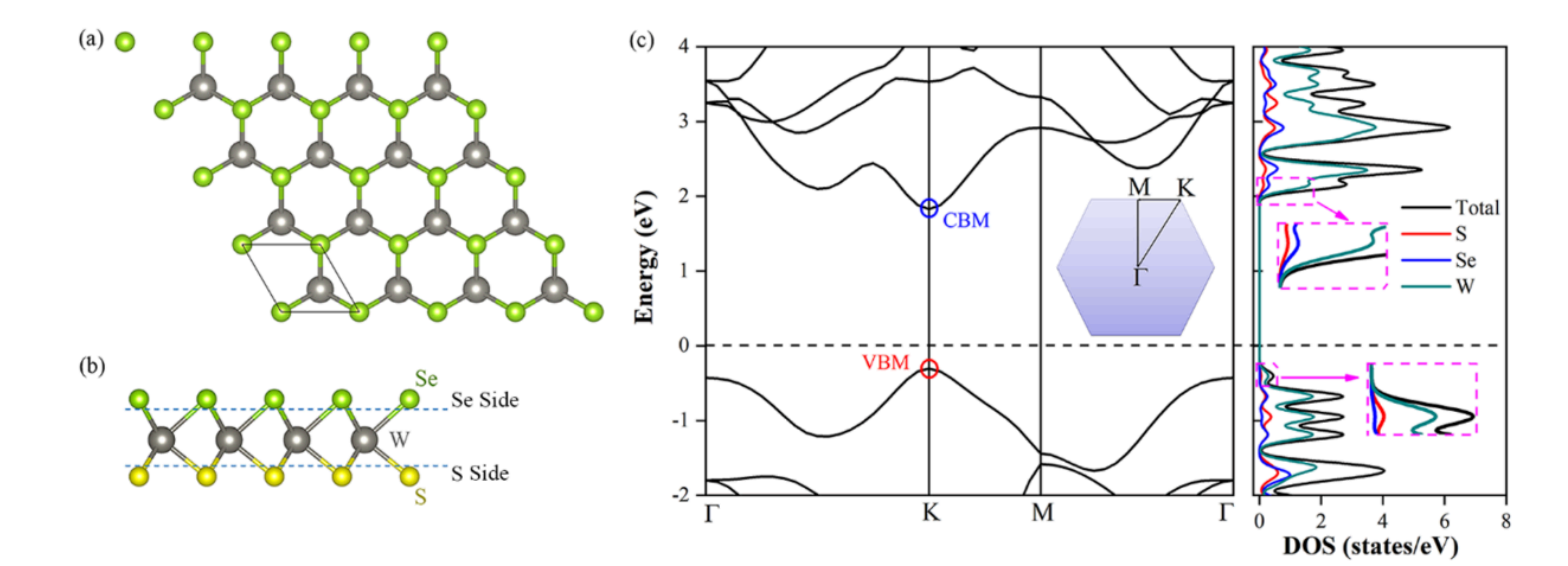
Progress report

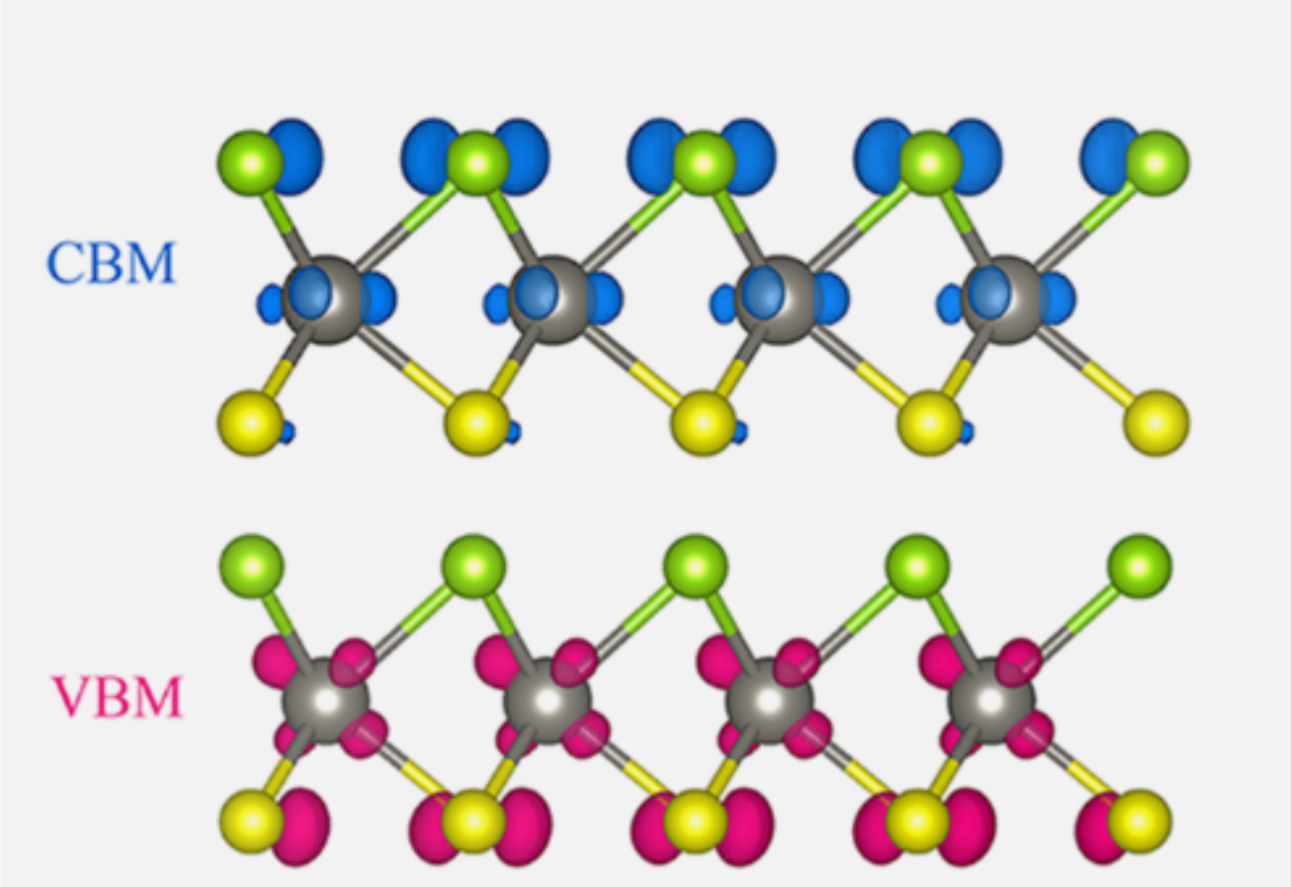
Tomoaki Kameda

Previous research

1.Ju, L., Bie, M., Tang, X., Shang, J. & Kou, L. Janus WSSe Monolayer: An Excellent Photocatalyst for Overall Water Splitting. *ACS Appl. Mater. Interfaces* **12**, 29335–29343 (2020).

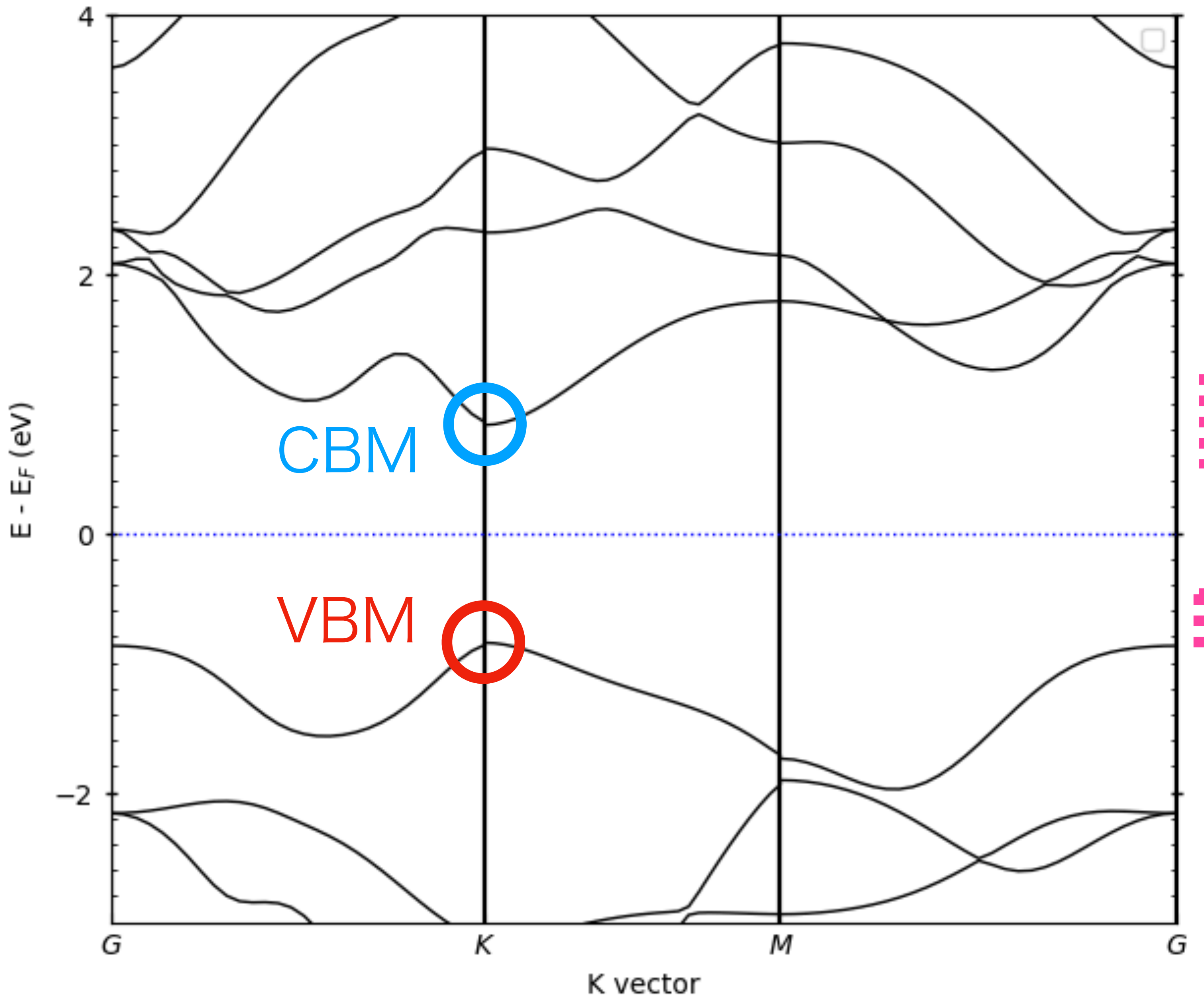
The PDOS of the valence and conduction bands and the charge density are localised on each side.

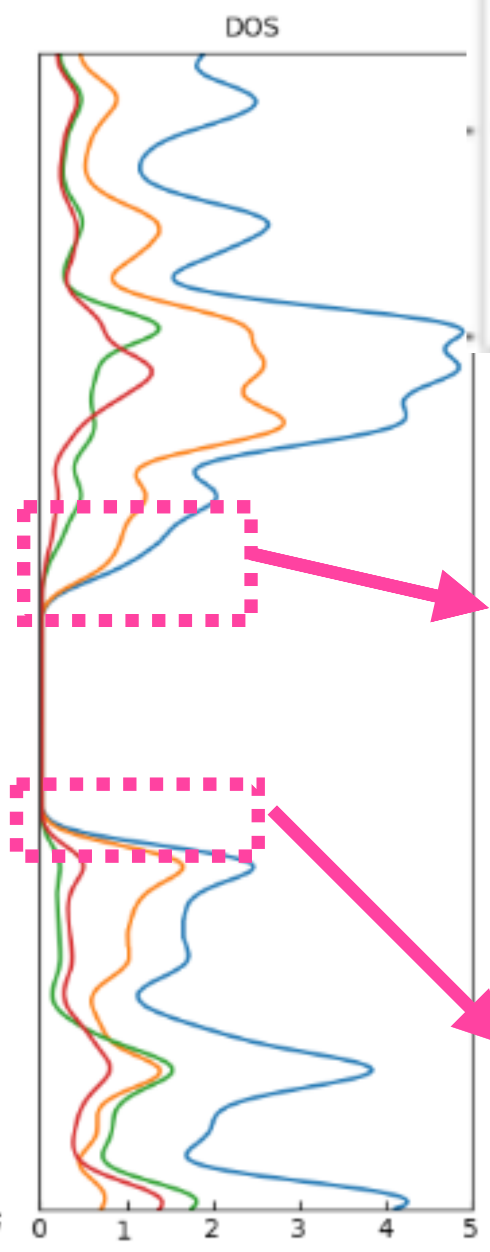


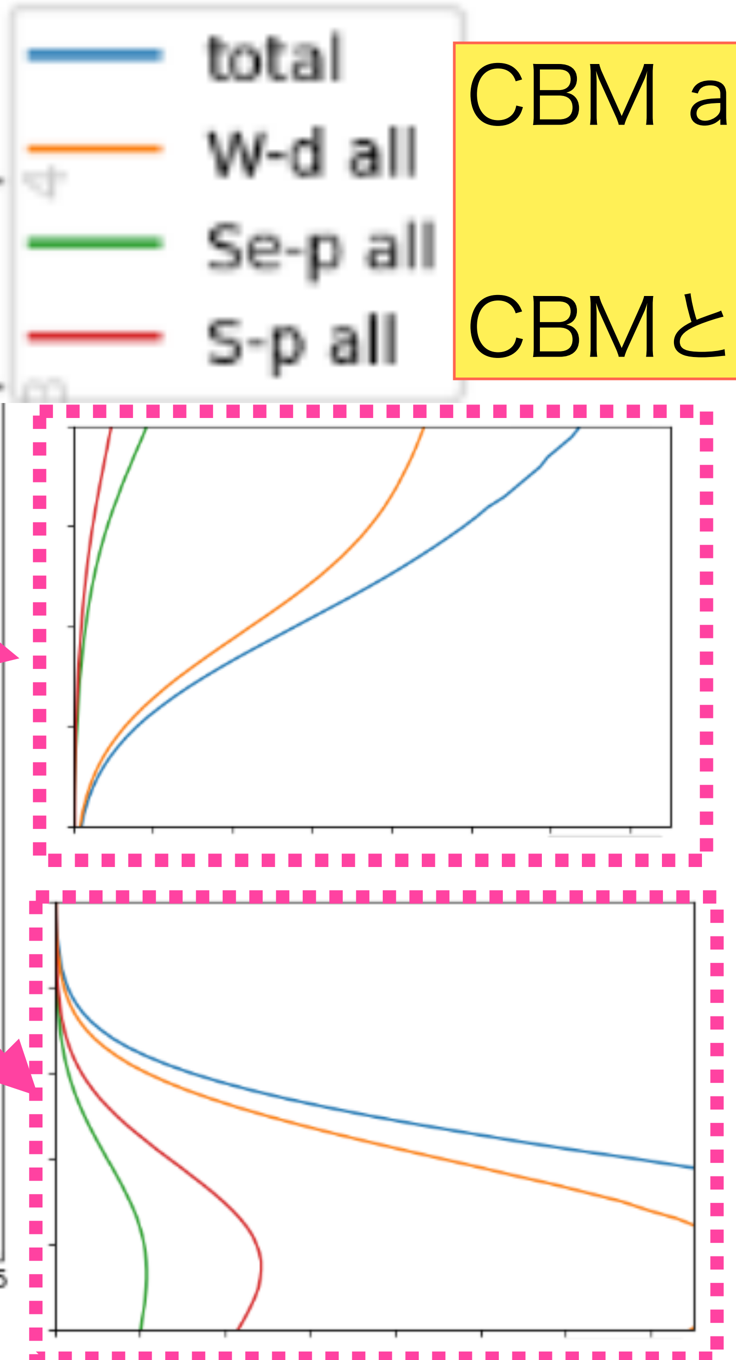


My calculation

WSeS@Q.E







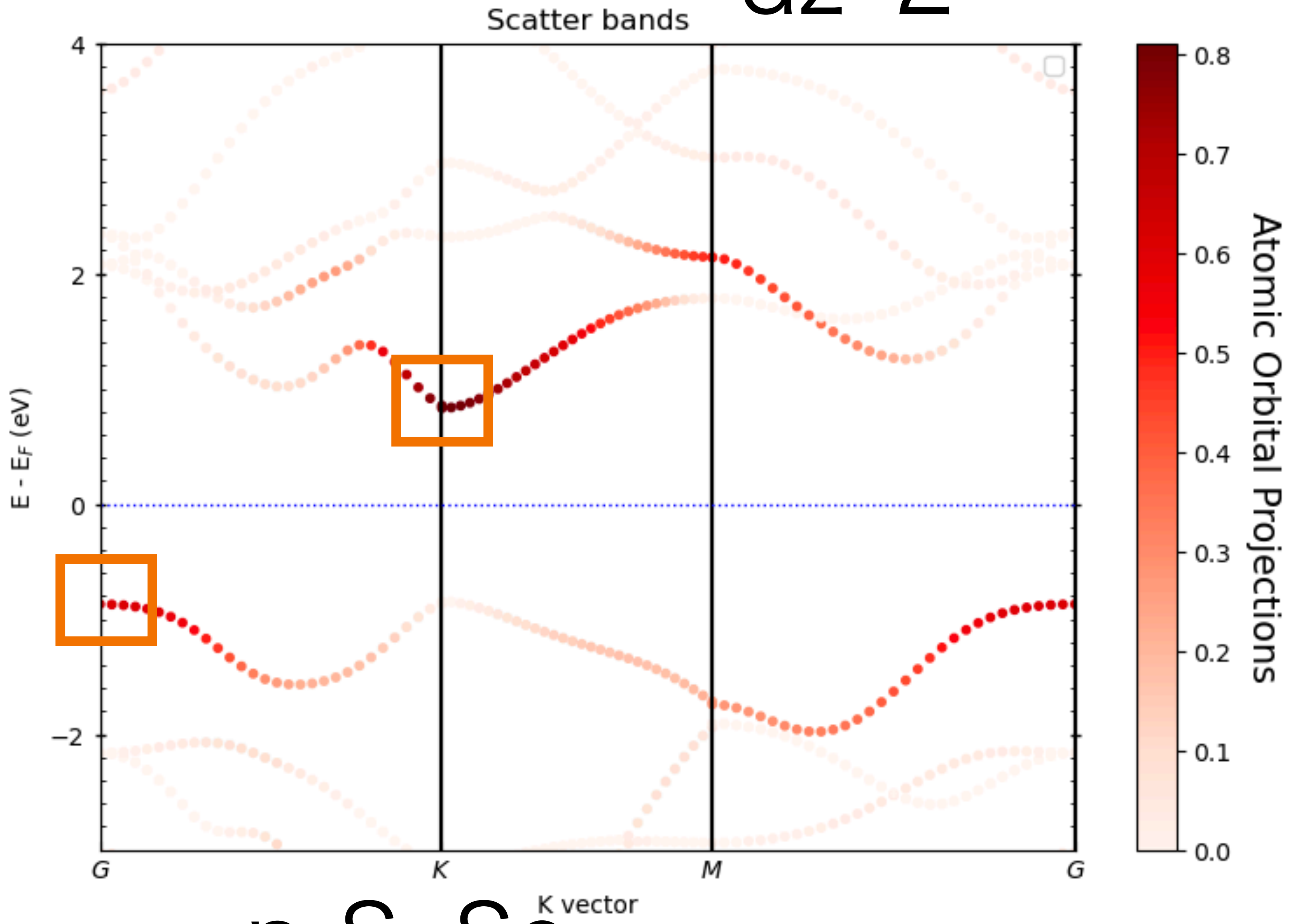
CBM and VBM swap the PDOS of S, Se in a large/small relationship

CBMとVBMでS, SeのPDOSの大小関係が入れ替わる->しかし寄与は小さい

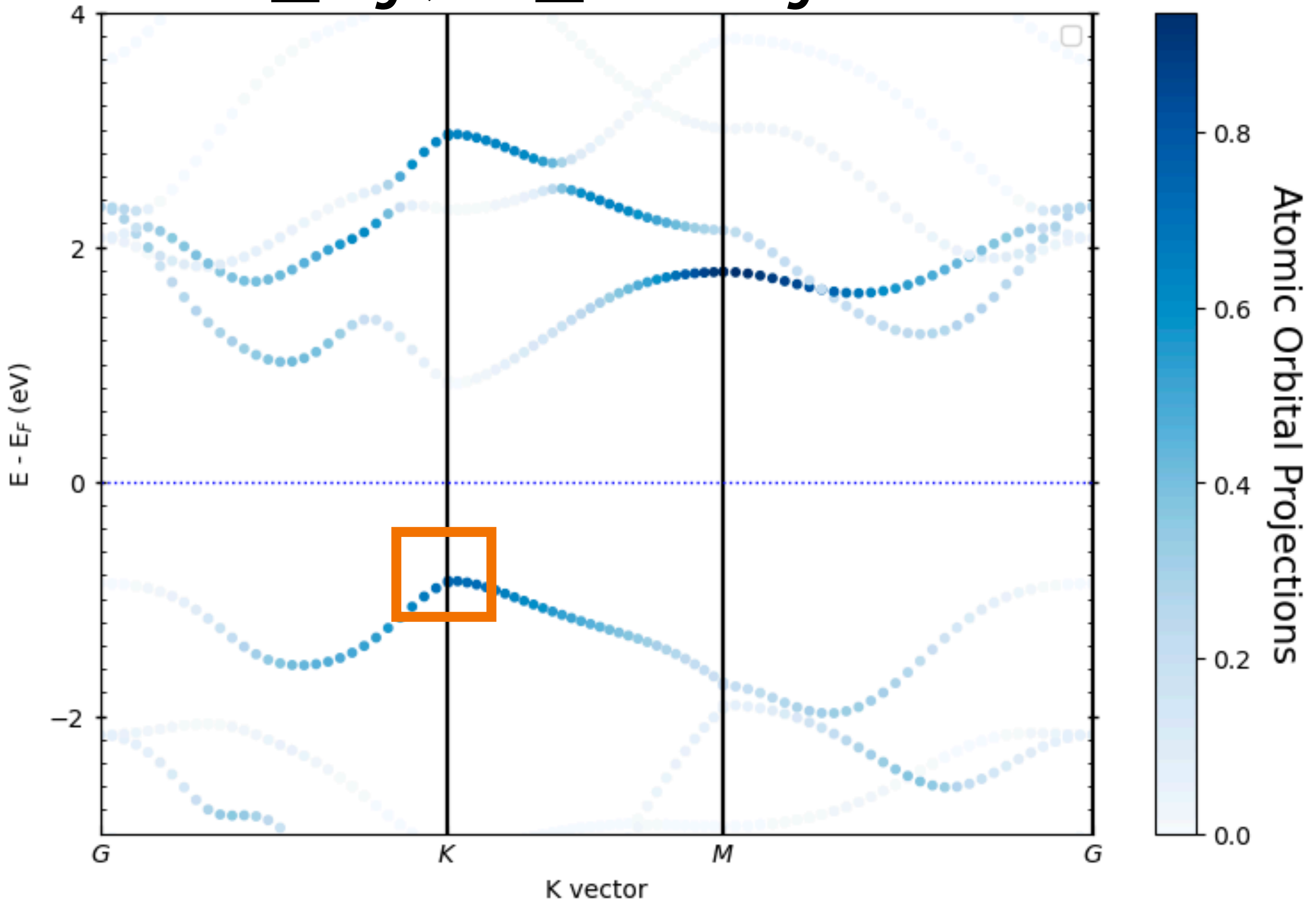
WSeS@Q.E

My calculation

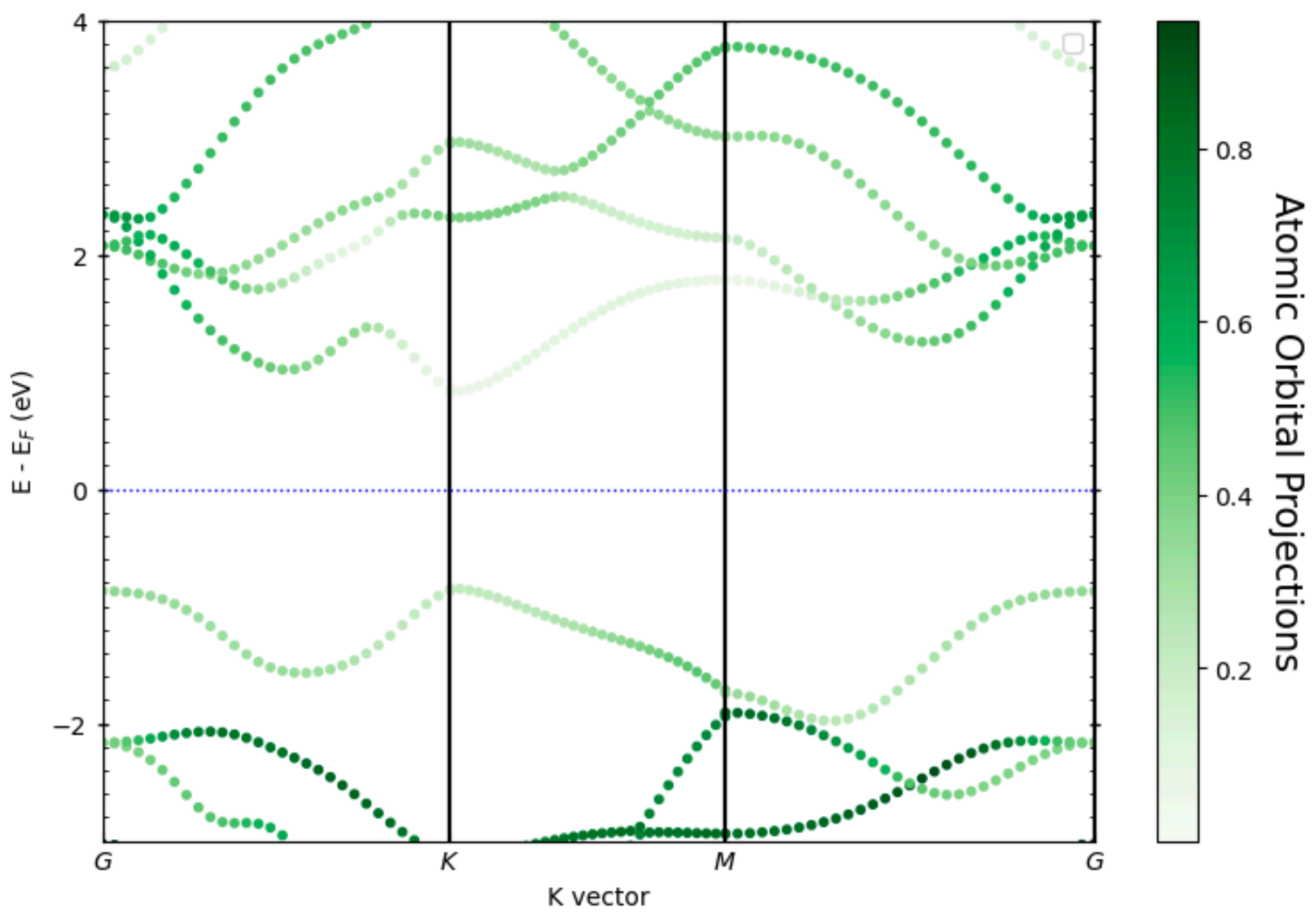
dz^2



d_xy, d_x^2-y^2



p-S, Se



Which orbitals are dominant?

Near the Fermi level, the d orbitals (three types) of the transition metal are dominate.

・Three-band tight binding models are useful.

Previous research

PHYSICAL REVIEW B **104**, 075435 (2021)

Spin Hall effect in the monolayer Janus compound MoSSe enhanced by Rashba spin-orbit coupling

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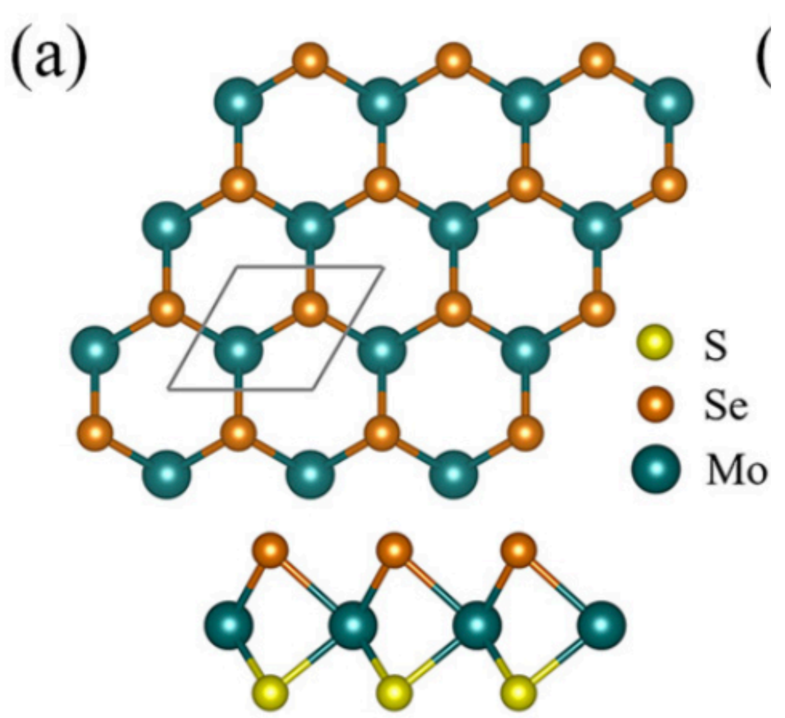
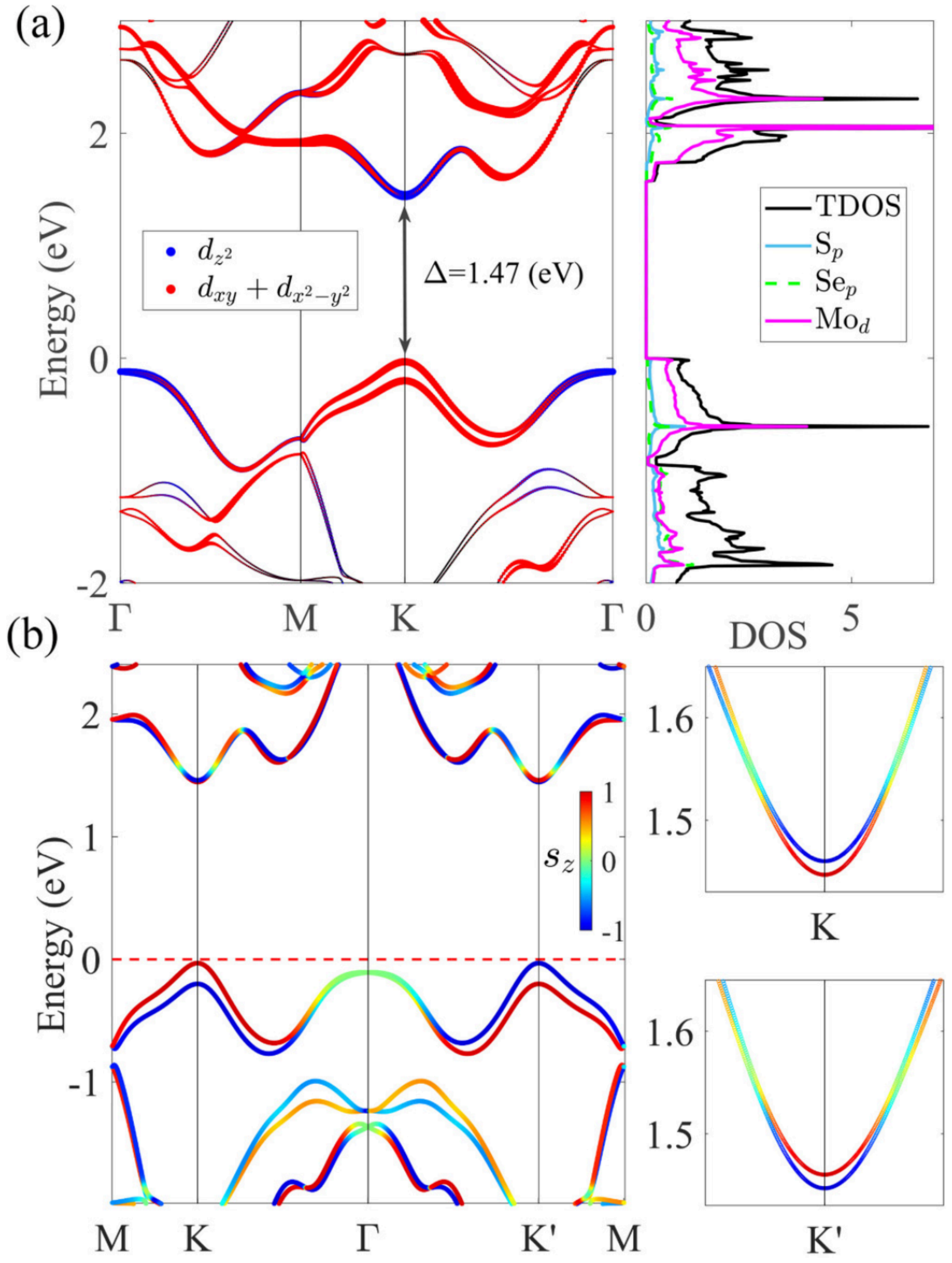
Band structures

・semiconductor with a direct band gap of about 1.47 eV (MoSe2 (1.33 eV) and MoS2 (1.61 eV))

The strong hybridization between the $d_{x^2-y^2}$ and d_{xy} orbitals of Mo atoms also cause the large Zeeman-like SOC splitting of the VBM at the K and K' points. The CBM is mainly comprised by the d_{z^2} orbital of the Mo atoms, which possesses sizable Rashba SOC. The large Rashba SOC also emerges at the Γ point of the valence bands because of the same dominant d_{z^2} orbital components, as shown in the d orbital-resolved projected band structures in the left panel of Fig. 2(a).





One can find spin splitting (≈169 meV) between the first and second valence bands at the K and K' valleys with opposite band sequences, which is larger than the reported values in monolayer MoS_2 (≈150 meV). Similar spin splittings also occur in the conduction bands, but with small values (≈13 meV), as shown in the right panel of Fig. 2(b). These differences indicate the existence of a large build-in vertical electric field.

⇒Spin polarisation occurs due to the Rashba effect.

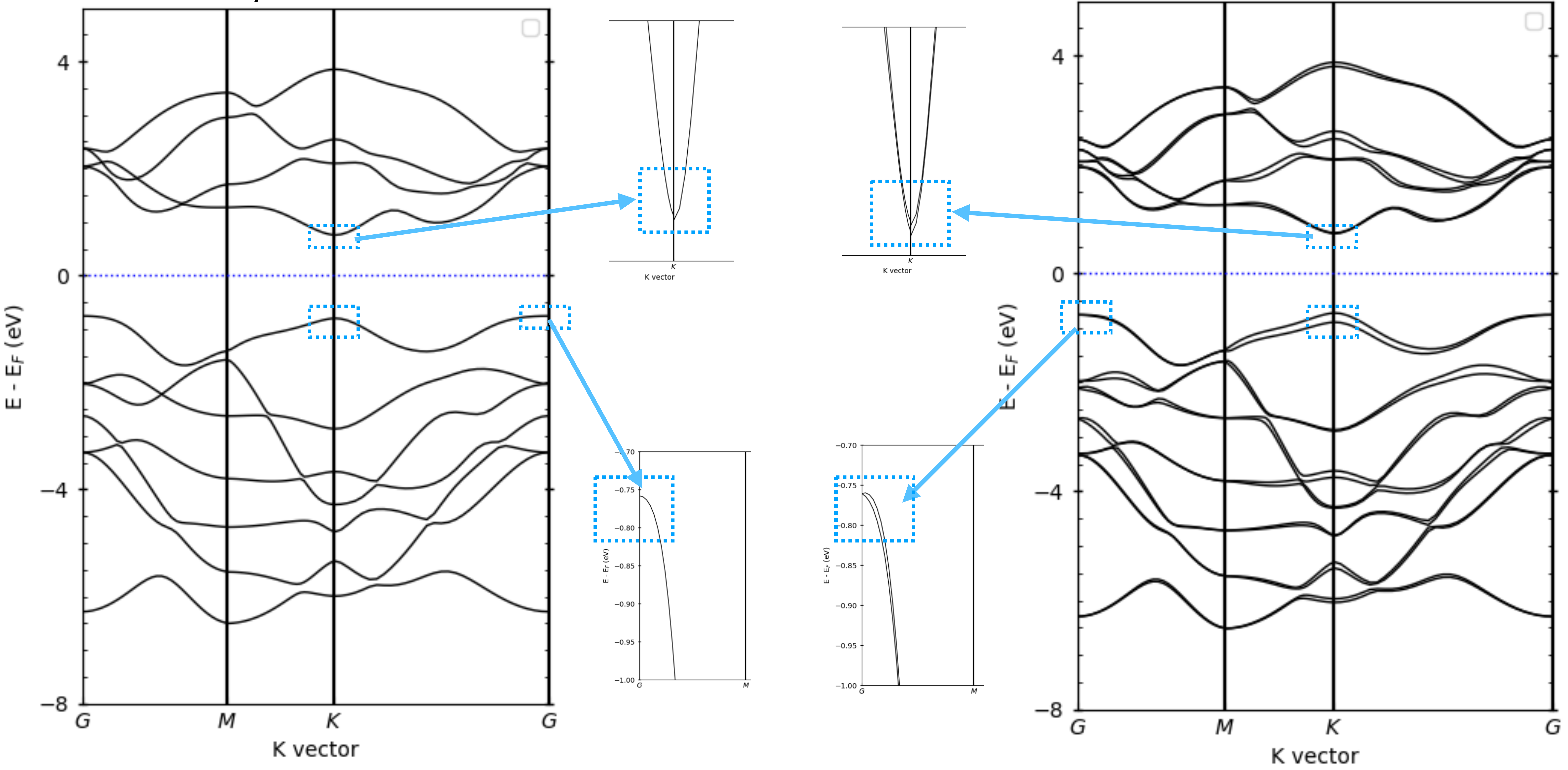
MoSSe@Q.E

My calculation

Chalcogenic contribution to Band structure appears in the SOC.

- Three-band tight binding models + SOC(Ising term & Rashba term)

W/O SOC | with SOC



Task

- Three-band tight binding models + SOC(Ising term & Rashba term).
- Wannier transform of Janus TMD band structure.
- calculation of janus TMD nanotube.
- optical conductivity(linear, nonlinear)
-