Electronic Structure of Topological Materials

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Topological phase of matter

What is topological phase in condensed matter physics?

Is that it?

Phase transition

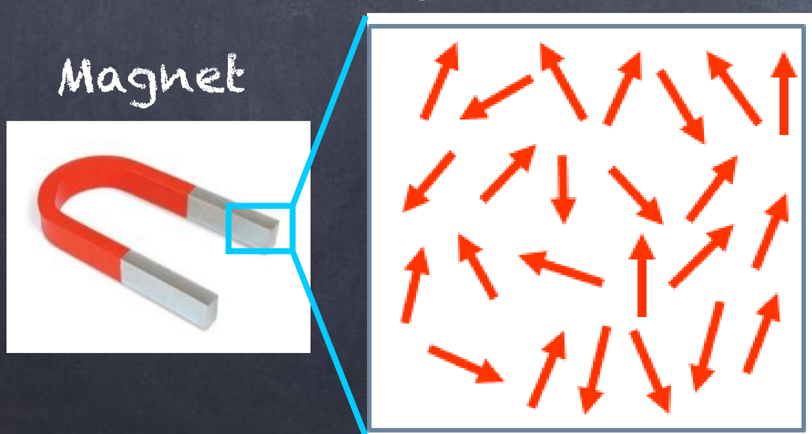
Ref: Lev Landau, Zh. Eksp. Teor. Fiz. 7, 19 (1937)

How physicists think about phase transitions?

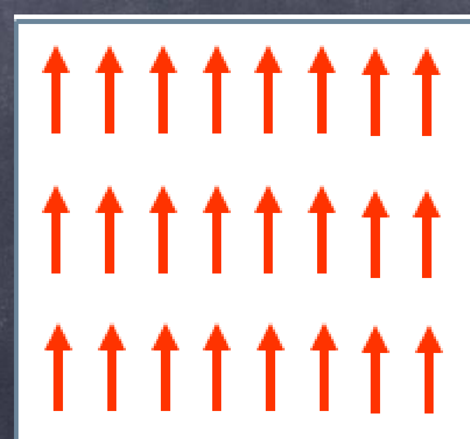
Landau theory
- Concept: symmetry breaking
- Observable: order parameter

Magnet

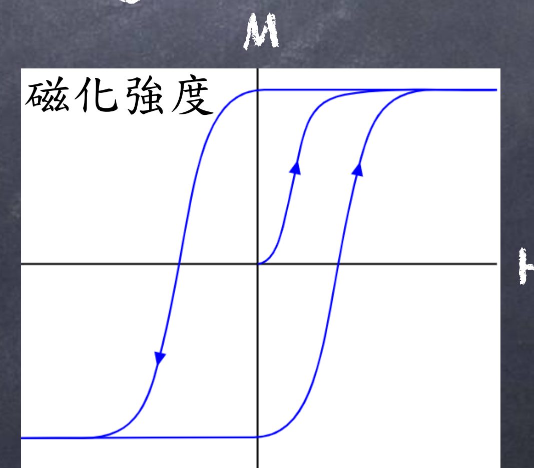
High T (disorder)



Low T (order)



Order parameter
(Magnetization)



Phase transition

Ref: Lev Landau, Zh. Eksp. Teor. Fiz. 7, 19 (1937)

How physicists think about phase transitions?

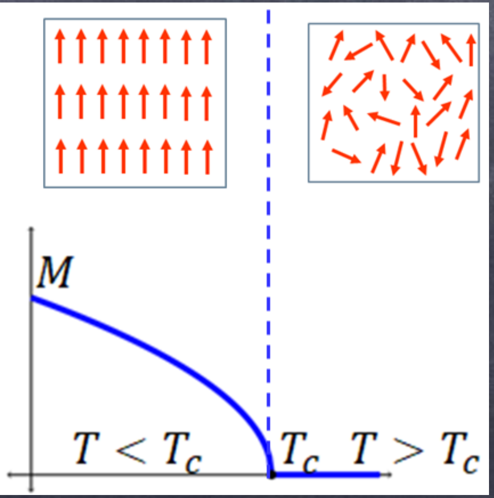
Second order phase transition:

$$F(T,M) = F_0 + a_0(T-T_c)M^2 + \frac{1}{2}b_0M^4 + \cdots$$

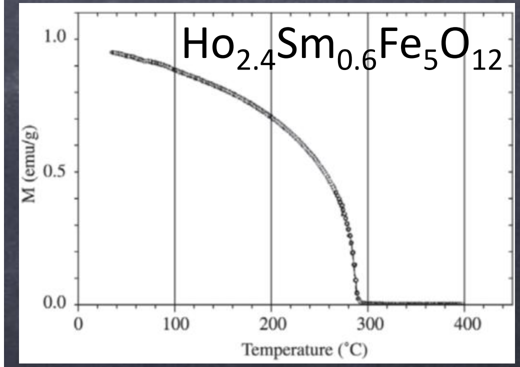
Magnetization (M)

$$\Rightarrow \frac{\partial F}{\partial M} = 2a_0(T-T_c)M + 2b_0M^3 = 0$$

$$\Rightarrow \begin{cases} M = 0 & , T>T_c \\ M = \sqrt{-\frac{a_0}{b_0}(T-T_c)} & , T<T_c \end{cases}$$



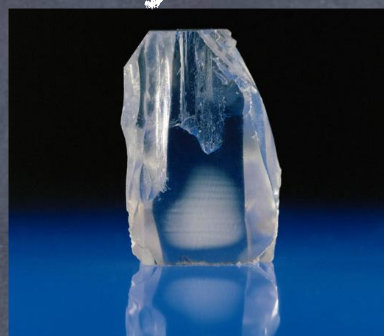
Materials Research **6**, 569 (2003)



Phase transition

Ref: Physics Today 63, 33 (2010)

Before 1970 ...

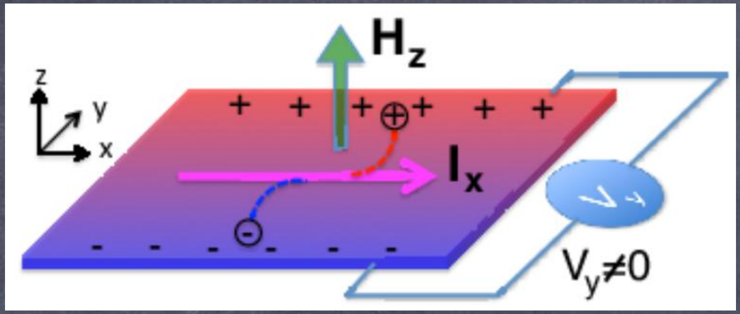
	Crystal	Magnet	Superconductor
			
Symmetry broken	translational symmetry	rotational symmetry	U(1) gauge symmetry
Order parameter	Charge density	Magnetization	Superconducting gap

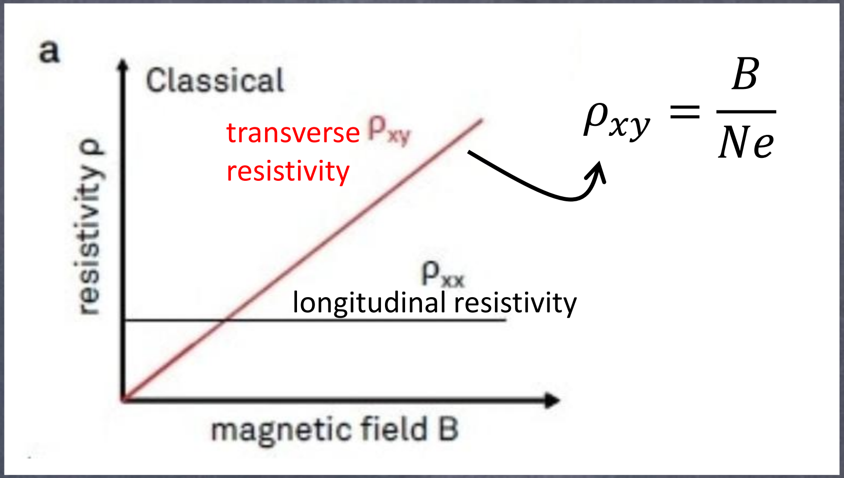
Quantum Hall effect

Ref: A-APPS Bulletin **23**, 3 (2013)

Hall effect

(1879, Edwin Herbert Hall)

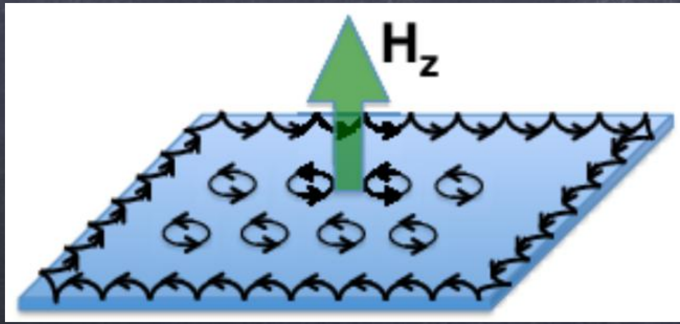


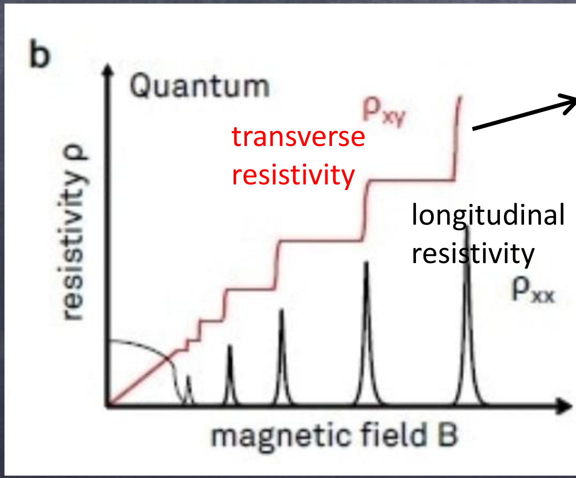


$$\rho_{xy} = \frac{B}{Ne}$$

Quantum Hall effect

(1980, Klaus von Klitzing)





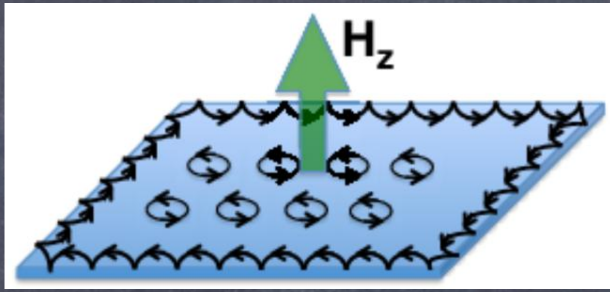
$$\rho_{xy} = \frac{1}{n}\frac{h}{e^2}$$
$$n = 1,2 \ldots$$

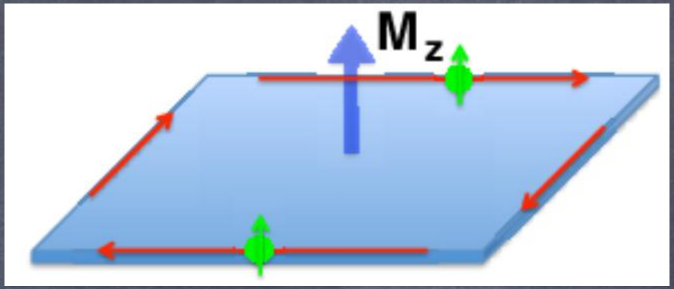
Quantum anomalous Hall effect

Ref: A-APPS Bulletin **23**, 3 (2013)
Ref: Phys. Rev. B 78, 195424 (2008)

External magnetic field ➡ Internal magnetization

Quantum Hall effect | Quantum anomalous Hall effect (量子異常霍爾效應)





Symmetry remains unchanged

⬇

Topological phase transitions
(Band theory point of view)

⬇

Topological materials

Outline

- **Band theory**

  Band structures: Bulk states, surface states

- **Topological band theory**

  Basic concepts and properties of topological band structure

- **Topological insulators (Non-magnetic)**

  Strong topological insulators

  Weak topological insulators

  topological crystalline insulators

- **Topological insulators (magnetic)**

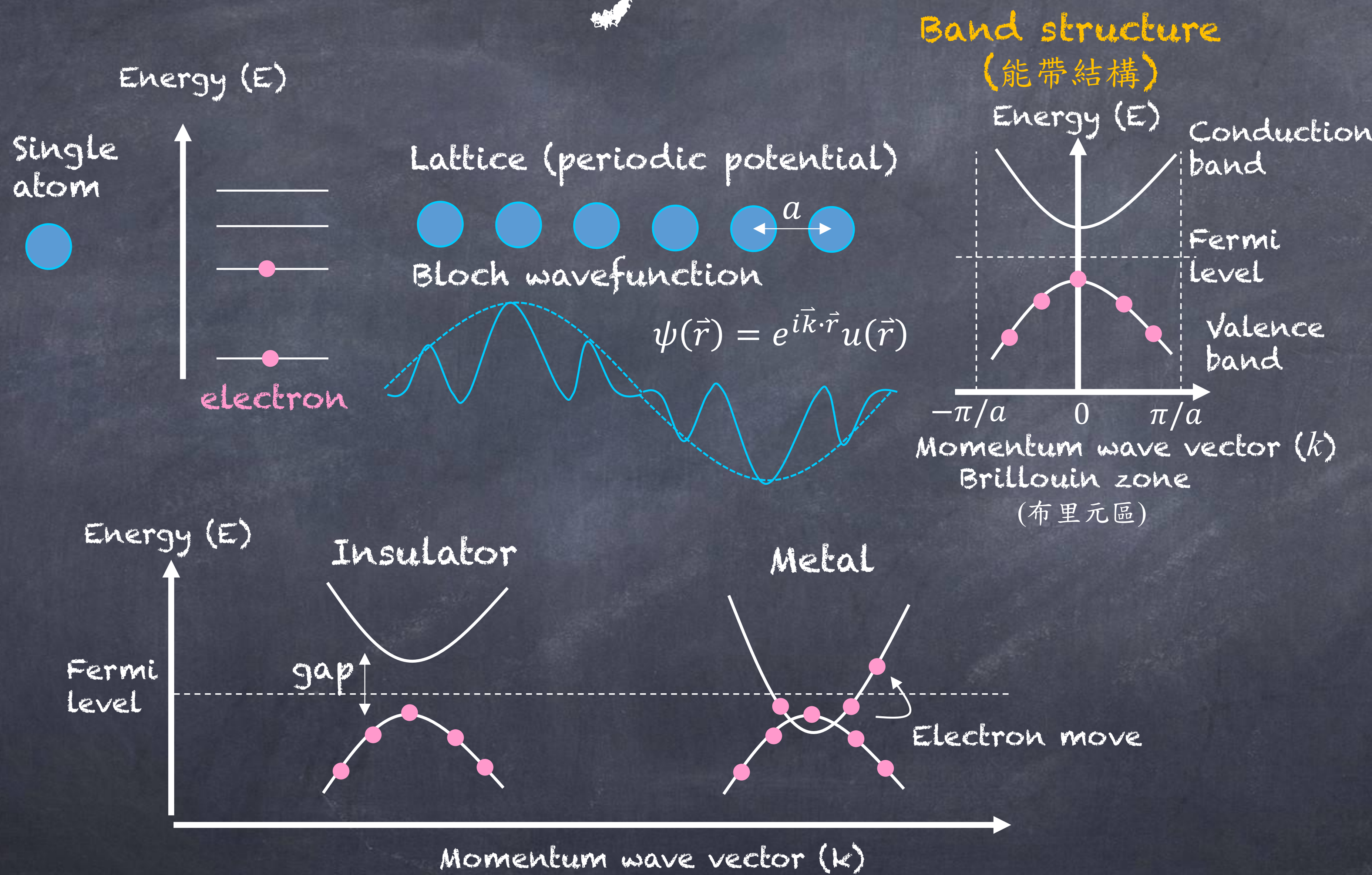
  Ferromagnetic topological insulators (axion insulators)

- **Orbital Hall effect**

  Feature spectrum topology

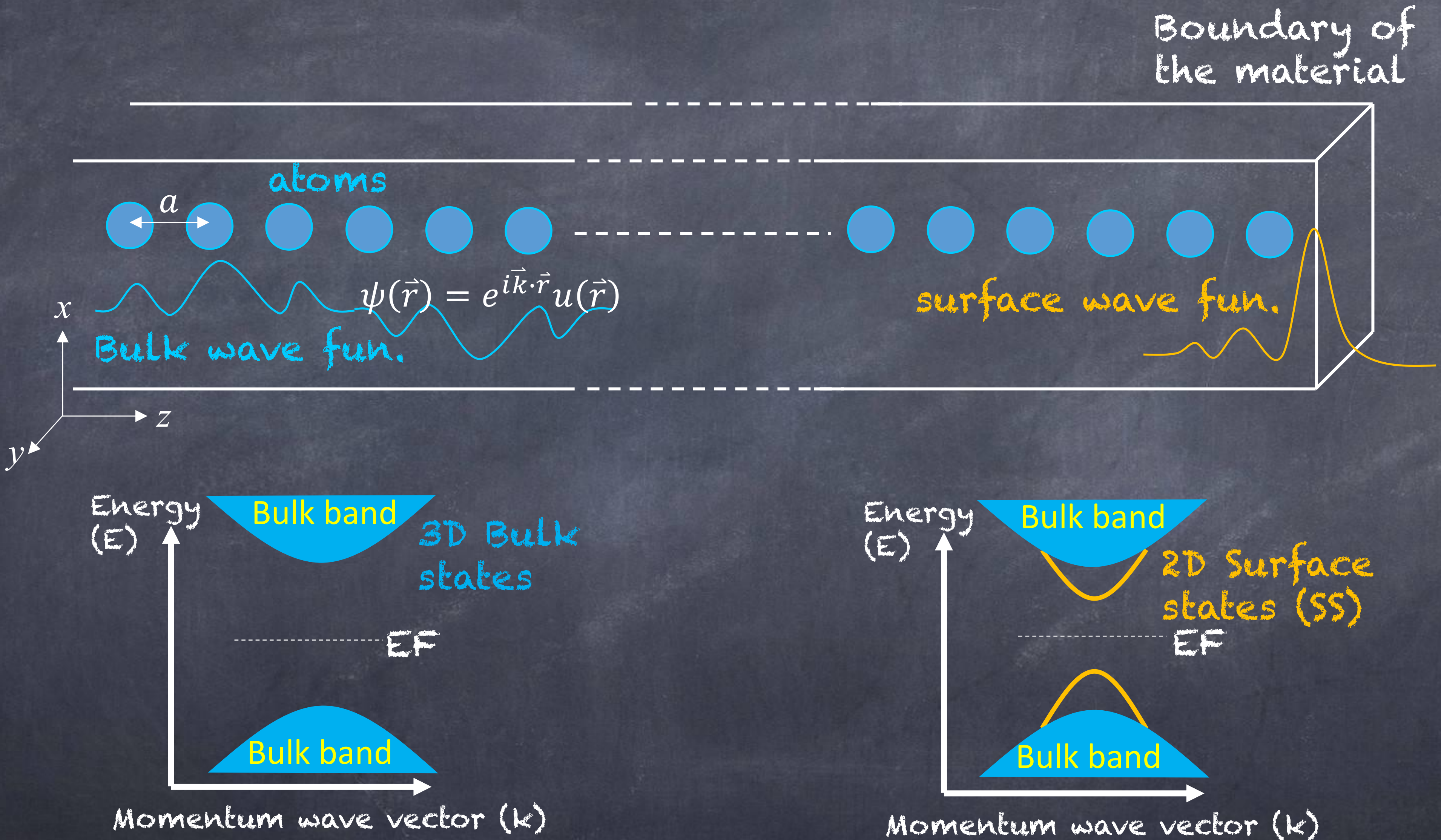
  Orbital Chern insulators

Band theory



Band structure
(能帶結構)
Energy (E)
Single
atom
electron
Lattice (periodic potential)
a
Bloch wavefunction
$\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}u(\vec{r})$
Energy (E)
Conduction
band
Fermi
level
Valence
band
$-\pi/a$
0
π/a
Momentum wave vector (k)
Brillouin zone
(布里元區)
Energy (E)
Insulator
Metal
Fermi
level
gap
Electron move
Momentum wave vector (k)

Band theory (surface state)



Outline

- Band theory
  - Band structures: Bulk states, surface states
- Topological band theory
  - Basic concepts and properties of topological band structure
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  - Strong topological insulators
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  - Feature spectrum topology
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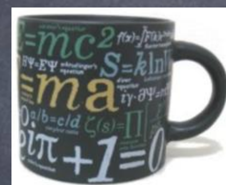
Band theory (topology)

Math => real space

Gauss-Bonnet Theorem:

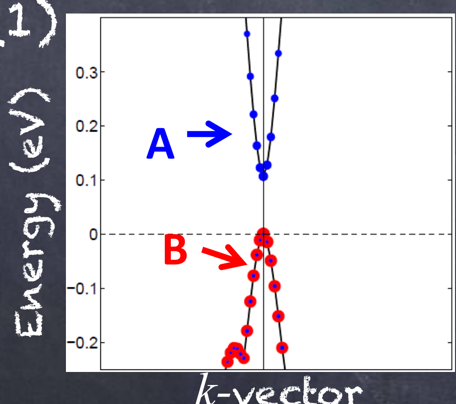

$\neq$

$=$


$$\int_S K_{Gauss} ds = 4\pi(1-g)$$

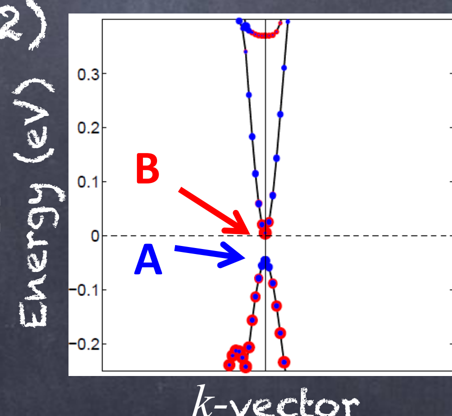
Gauss curvature   genus

genus   g=0   g=1   g=1

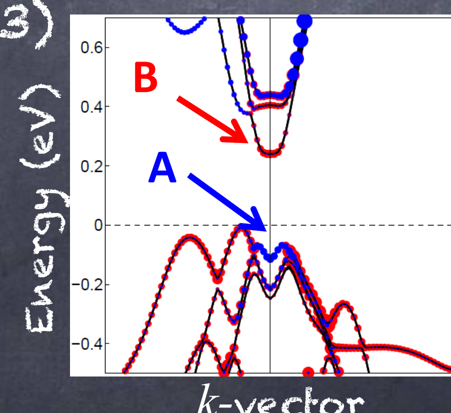
Phys => momentum space

(1)


$\neq$

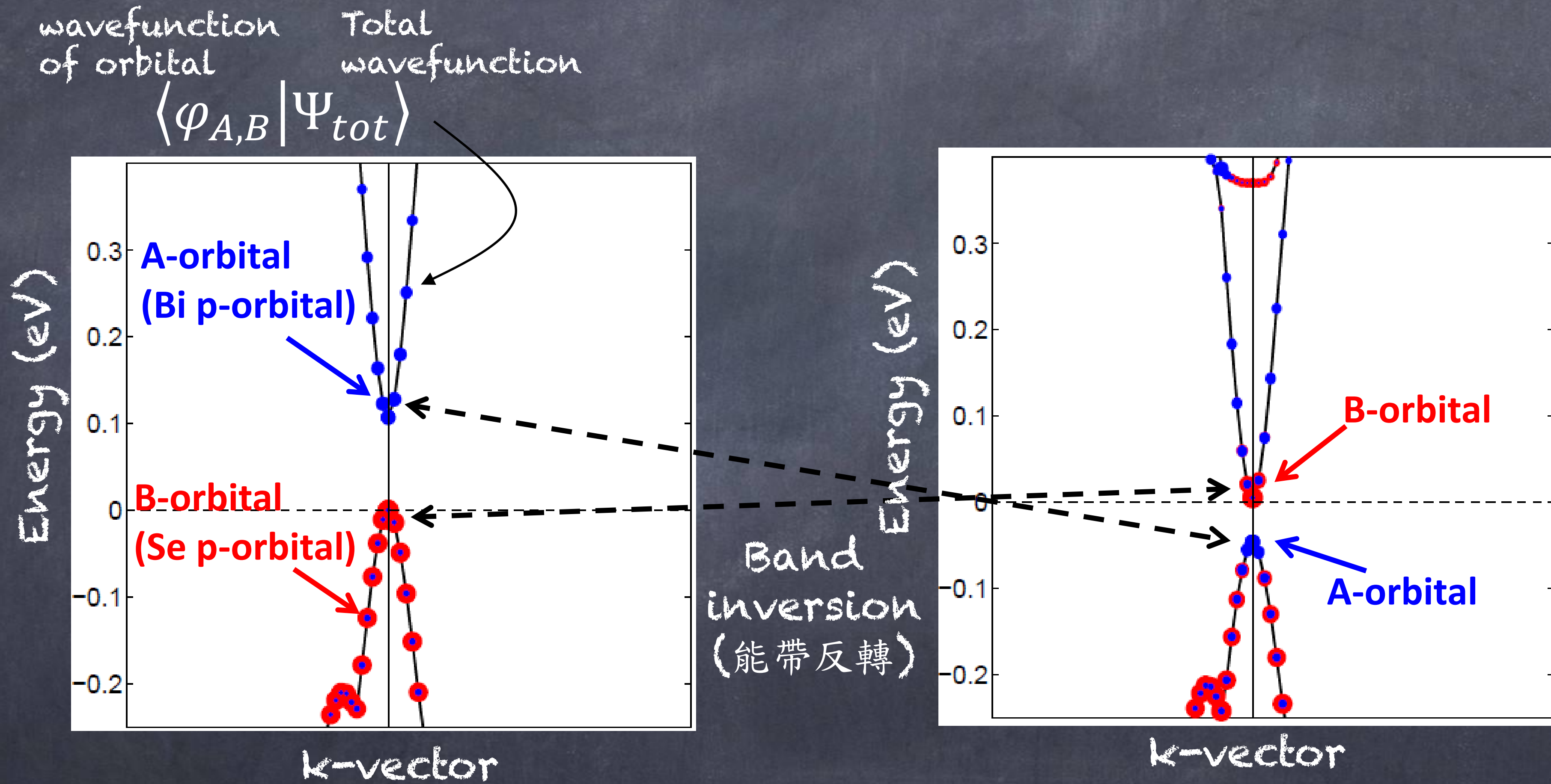
(2)


$=$

(3)


物理雙月刊（2017）藏在邊緣的物理：拓樸材料與拓樸能帶理論（張泰榕）

Band theory (topology)



Band theory (topology)

Ref: Phys. Rev. Lett. 49, 405 (1982)
Ref: Phys. Rev. Lett. 61, 2015 (1988)

Math => real space

Gauss-Bonnet Theorem:

$$\int_S K_{Gauss} ds = 4\pi(1-g)$$

Gauss curvature

genus

Phys => momentum space

TKNN theorem:

Topological invariants
(拓樸不變量)

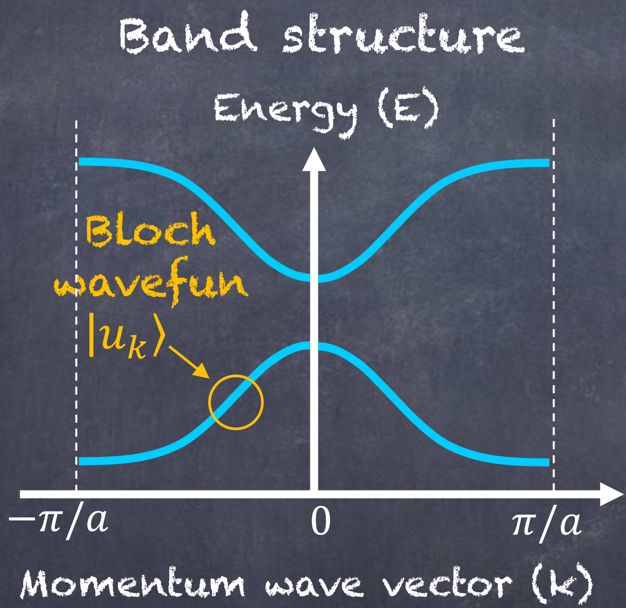
$$\frac{1}{2\pi}\sum_m \int_{BZ} d^2k\, \underbrace{\vec{\nabla} \times i\left\langle u_m \middle| \vec{\nabla} \middle| u_m \right\rangle}_{\text{Berry curvature}} = n$$

Berry curvature
(貝里曲率)

Bloch wavefun

Berry curvature: $\vec{\Omega} = \vec{\nabla} \times \vec{A} = \vec{\nabla} \times i\left\langle u_m \middle| \vec{\nabla} \middle| u_m \right\rangle$?

Band theory (topology)



Quantum (Momentum space)	Classical (Real space)
Berry connection	Vector potential
$\vec{A}_k = i\left\langle u_k \middle\| \vec{\nabla}_k \middle\| u_k \right\rangle$	$\vec{A}$
Berry curvature	Magnetic field
$\vec{\Omega}_k = \vec{\nabla}_k \times \vec{A}_k$	$\vec{B} = \vec{\nabla} \times \vec{A}$
Topological invariants	Gauss's law
$n = \frac{1}{2\pi}\sum_m \int_{BZ} d^2k\, \vec{\Omega}_{m,k}$	$\oint \vec{B} \cdot d\vec{S} = 0$

n = 0 : Ordinary insulator
n = integer : Topological nontrivial

Band theory (topology)

Berry connection

$$\vec{A}_k = i \left\langle u_k \middle| \vec{\nabla}_k \middle| u_k \right\rangle$$

Berry curvature

$$\vec{\Omega}_k = \vec{\nabla}_k \times \vec{A}_k$$

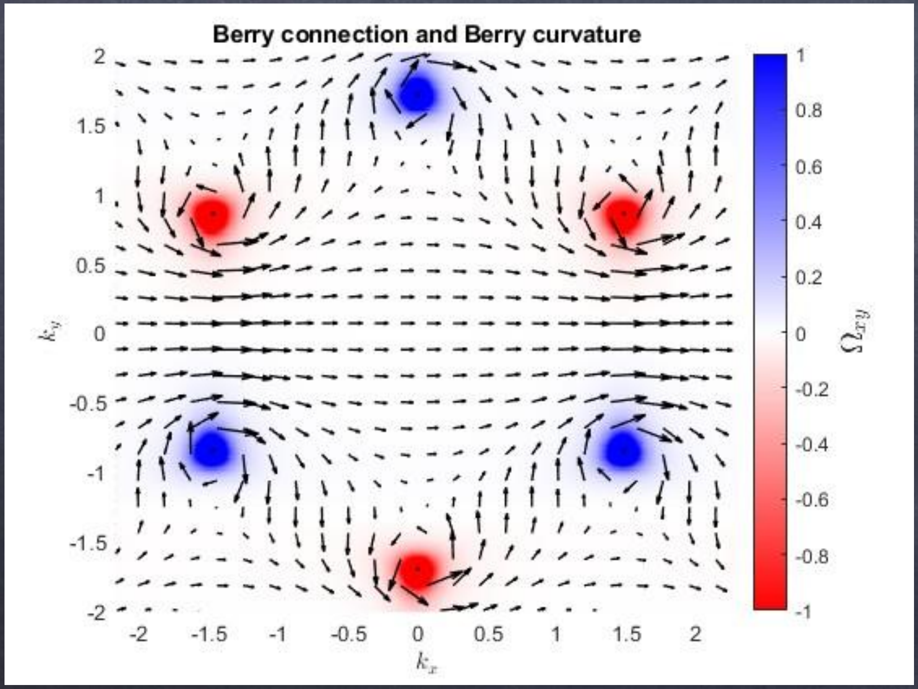
Topological invariants

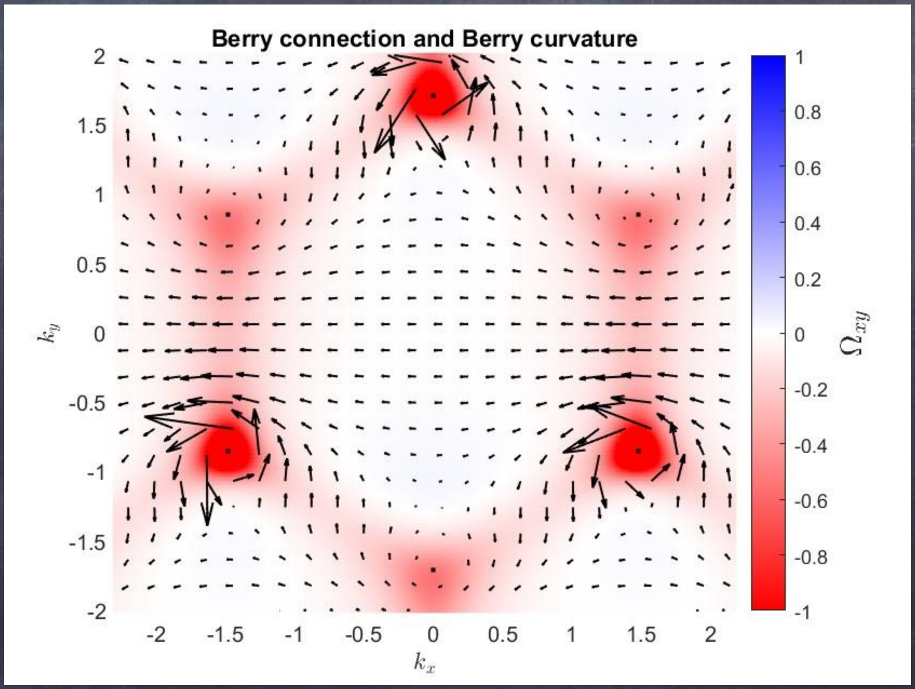
$$n = \frac{1}{2\pi} \sum_m \int_{BZ} d^2k\, \vec{\Omega}_{m,k}$$

e.g. Haldane model   Ref: F. D. M. Haldane, PRL 61, 2015 (1988)

$n = 0$ Ordinary insulator (topologically trivial)

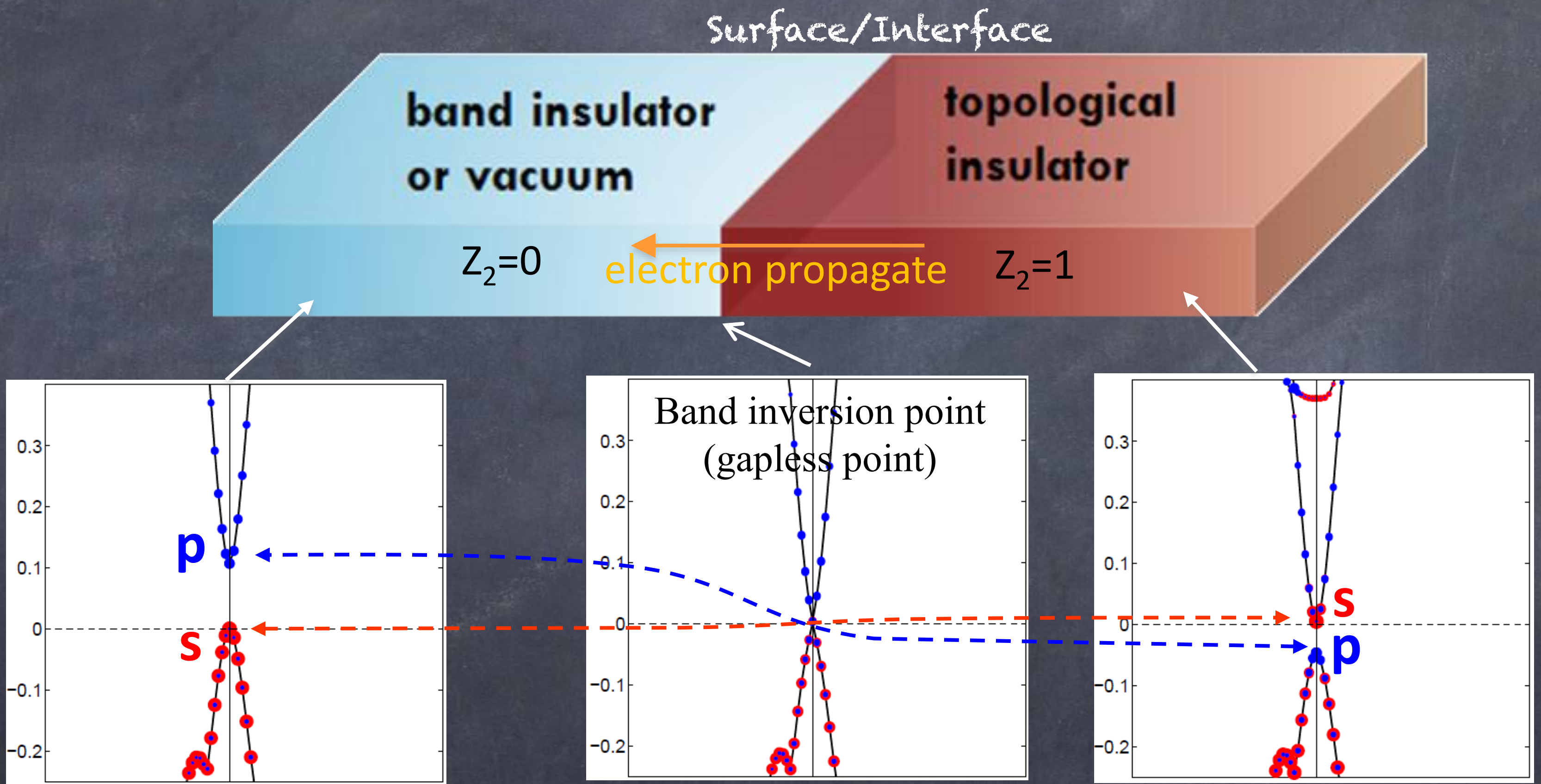
$n = 1$ Chern insulator (topologically nontrivial)





Band theory (topology)

Bulk-boundary correspondence(體-邊界對應)

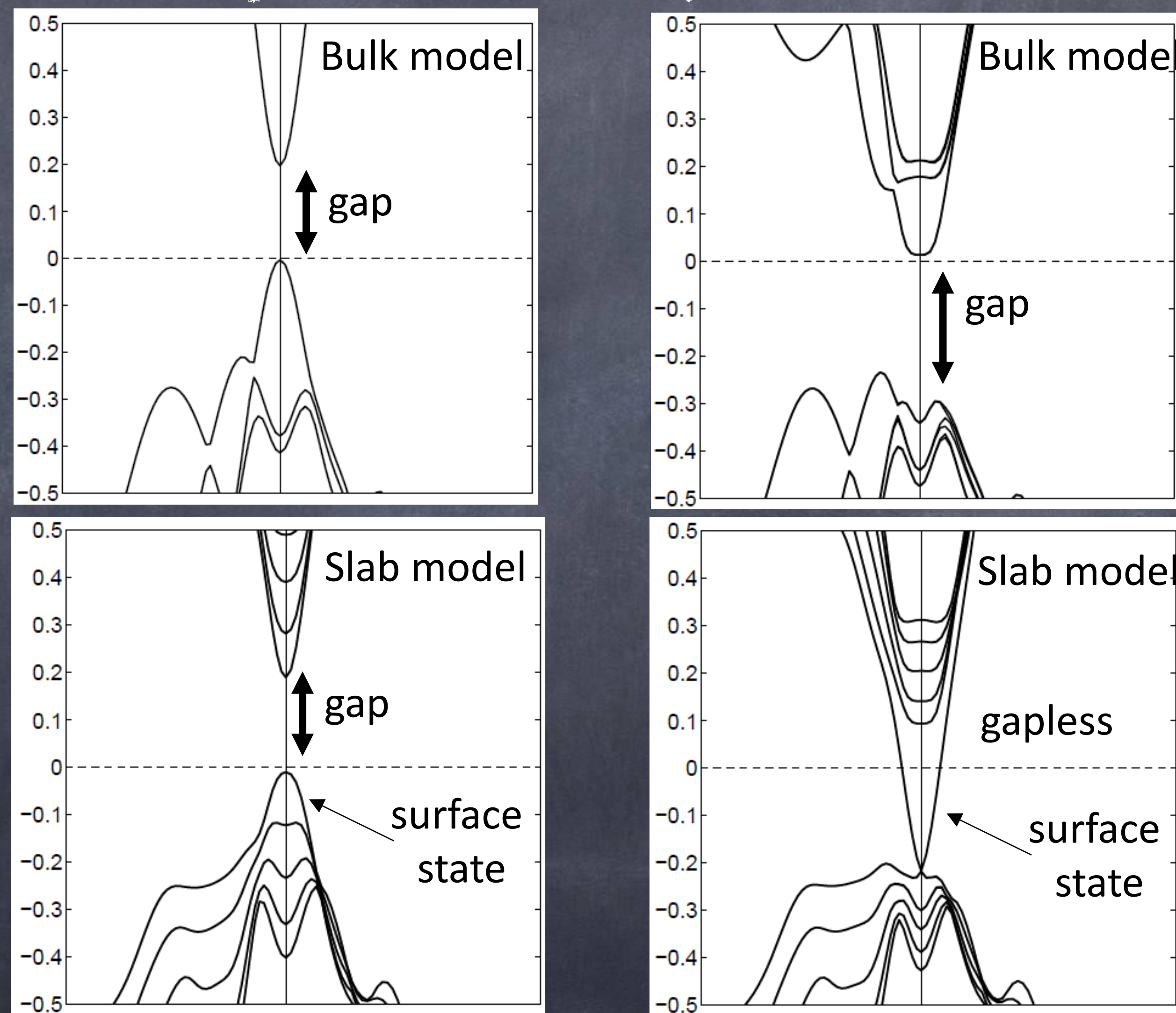


The gapless boundary state is the hallmark of topological phase

Ref: Rev. Mod. Phys. 82, 3045 (2010)
Ref: Rev. Mod. Phys. 83, 1057 (2011)

Band theory (topology)

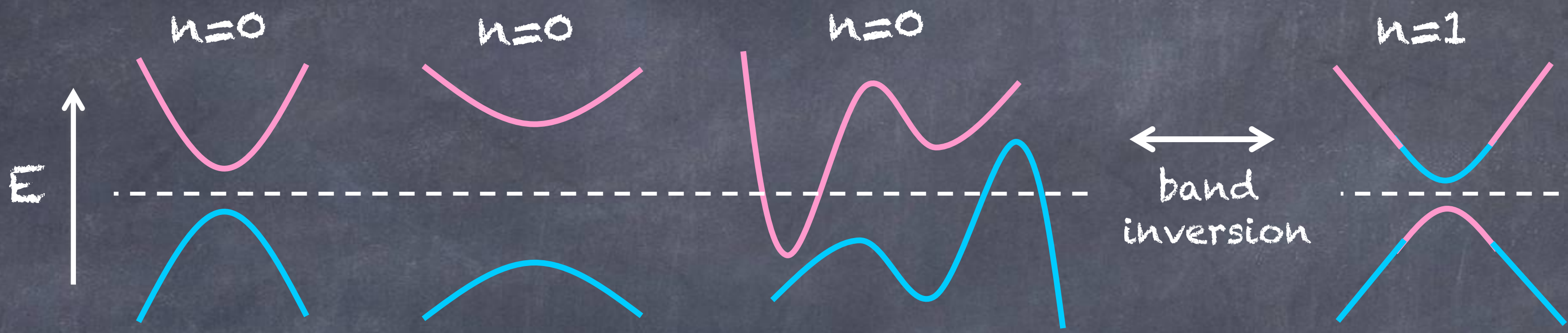
Ordinary insulator | Topological insulator



Momentum wave vector (k) | Momentum wave vector (k)

Topological band theory (Summary)

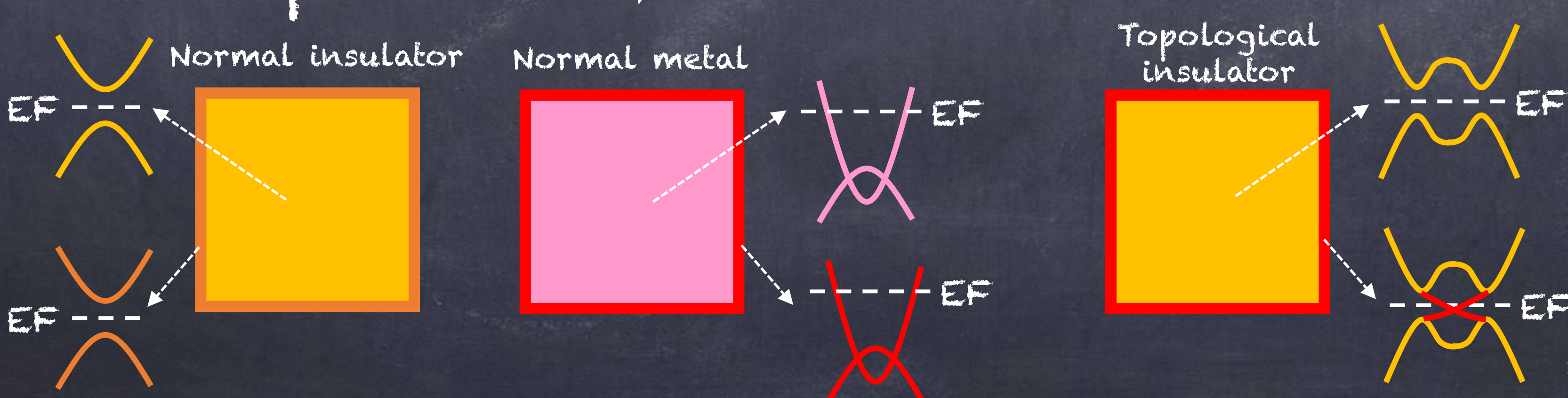
(1) Robust



(2) Topological invariants (math)

Chern number, Z_2 index, mirror Chern number, chiral charge, winding number ... etc

(3) Gapless surface states (measurable)



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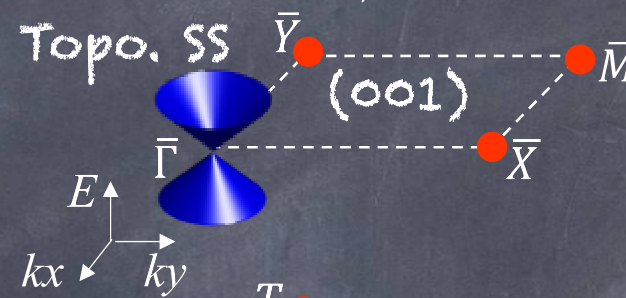
Strong topological insulator

Topological invariant of topological insulators: $\mathbb{Z}_2$ index

$\mathbb{Z}_2 \oplus \mathbb{Z}_2 \oplus \mathbb{Z}_2 \oplus \mathbb{Z}_2 = (1;\underbrace{0,0,0}_{\text{weak index}})$ $\xrightarrow{\text{simplify}}$ $Z_2=1$ Strong topological insulator

strong index   weak index

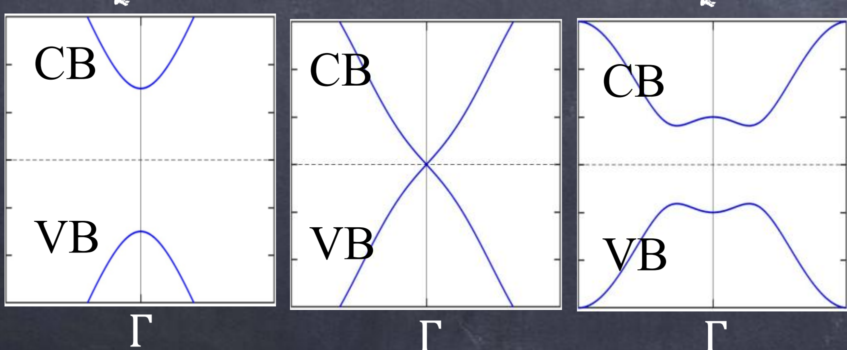
Surface 2D BZ



e.g. Bi_2Se_3 (strong TI)

small   SOC strength   large

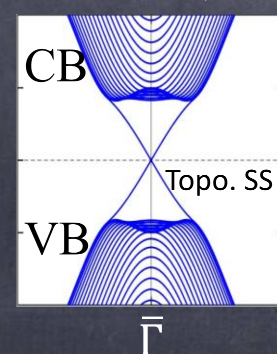
$Z_2=0$ critical $Z_2=1$

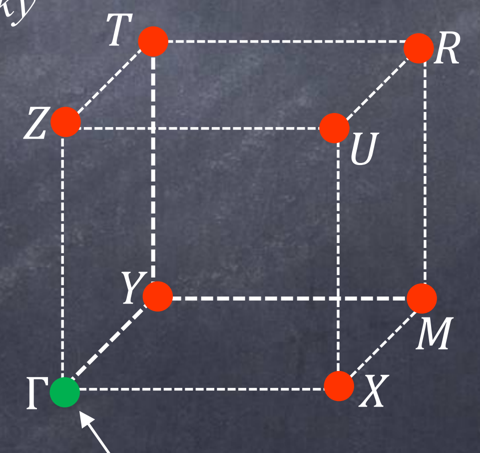


Normal insulator   Strong TI

Cleave sample

(001)



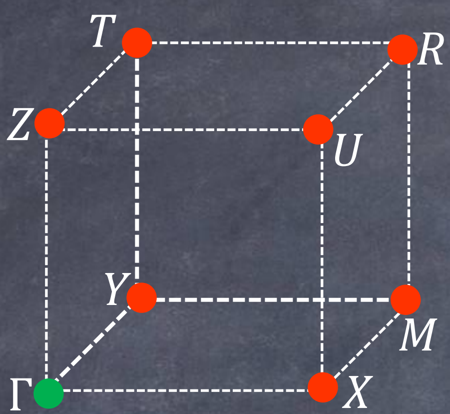


Band inversion position in Bulk 3D BZ

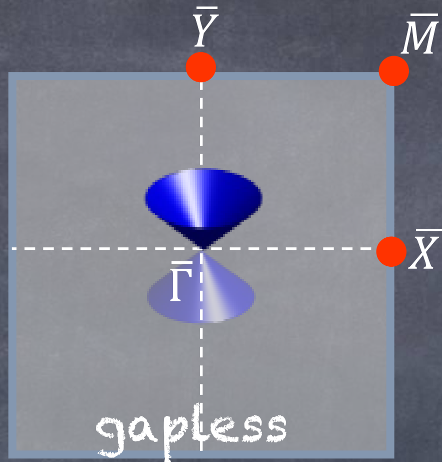
Strong topological insulator $Z_2=(1;0,0,0)$

Ref: Phys. Rev. B 76, 045302 (2007)

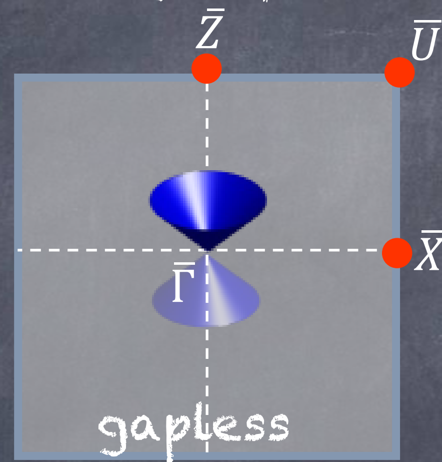
e.g. Bi_2Se_3



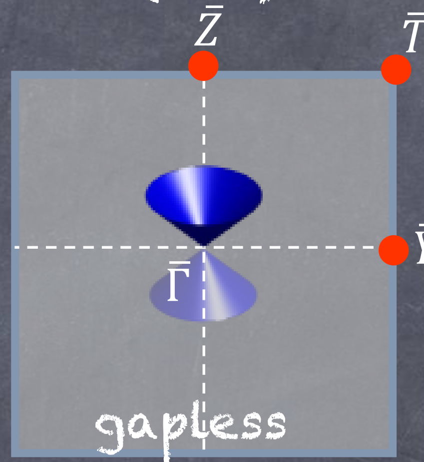
(001)



(010)



(100)

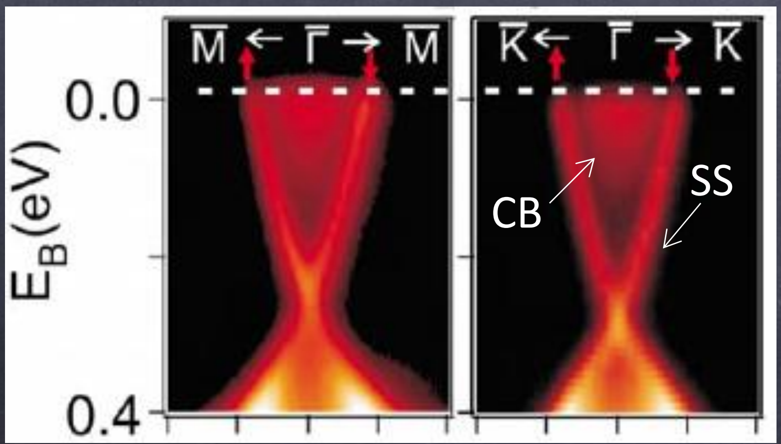


e.g. Bi_2Se_3

ARPES

(**A**ngle **R**esolved **P**hoto**E**mission **S**pectroscopy)

(角解析光電子能譜學)

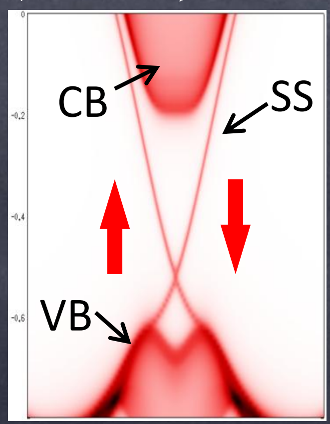


k-vector

Ref: Nat. Phy.s 5, 398 (2009)

Theory

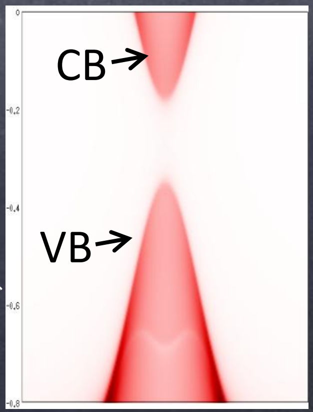
Non-trivial



k-vector

band inversion

trivial

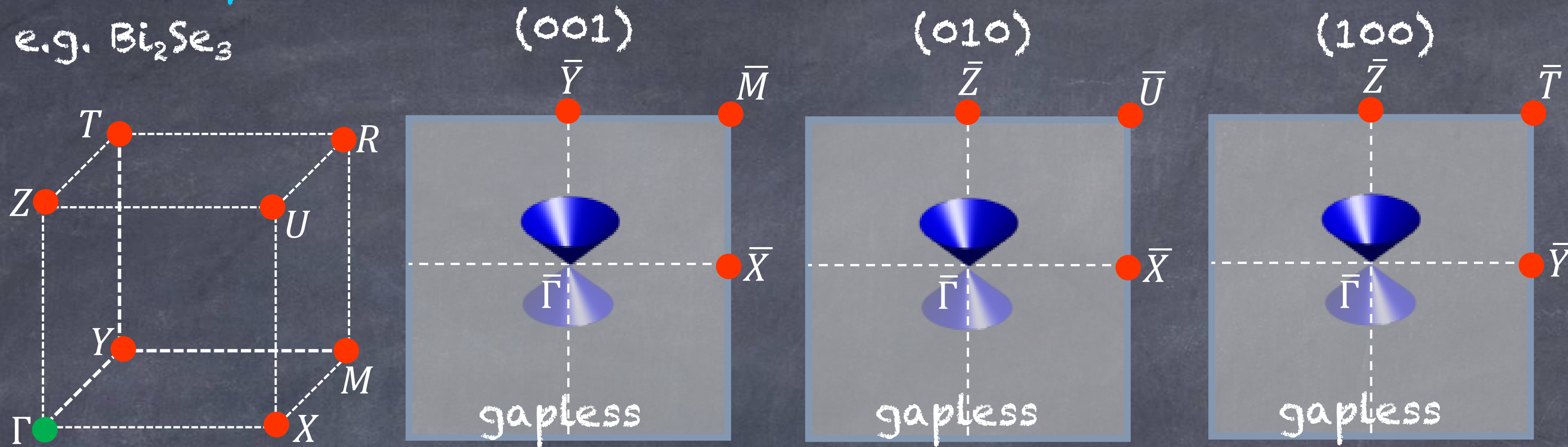


k-vector

Strong topological insulator $Z_2=(1;0,0,0)$

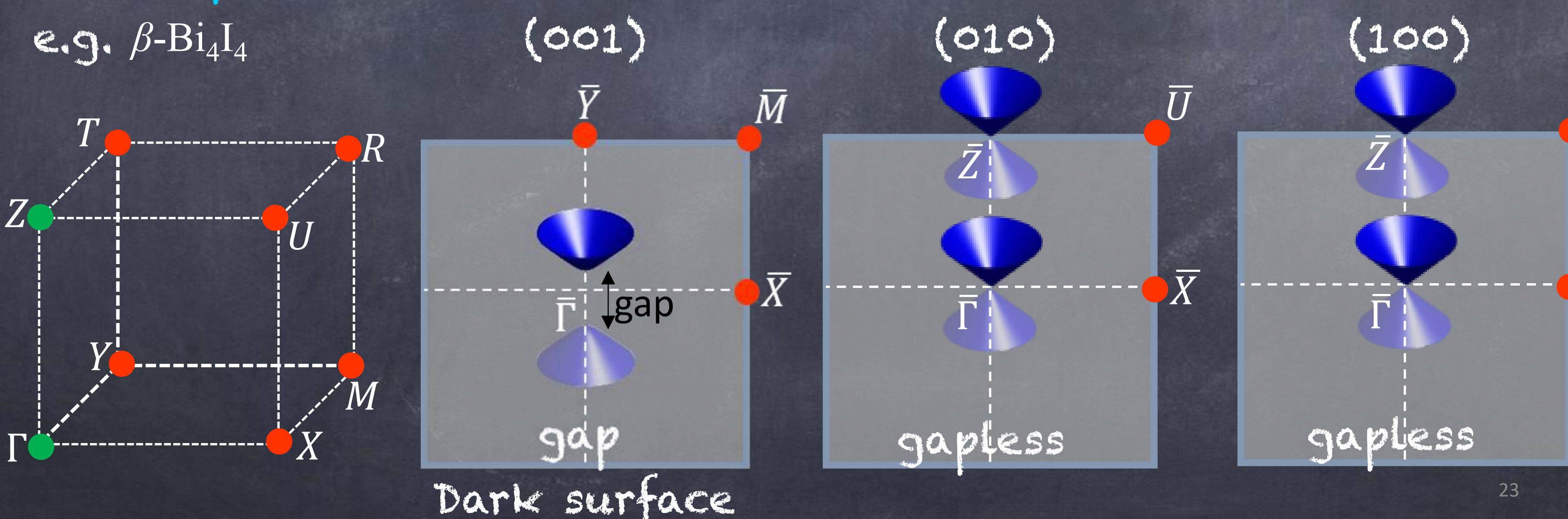
Ref: Phys. Rev. B 76, 045302 (2007)

e.g. Bi_2Se_3



Weak topological insulator $Z_2=(0;0,0,1)$

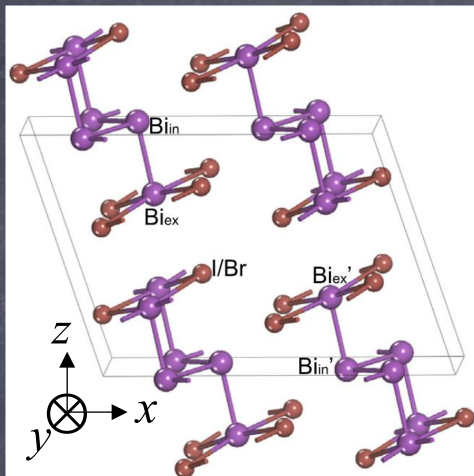
e.g. β-Bi_4I_4

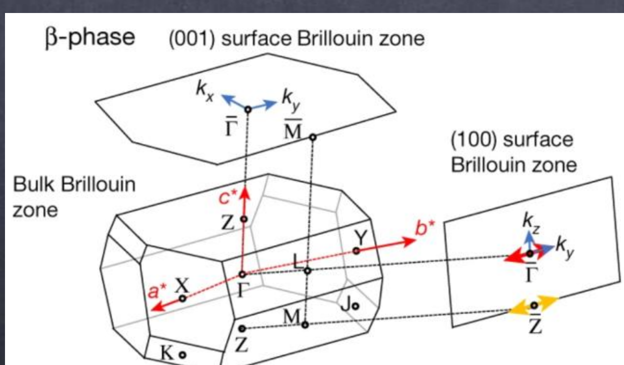


Weak topological insulator: ARPES measurements

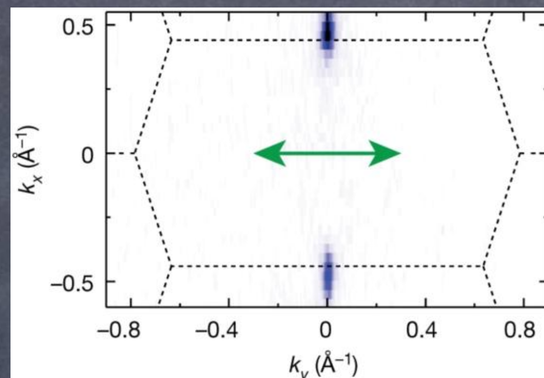
Ref: Phys. Rev. B 76, 045302 (2007)
Ref: Phys. Rev. Lett. 116, 066801 (2016)
Ref: Nature 566, 518 (2019)

β-Bi_4I_4

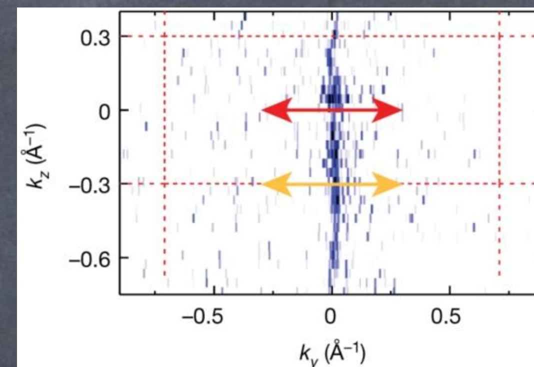


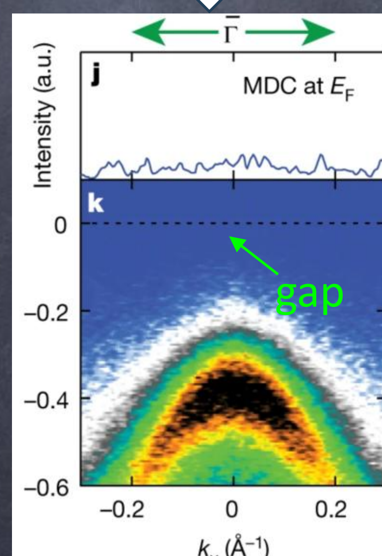


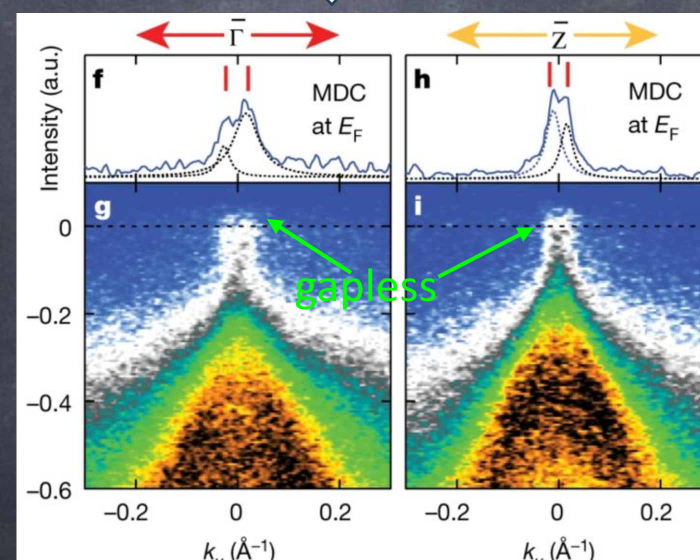
(001) Dark surface



(100) Side surface







Topological crystalline insulators

Strong topological insulators $Z_2=(1;0,0,0)$

Weak topological insulators $Z_2=(0;0,0,1)$

If $Z_2=(0;0,0,0)$ $\xrightarrow{?}$ Ordinary band insulators

↓ additional crystal symmetries:
mirror plane, rotation … etc

Gapless topological surface states

↓

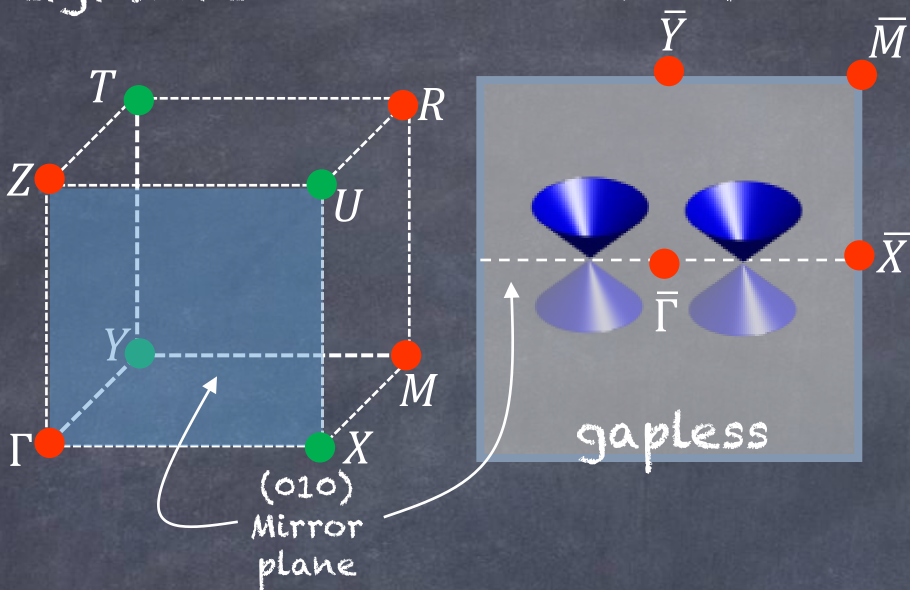
Topological crystalline insulators

Topological crystalline insulator (mirror) $Z_2=(0;0,0,0)$

e.g. SnTe

(001)

Ref: Nat. Commun. 3, 982 (2012)



Mirror Chern number:

$$C_M = \frac{(C_{+i} - C_{-i})}{2}$$

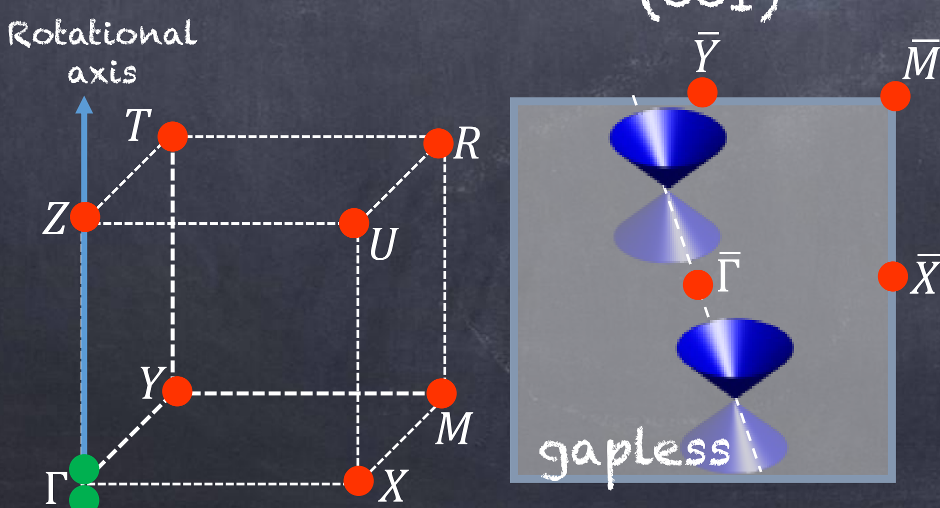
where $C_{\pm i}$ is mirror eigenvalue

e.g. $C_M = 2$ => two gapless SS

Topological crystalline insulator (rotation) $Z_2=(0;0,0,0)$

(001)

Ref: Nat. Commun. 8, 50 (2017)
Ref: Nat. Commun. 9, 3530 (2018)



Symmetry indicators:

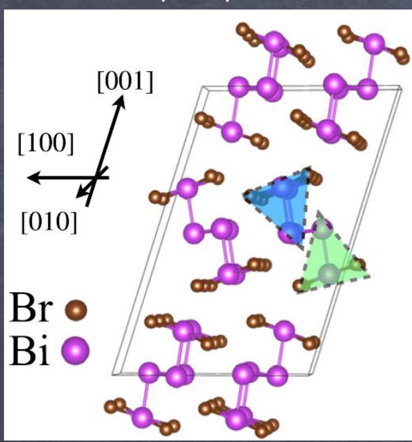
Z_2 index | Z_2 invariant for C_2 rotation | Mirror chern

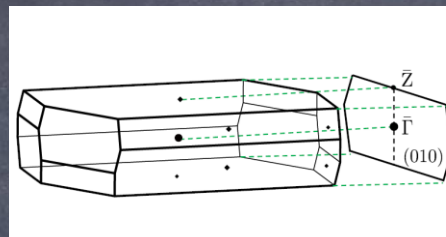
$(\nu_0;\nu_1\nu_2\nu_3)$	$n_{2_{[1\bar{1}0]}}$	$n_{\mathcal{M}_{[1\bar{1}0]}}$
(0;000)	1	0
(0;000)	0	2

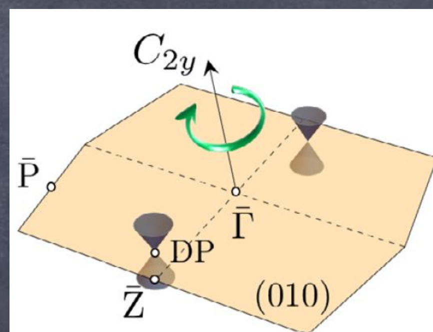
Topological crystalline insulator (rotation): Materials prediction

2D Mater. 6 031004 (2019)
PNAS 116, 13255 (2019)
Nat. Mater. 21, 1111 (2022)

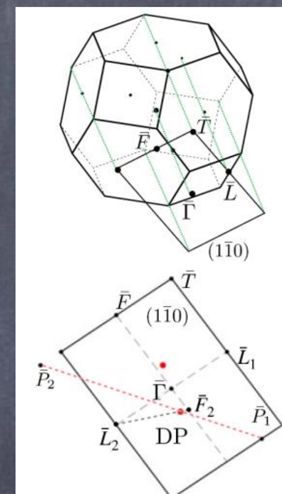
α-Bi_4Br_4

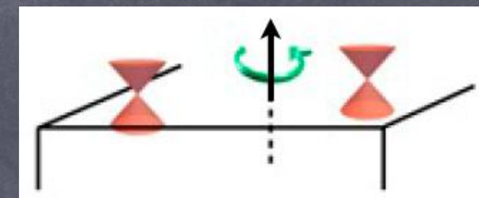


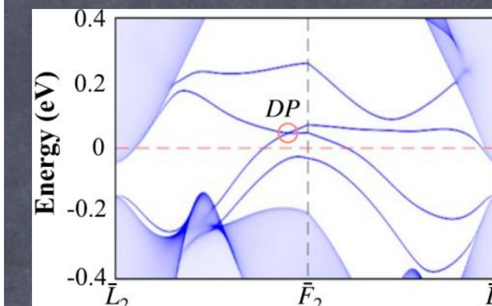




Bulk Bi



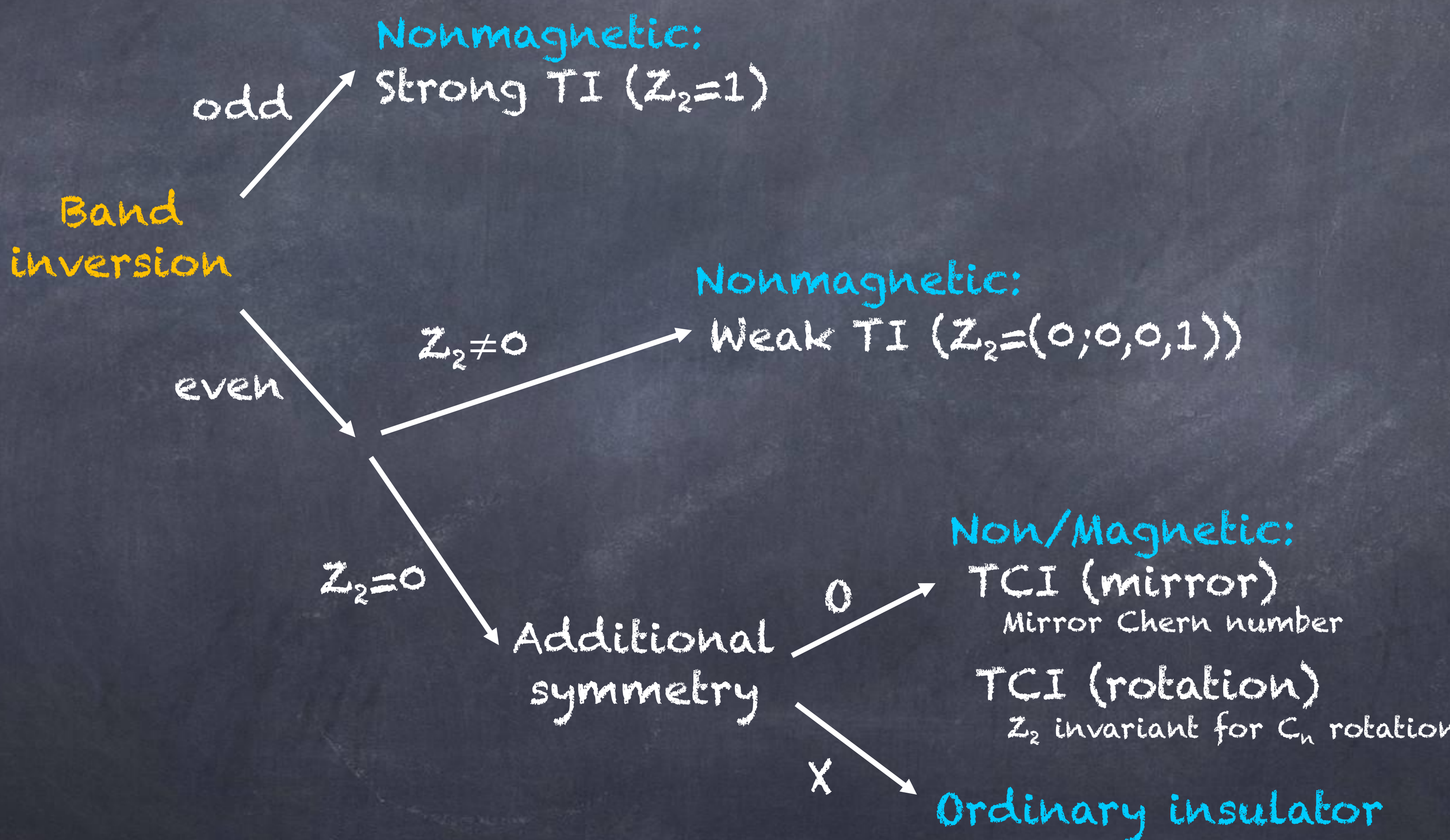




Previous studies: Normal insulators

Our studies: Rotational TCI

Odd vs Even number of band inversions



Outline

- Topological band theory

  Basic concepts and properties of topological band structure

- Topological insulator (Non-magnetic)

  Strong topological insulators

  Weak topological insulators

  topological crystalline insulators

- Topological insulator (magnetic)

  Ferromagnetic topological insulators (axion insulator)

- 2D topological phases w/o symmetry

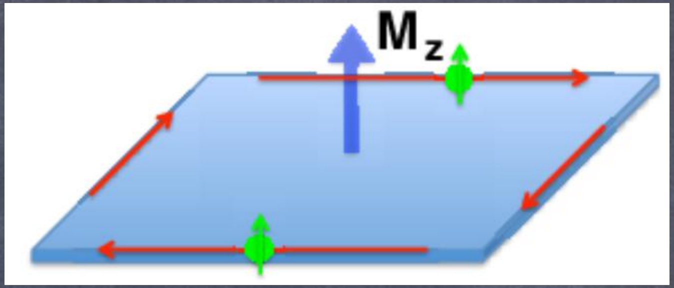
  Feature spectrum topology

  Orbital Hall effect

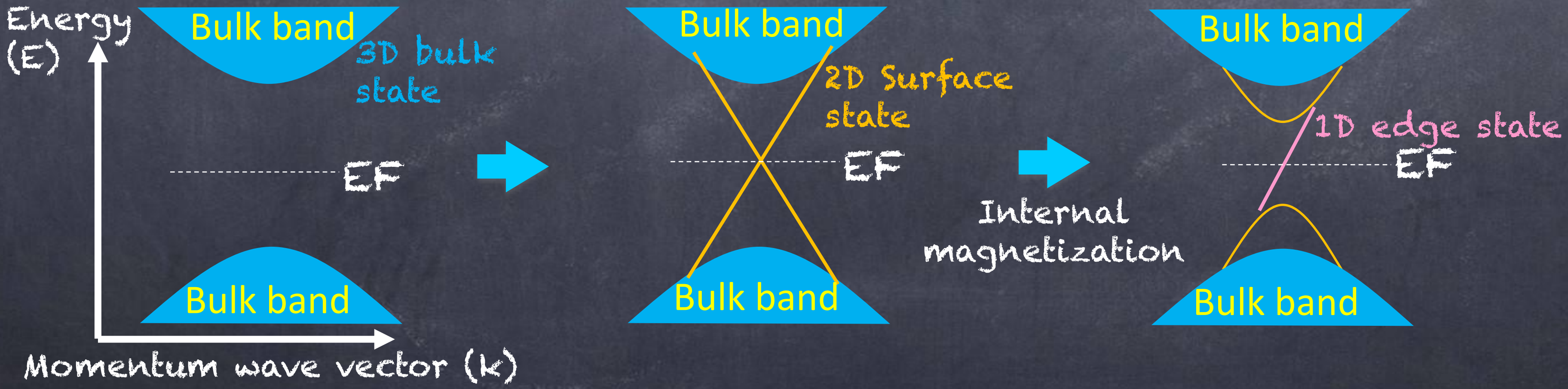
Magnetic topological materials

Internal magnetization

Quantum anomalous Hall effect



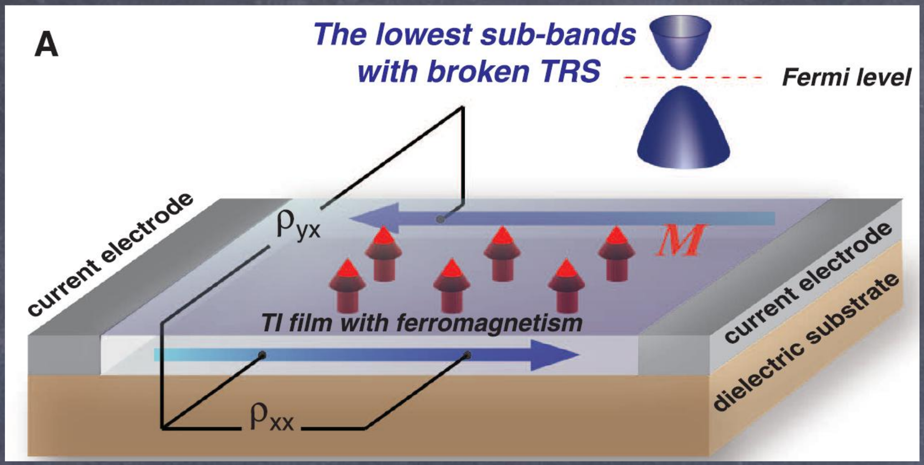
Ref: Phys. Rev. Lett. 101, 146802 (2008)
Ref: Science 329, 61 (2010)

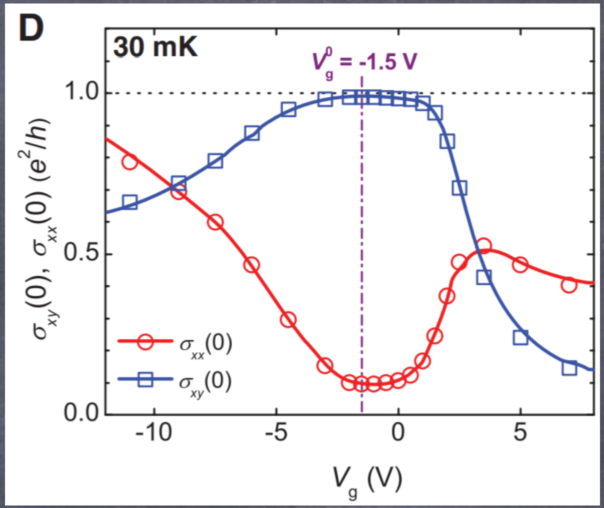


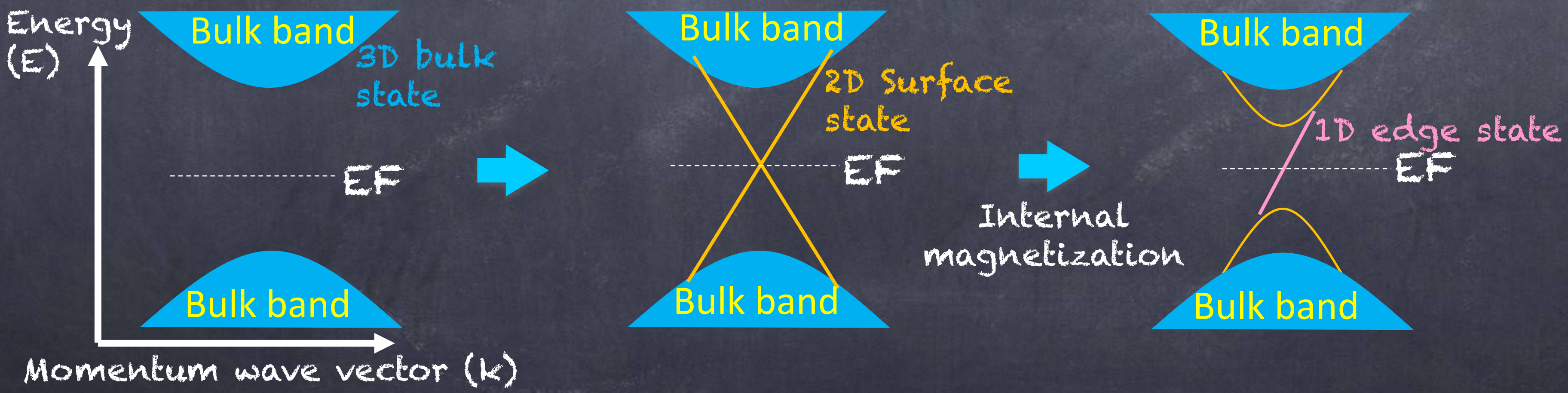
Magnetic topological materials

Ref: Science **340**, 167 (2013)

$Cr_{0.15}(Bi_{0.1}Sb_{0.9})_{1.85}Te_3$



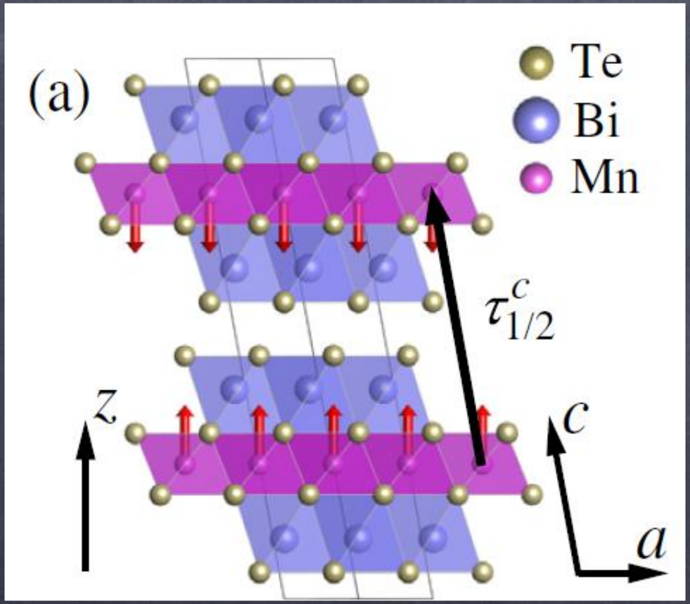




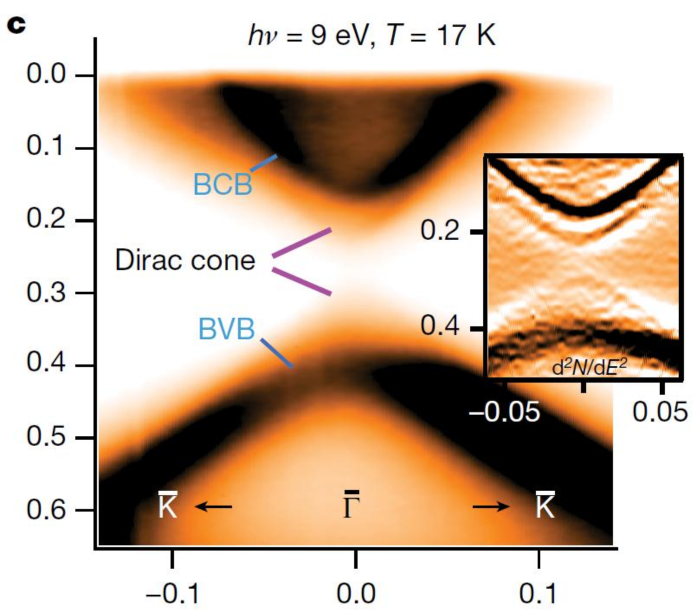
Antiferromagnetic topological material: $MnBi_2Te_4$ (MBT-124)

Ref: Nature 576, 19 (2019)
Ref: Phys. Rev. X 9, 041038 (2019)
Ref: Science 367, 895 (2020)

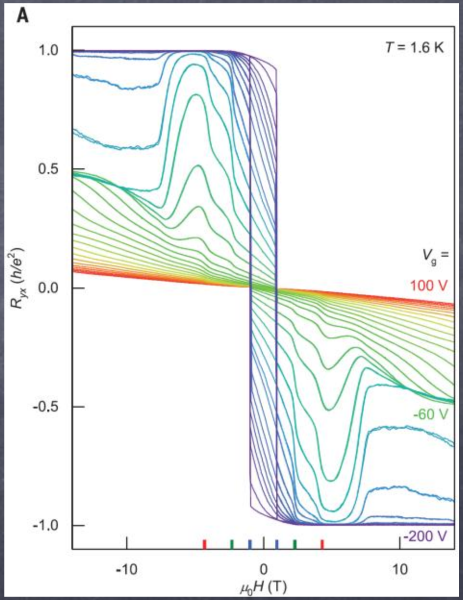
Crystal



ARPES



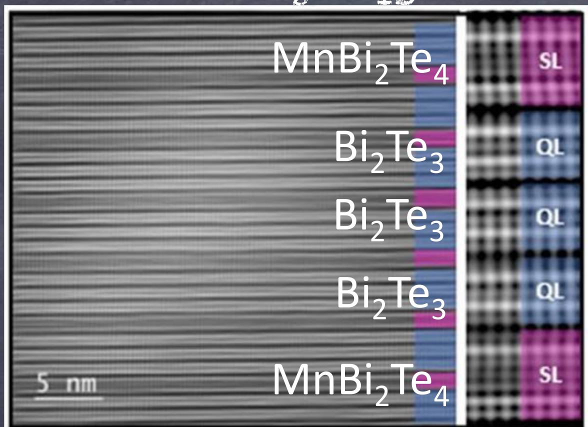
Hall effect (strong $\vec{B}$ field)

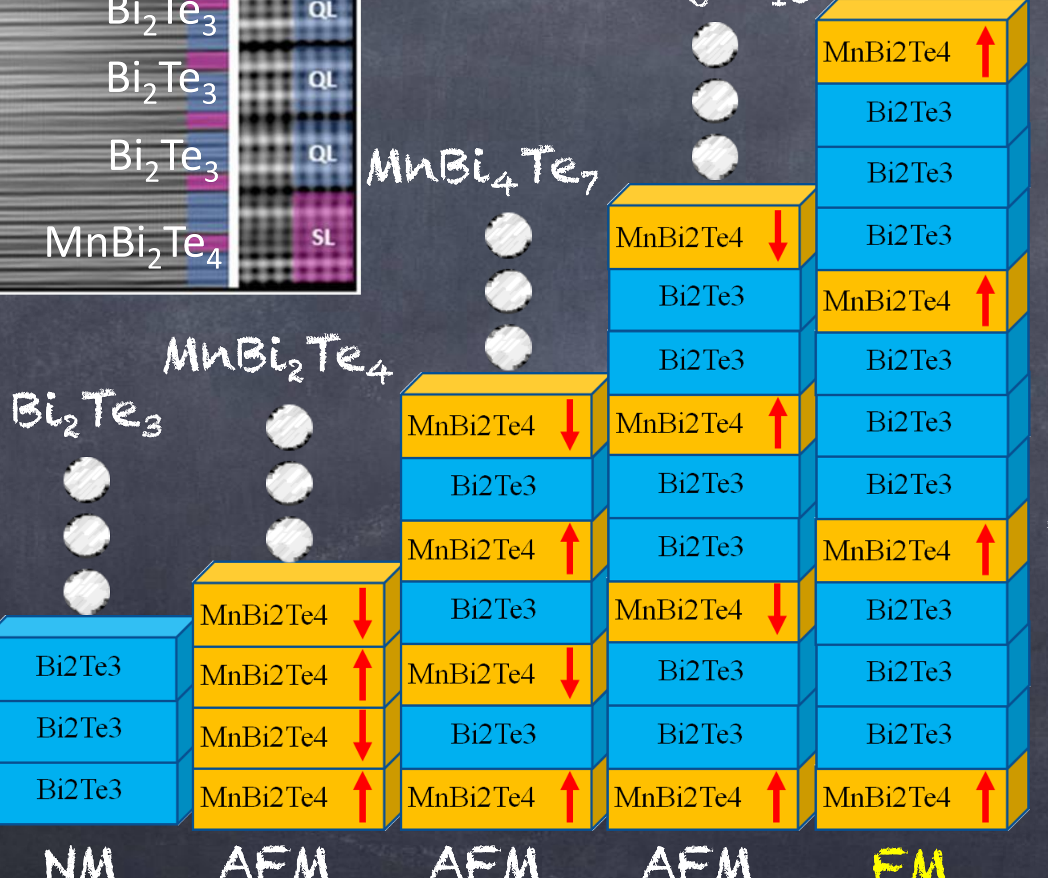


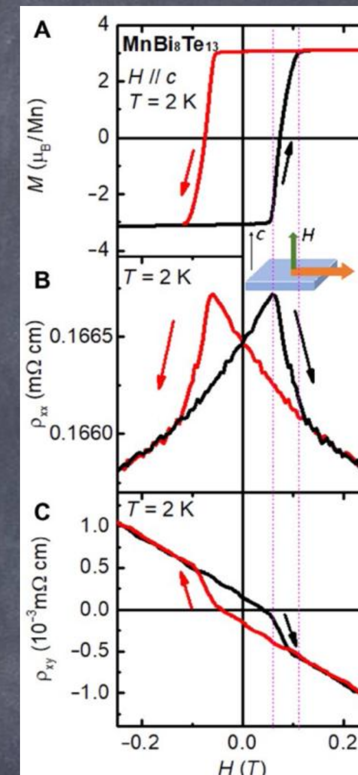
Ferromagnetic topological material: $MnBi_8Te_{13}$ (MBT-1813)

Science advances 6, eaba4275 (2020)

TEM: $MnBi_8Te_{13}$







Topological invariant

$$Z_4 = \sum_{i=1}^{8} \sum_{n=1}^{occ} \frac{1+\eta_n(\Gamma_i)}{2} mod4 = 2$$

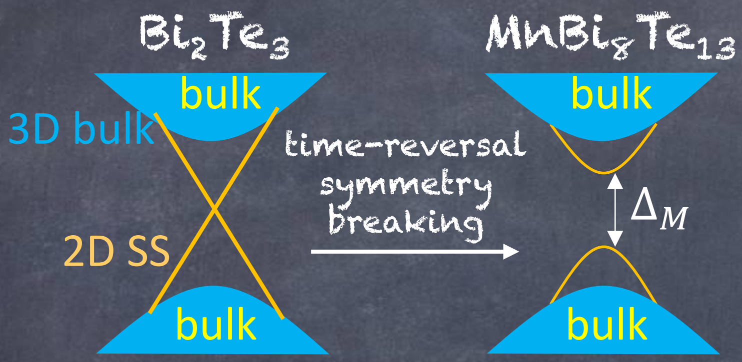
FM axion insulator!
(軸子絕緣體)

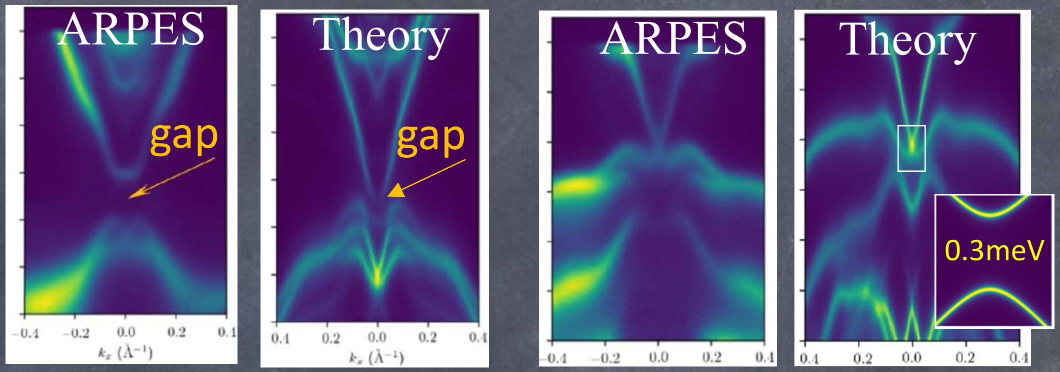
Axion insulator: $MnBi_8Te_{13}$

Science advances 6, eaba4275 (2020)
Phys. Rev. B 104, 054422 (2021)
Nature 595, 521 (2021)

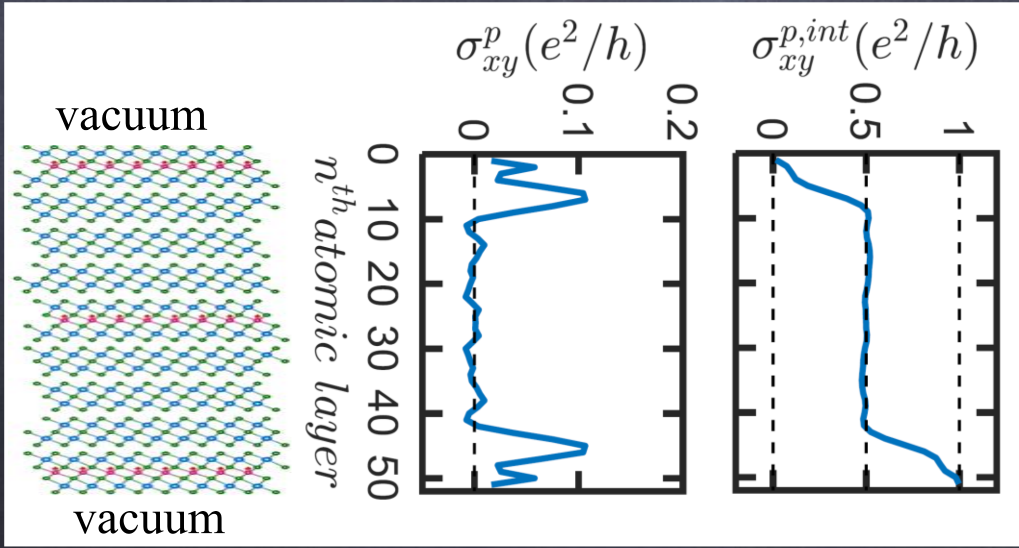
Expected observations in axion insulator:

(1) Gapped surface states for all terminations





(2) Half-integer surface Hall conductivity



$$\vec{J}_\theta = \frac{e^2}{2\pi h}\frac{\partial\theta}{\partial z}\hat{z}\times\vec{E} = \sigma\hat{z}\times\vec{E}$$

at the surface $\frac{\partial\theta}{\partial z} = \pi\delta(z_0)$

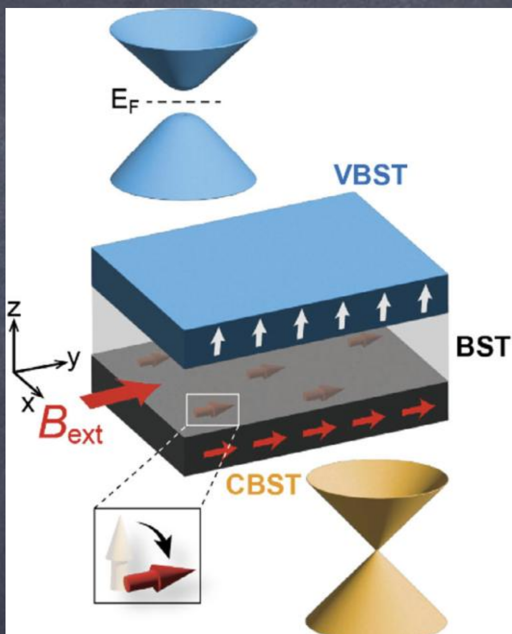
$$\Rightarrow \sigma_H^{surf} = \frac{e^2}{2\pi h}\pi = \frac{1}{2}\frac{e^2}{h}$$

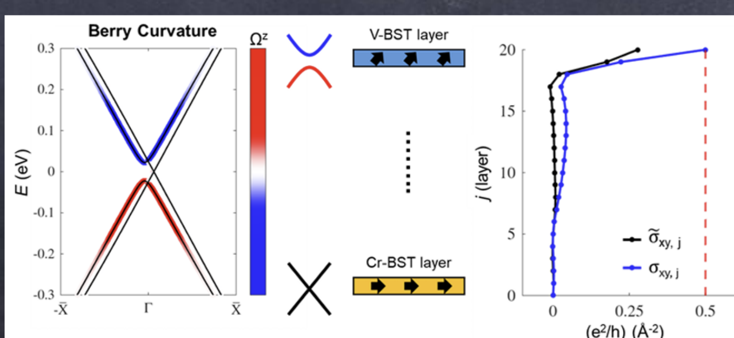
Ref: PRB 98, 115108 (2018)
Ref: PRB 98, 245117 (2018)

Unique phenomena in magnetic TI

Single Dirac cone (parity anomaly ?)

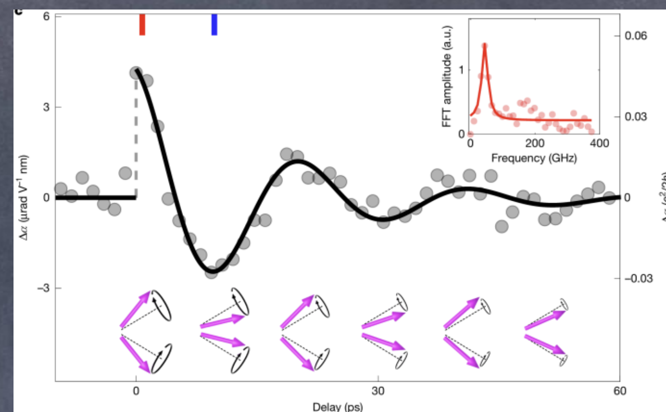
Advanced Materials 38, e10754 (2026)

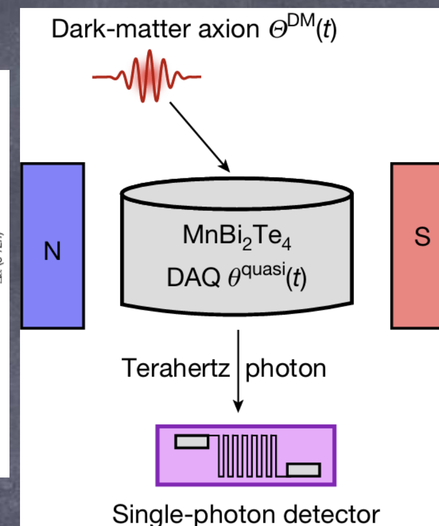


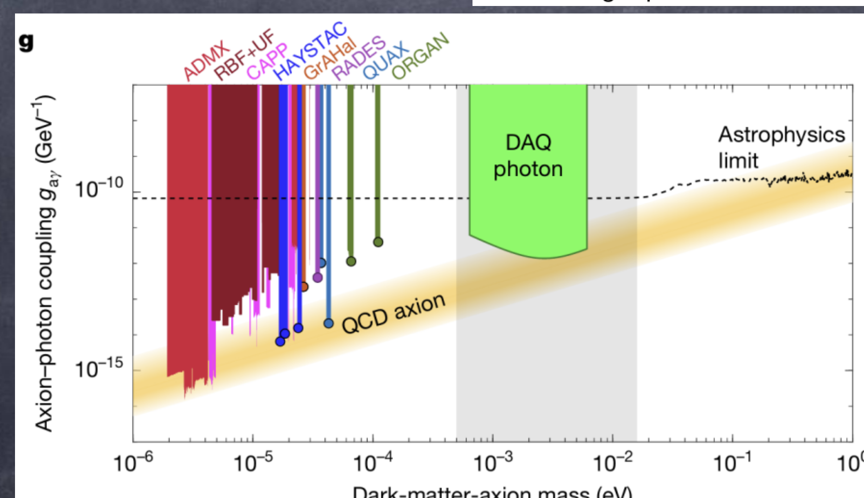


Dynamical axion quasiparticle (axion detector ?)

Nature 641, 62 (2025)







Outline

- Band theory

  Band structures: Bulk states, surface states

- Topological band theory

  Basic concepts and properties of topological band structure

- Topological insulators (Non-magnetic)

  Strong topological insulators

  Weak topological insulators

  topological crystalline insulators

- Topological insulators (magnetic)

  Ferromagnetic topological insulators (axion insulators)

- Orbital Hall effect

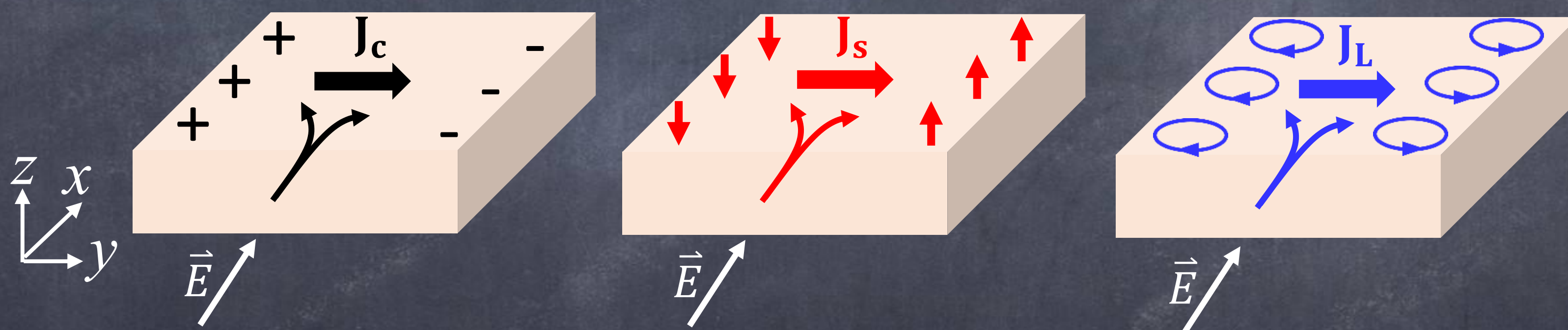
  Feature spectrum topology

  Orbital Chern insulators

Hall effect (metal)

		Ref: Science 306, 1910 (2004) Ref: PRL 94, 047204 (2005)	Ref: Nature 619, 52 (2023)
Degree of freedom	e^- Charge	$\hat{S}_i$ Spin	$\hat{L}_i$ Orbital
Hall responses	(Anomalous) Hall effect	Spin Hall effect	Orbital Hall effect

Metal



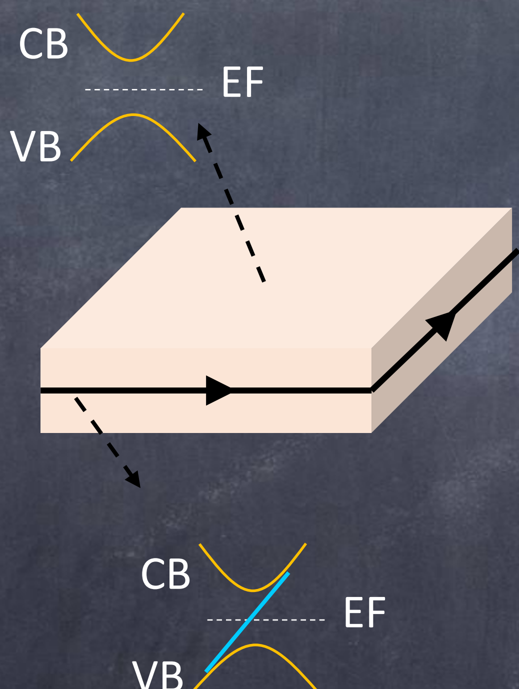
Hall effect (insulator)

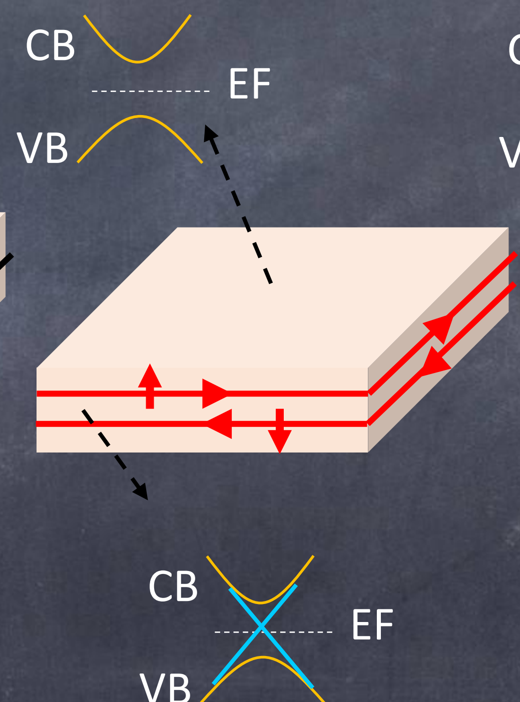
Ref: PRL 61, 2015 (1988)

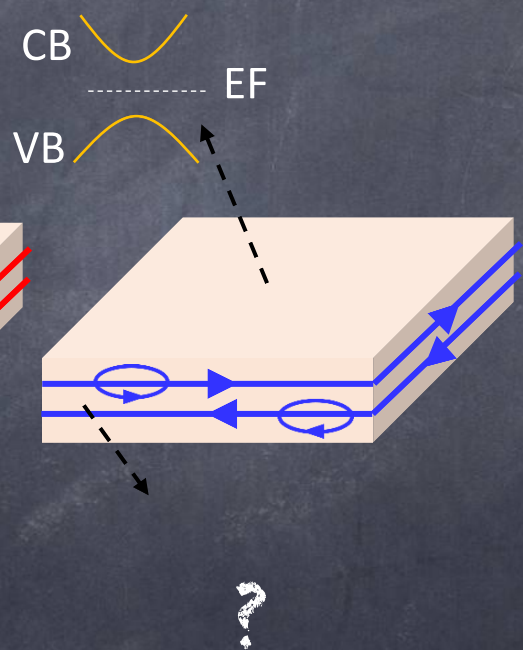
Ref: PRL 95, 226801 (2005)
Ref: PRL 95, 146802 (2005)

Topological state	Chern insulator	2D Topological insulator (Spin Chern insulator)	Orbital Chern insulator This work

Insulator







Topological invariants	C	$C_s, \mathbb{Z}_2$	$C_L = ?$

Feature Spectrum Topology

Ref: E. Prodan PRB 80, 125327 (2009)
Ref: H. Lin et al. Communications Physics (2026)
YT Yao et al., PRB 109, 155143 (2024)

$$\widehat{\mathbb{F}}_O|\tilde{\phi}_{mk}\rangle = (P\hat{O}P)|\tilde{\phi}_{mk}\rangle = O_{mk}|\tilde{\phi}_{mk}\rangle$$

$\widehat{\mathbb{F}}_O =$ feature operator

$\hat{O} =$ operator, e.g. $\hat{S}_z$, $\hat{L}_z \cdots$

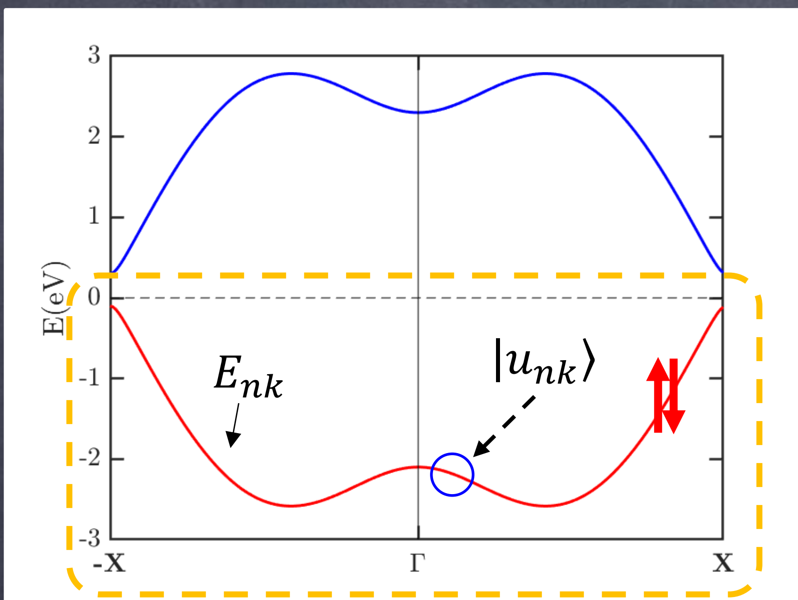
$P =$ projector $= \sum_{n \in occ.} |u_{nk}\rangle\langle u_{nk}|$ ← Bloch wavefunction of valence bands

Feature Spectrum Topology

Ref: E. Prodan PRB 80, 125327 (2009)
Ref: H. Lin et al. Communications Physics (2026)
YT Yao et al., PRB 109, 155143 (2024)

$$\widehat{\mathbb{F}}_O|\tilde{\phi}_{mk}\rangle = (P\hat{O}P)|\tilde{\phi}_{mk}\rangle = O_{mk}|\tilde{\phi}_{mk}\rangle$$

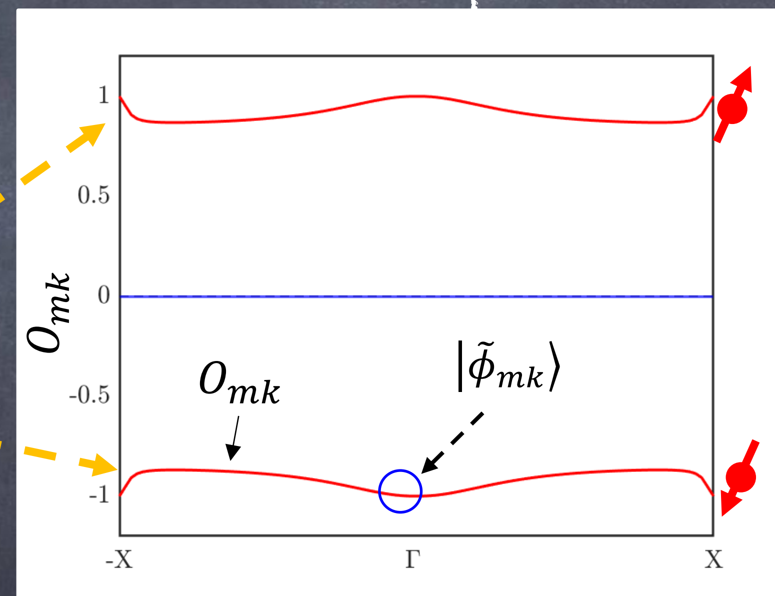
Band structure



Feature operator

$\widehat{\mathbb{F}}_O = (P\hat{S}_z P)$

Feature spectrum



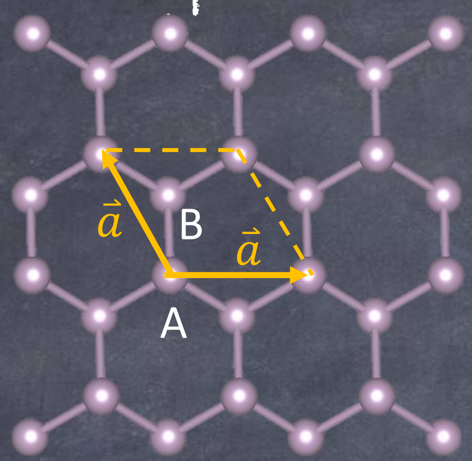
Topological invariant : Orbital Chern number

$$\widehat{\mathbb{F}}_{L_z} = P\hat{L}_z P \quad \Rightarrow \quad C_L = \frac{C_L^{\mathbb{I}+} - C_L^{\mathbb{I}-}}{2}$$

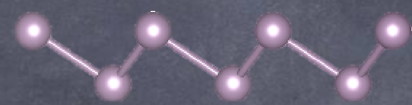
Orbital Chern number

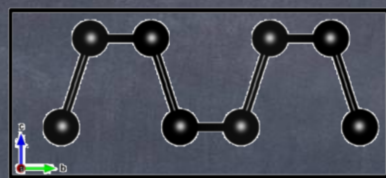
YT Yao et al., Rep. Prog. Phys. 89, 018001 (2026)

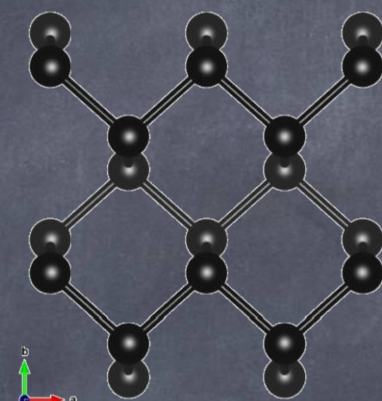
Phosphorene



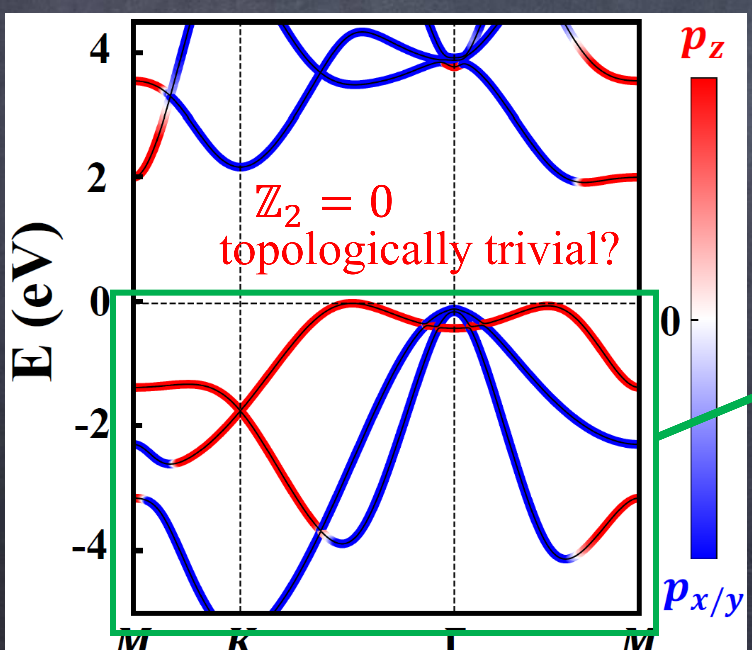
side view



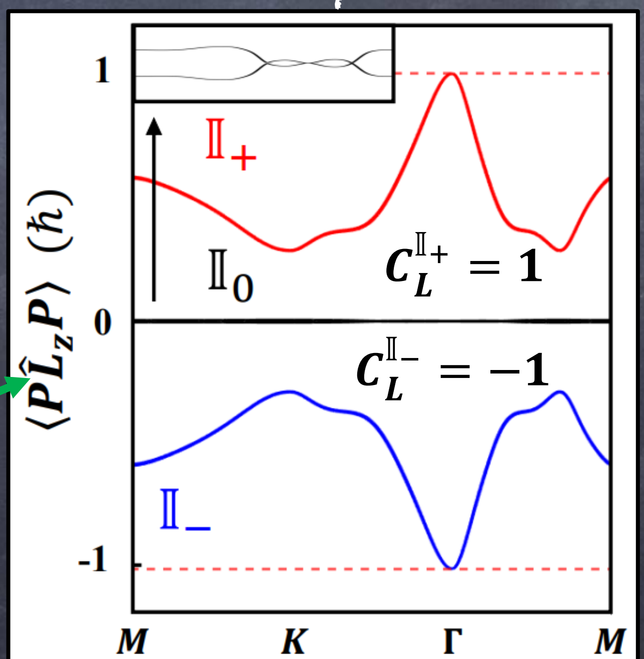




Band structure



Feature spectrum



Feature operator:

$$\widehat{\mathbb{F}}_{L_z} = P\hat{L}_z P$$

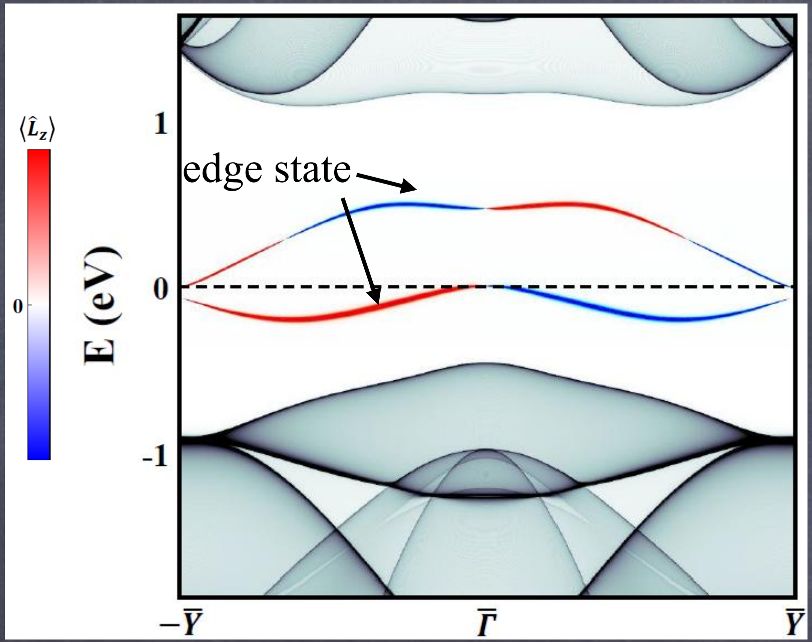
Orbital Chern number:

$$C_L = \frac{C_L^{\mathbb{I}_+} - C_L^{\mathbb{I}_-}}{2} = 1$$

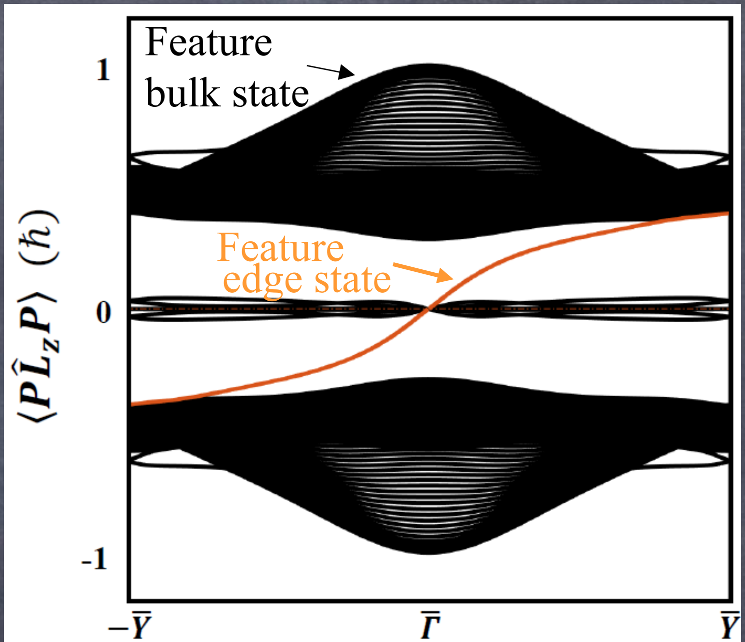
Bulk-Boundary Correspondence

YT Yao et al., Rep. Prog. Phys. 89, 018001 (2026)

Edge band structure



Edge feature spectrum



$$\mathbb{Z}_2 = 0$$

$$C_L = \frac{C_L^{\mathbb{I}_+} - C_L^{\mathbb{I}_-}}{2} = 1$$

Feature - energy duality: $C_L = 0 + 1$

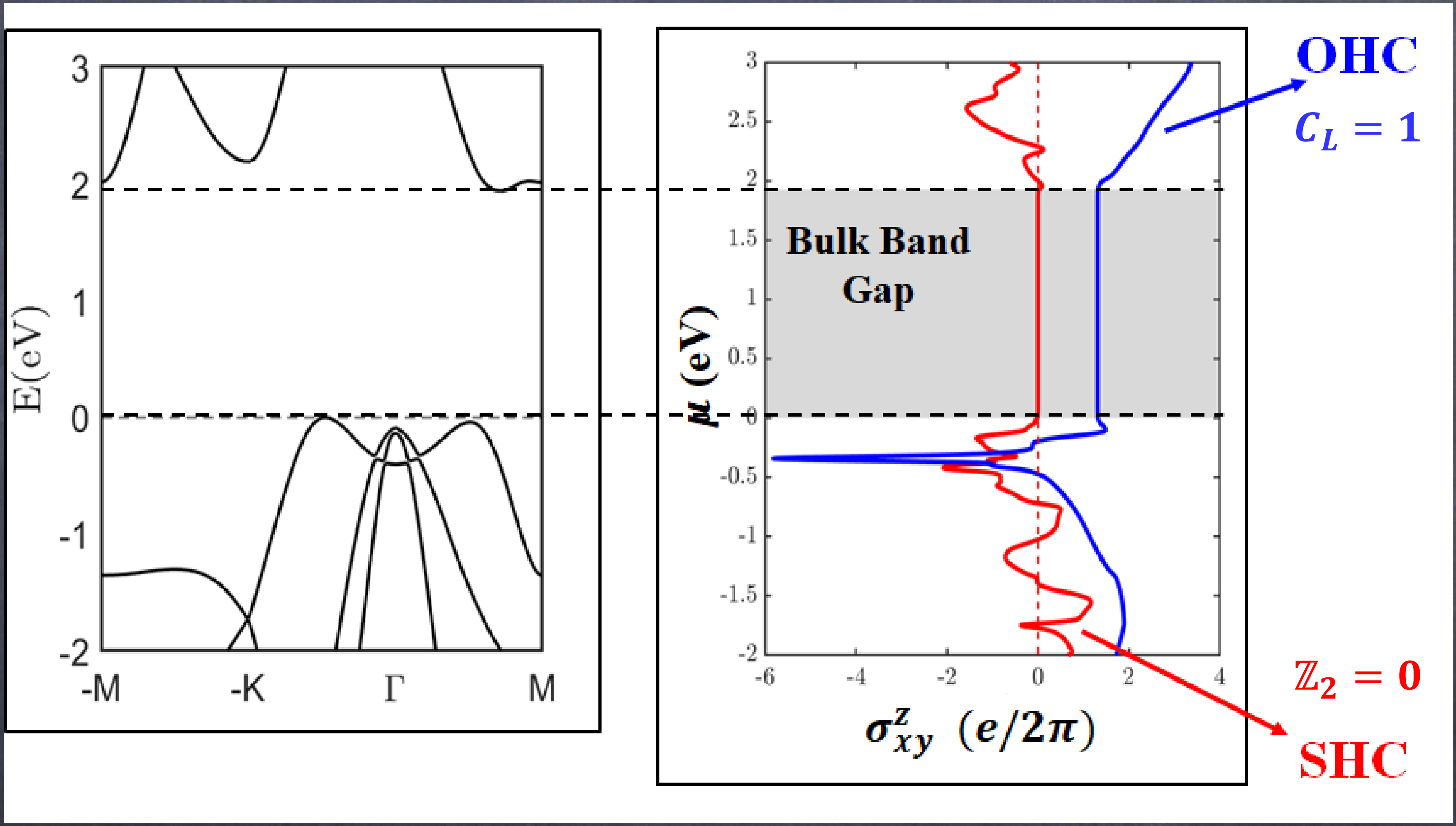
YT Yao et al., PRB109, 155143 (2024)

Gapless edge states in band structure

Gapless edge states in feature spectrum

Orbital Hall conductivity

YT Yao et al., Rep. Prog. Phys. 89, 018001 (2026)



Orbital Chern insulator

Conclusion

Band inversion

odd

Nonmagnetic:
Strong TI (Z_2=1)
Magnetic:
AFM-TI (Z_2=1;S-symmetry)

even

$Z_2 \neq 0$
$Z_4 \neq 0$
...etc

Nonmagnetic:
Weak TI (Z_2=(0;0,0,1))
Magnetic:
FM axion (Z_4=2)

Z_2=0
Z_4=0
...etc

Additional symmetry

O

Non/Magnetic:
TCI (mirror)
Mirror Chern number
TCI (rotation)
Z_2 invariant for C_n rotation

X

Ordinary insulator

w/o symmetry

Feature Spectrum Topology
e.g. Orbital Chern insulator

Geometrical structure of electron wave function

$$Q_{\mu\nu} = g_{\mu\nu} - \frac{i}{2}\Omega_{\mu\nu}$$

Quantum geometry engineering: How to manipulate the geometric properties of electron wave function

Acknowledgements

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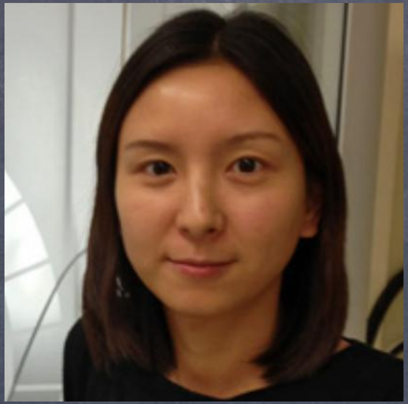

Su-Yang Xu
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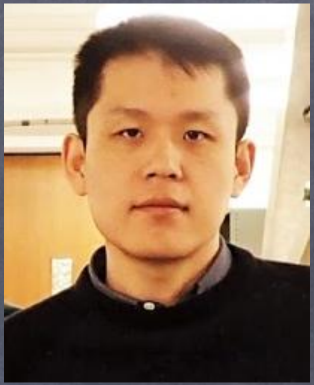

Kang L. Wang
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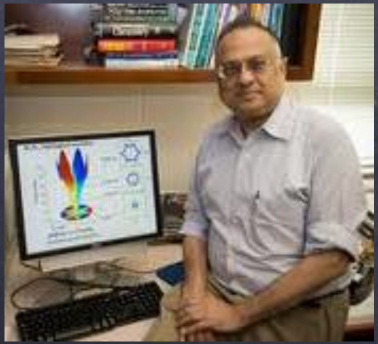

Hsin Lin
(Academia Sinica)

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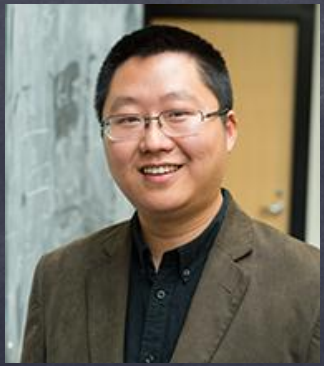
(MIT)



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林庭永

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廖俊德

Thank you !

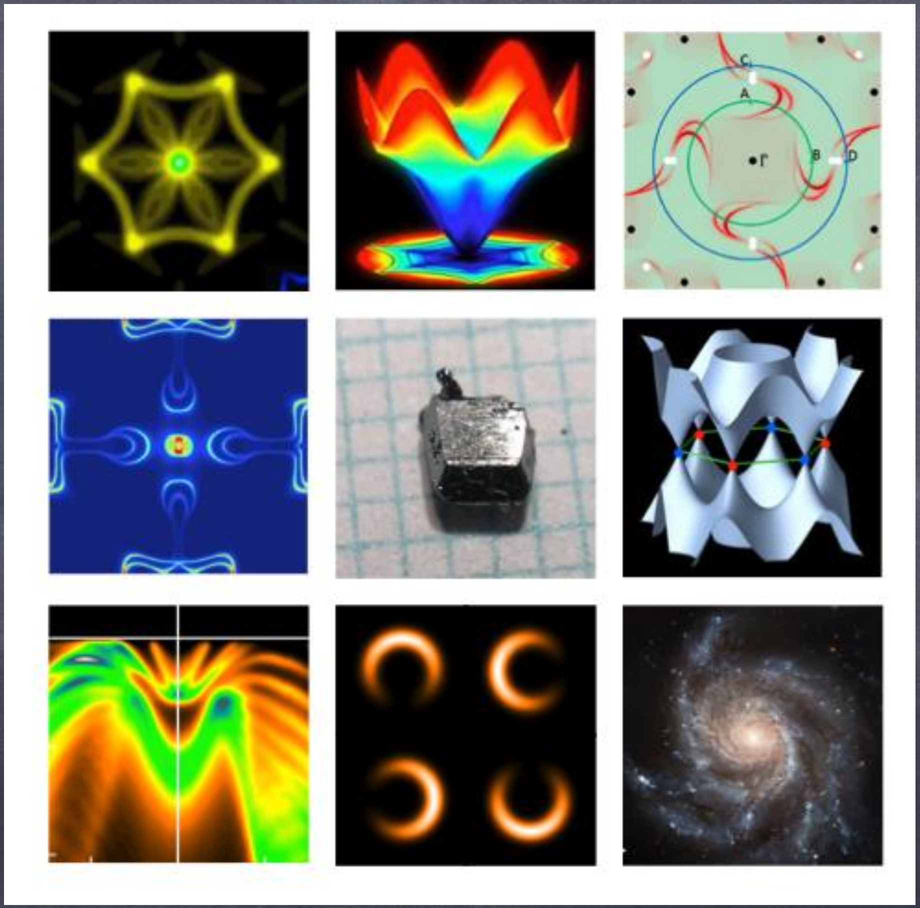
NSTC 國家科學及技術委員會
National Science and Technology Council

國立成功大學
National Cheng Kung University
1931

前沿量子科技研究中心
Center for Quantum Frontiers of Research & Technology

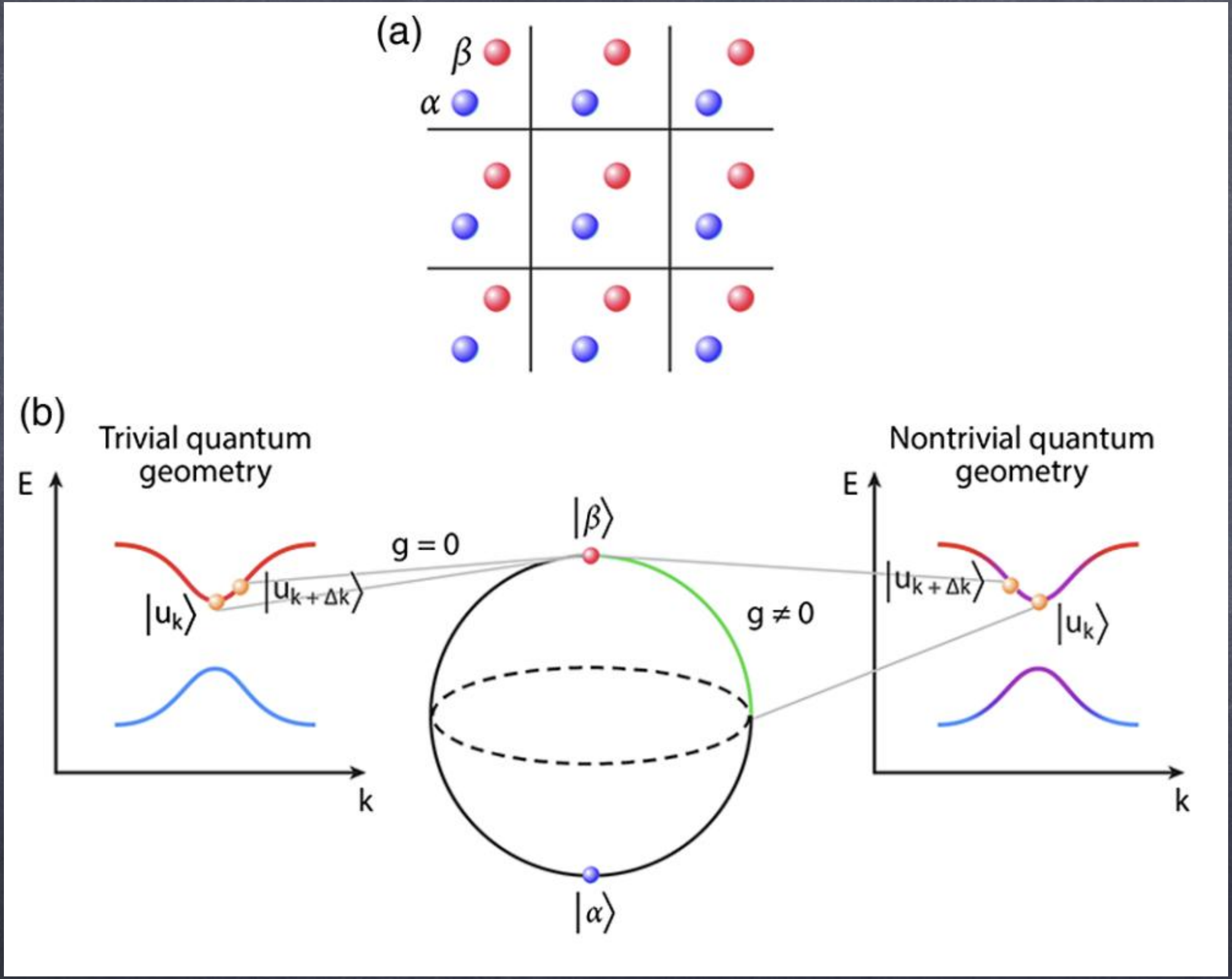
NCTS
Physics Division

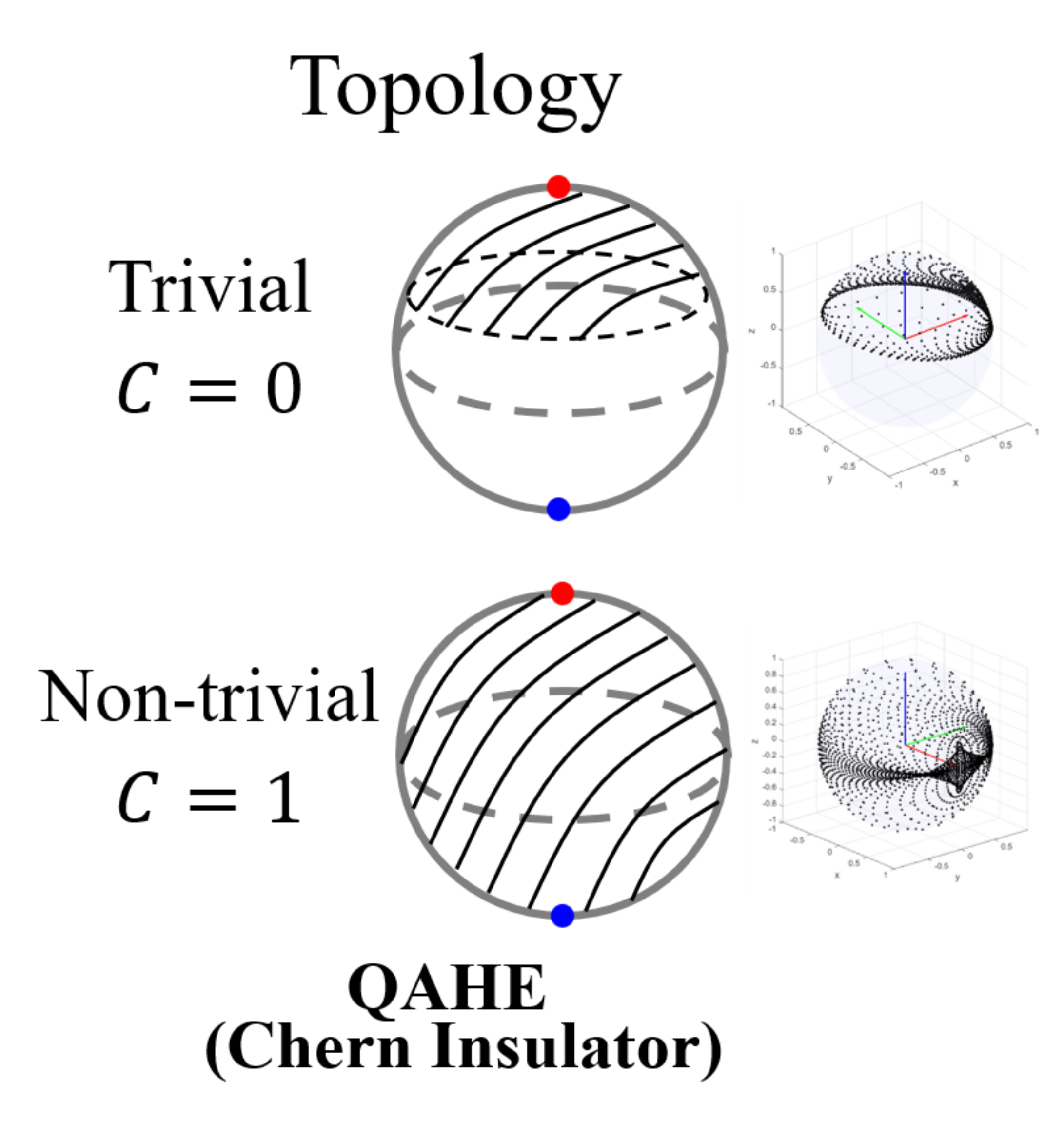
To see a world in a grain of sand … —William Blake



APPENDIX

Ref: Phys. Rev. Lett. 131, 240001 (2023)





毛球定理(Hairy ball theorem)

在偶數維的單位球面上，連續且處處不為零的切向量場是不存在的

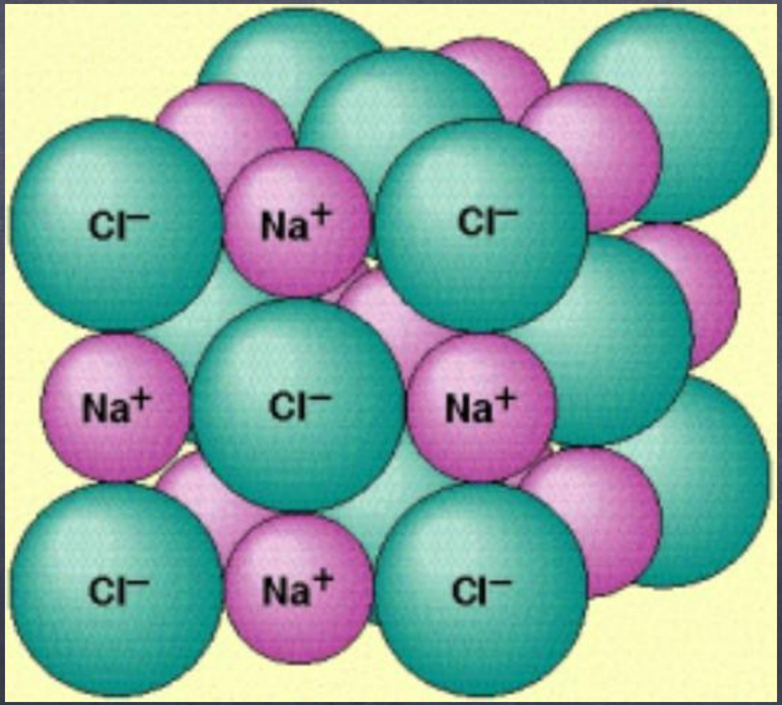
On the even-dimensional unit sphere, a continuous and everywhere non-zero tangent vector field does not exist.

Z2=0
E
Z2=0

Band theory (topology)

Practically...

Na+Cl → NaCl (Na^++Cl^-)



chemical bond order

Energy state

obey

Na^+

Cl^-

Topological trivial

Cl^-

violate

Na^+

Topological nontrivial

Vector of wavefunction is well-defined (smooth and continue) in the whole BZ

$$\oint \vec{A} dk = 0,$$

where $\vec{A} = i \left\langle u_k \middle| \vec{\nabla} \middle| u_k \right\rangle$

Brillouin zone

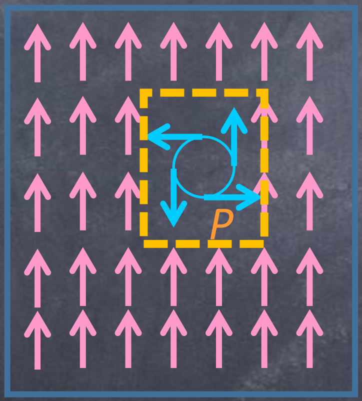
wavefunction is smooth

Vector of wavefunction is ill-defined in the whole BZ

$$\oint_{Bz-P} \vec{A}_1 dk - \oint_{P} \vec{A}_2 dk = 2\pi n,$$

where $n = 0,1,2,3 \ldots$

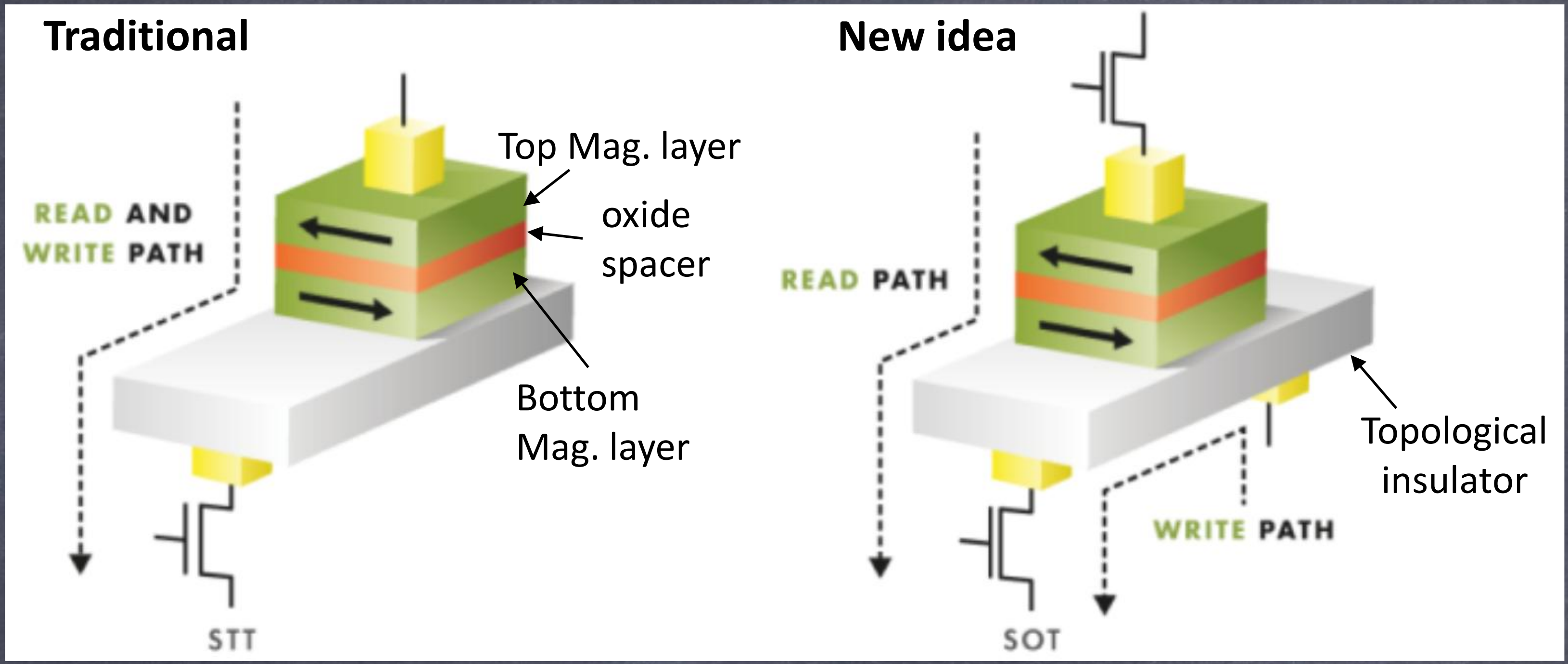
Brillouin zone

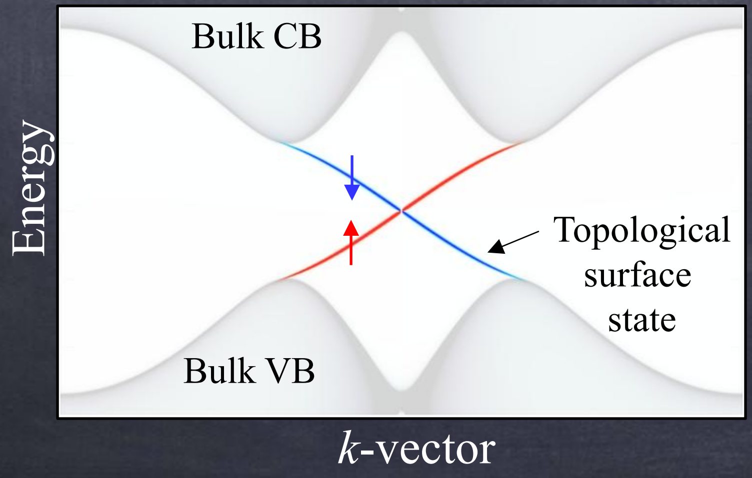


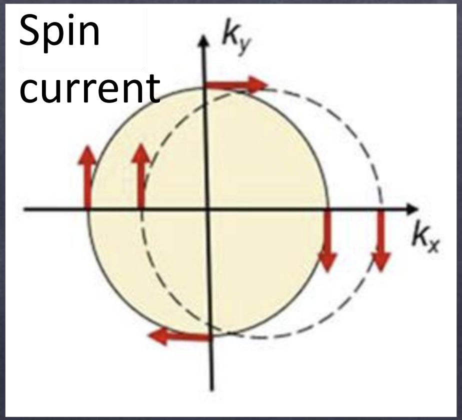
wavefunction is NOT smooth

Magnetic memory

Ref: EE Times, Gary Hilson 09.26.2021
Ref: Nat. Commun. 12, 6251 (2021)
Ref: APL Mater. 9, 060901 (2021)







Ferromagnetic topological material: $MnBi_8Te_{13}$

Ref: Phys. Rev. Lett. 58, 1799 (1987)
Ref: Phys. Rev. Lett. 102, 146805 (2009)

High energy field theory:

hypothetical particle to resolve the strong CP problem in QCD.

F. Wilczek (1987):

Axion electrodynamics Lagrangian $\Delta\mathcal{L}_{axion} = \kappa\theta = \frac{\theta e^2}{2\pi h}\vec{E}\cdot\vec{B}$ strength of axion field

Maxwell's equations with axion modifications:

$$\vec{\nabla}\cdot\vec{E} = \rho - \kappa(\vec{\nabla}\theta\cdot\vec{B}), \quad \vec{\nabla}\cdot\vec{B} = 0, \quad \vec{\nabla}\times\vec{E} = -\frac{\partial\vec{B}}{\partial t}, \quad \vec{\nabla}\times\vec{B} = \vec{J} + \frac{\partial\vec{E}}{\partial t} + \kappa(\vec{\nabla}\theta\times\vec{E} + \frac{\partial\theta}{\partial t}\vec{B}).$$

Condensed matter theory:

Free energy: $F = F_0 - P_i^s E_i - M_i^s B_i - \frac{1}{2}\epsilon_0\epsilon_{ij}E_iE_j - \frac{1}{2}\mu_0\mu_{ij}B_iB_j - \alpha_{ij}E_iB_j$

Polarization: $P_i = P_i^s + \epsilon_0\epsilon_{ij}E_j + \alpha_{ij}B_j$ Magnetization: $M_i = M_i^s + \mu_0\mu_{ij}B_j + \alpha_{ij}E_j$

Magnetoelectric coupling factor: $\alpha_{ij} = \tilde{\alpha}_{ij} + \frac{\theta e^2}{2\pi h}\delta_{ij}$

Insulator: $\theta = -\frac{1}{4}\int_{BZ} d^3k\epsilon^{ijk}Tr\left[\mathcal{A}_i\partial_j\mathcal{A}_k - i\frac{2}{3}\mathcal{A}_i\mathcal{A}_j\mathcal{A}_k\right]$

Normal insulator
$\theta = 0$

Axion insulator
$\theta = \pi$

Ferromagnetic topological material: $MnBi_8Te_{13}$

Science advances 6, eaba4275 (2020)
Phys. Rev. B 104, 054422 (2021)

(2) Half-integer surface Hall conductivity

Maxwell eq. in an axion insulator

$$\vec{\nabla}\cdot\vec{D} = \rho_f + \rho_\theta = \rho_f - \vec{\nabla}\alpha\cdot\vec{B} \quad \text{where } \alpha = \frac{e^2}{2\pi h}\theta$$

strength of axion field

$$\vec{\nabla}\cdot\vec{B} = 0$$

$$\vec{\nabla}\times\vec{E} = -\frac{\partial\vec{B}}{\partial t}$$

$$\vec{\nabla}\times\vec{H} = \vec{J}_f + \frac{\partial\vec{D}}{\partial t} + \vec{J}_\theta = \vec{J}_f + \frac{\partial\vec{D}}{\partial t} + \vec{\nabla}\alpha\times\vec{E} + \frac{\partial\alpha}{\partial t}\cdot\vec{B}$$

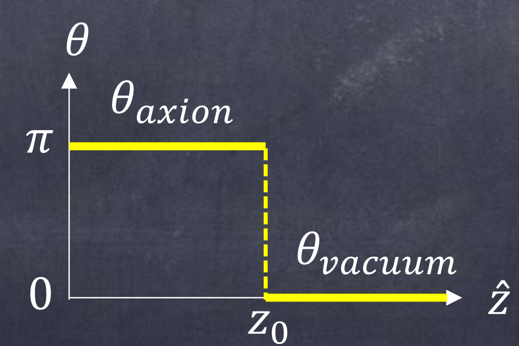
assume $\theta = \theta(z)$ is a step function, and $\vec{B} = 0$

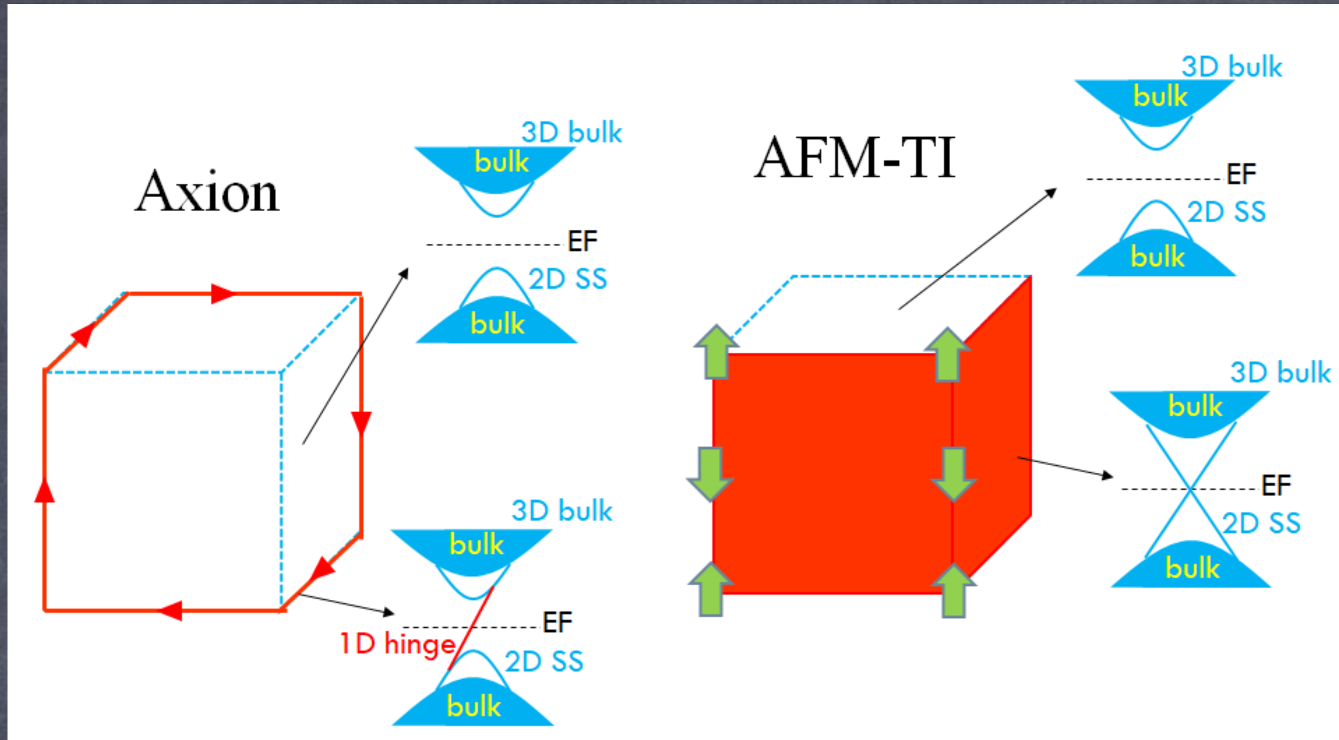
Ref: PRB 98, 115108 (2018)
Ref: PRB 98, 245117 (2018)

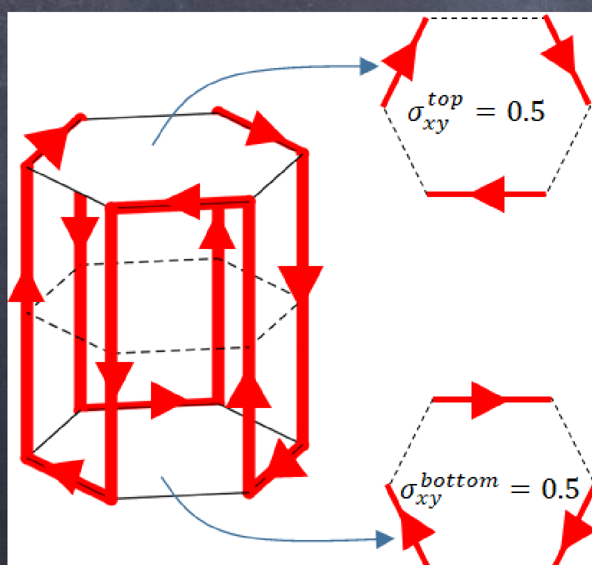
$$\vec{J}_\theta = \frac{e^2}{2\pi h}\frac{\partial\theta}{\partial z}\hat{z}\times\vec{E} = \sigma\hat{z}\times\vec{E}$$

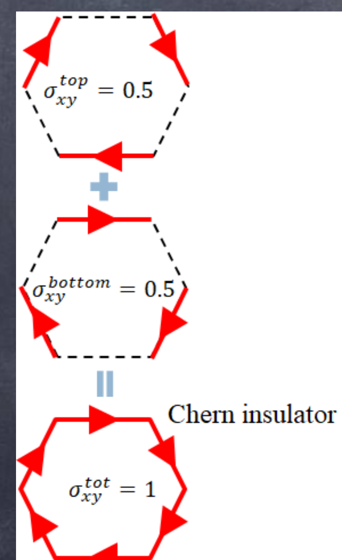
at the surface $\dfrac{\partial\theta}{\partial z} = \pi\delta(z_0)$

$$\Rightarrow \sigma = \sigma_H^{surf} = \frac{e^2}{2\pi h}\pi = \frac{1}{2}\frac{e^2}{h}$$



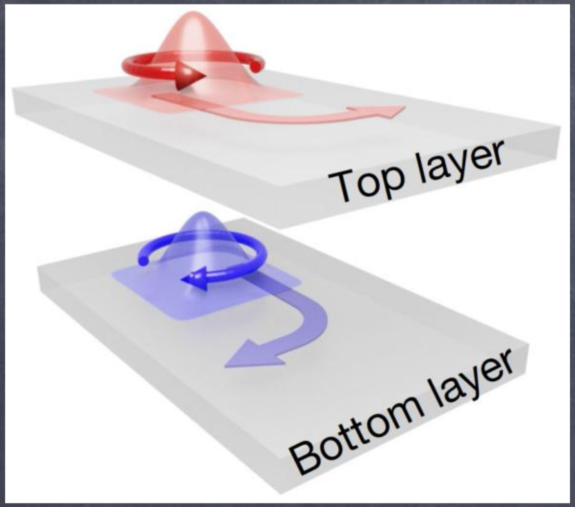

Axion
3D bulk
bulk
EF
2D SS
bulk
3D bulk
bulk
EF
1D hinge
2D SS
bulk
AFM-TI
3D bulk
bulk
EF
2D SS
bulk
3D bulk
bulk
EF
2D SS
bulk

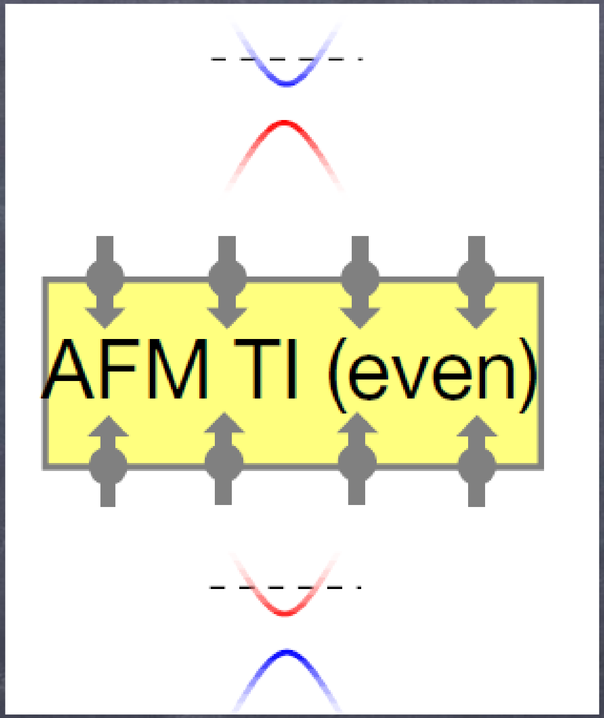

$\sigma_{xy}^{top} = 0.5$
$\sigma_{xy}^{bottom} = 0.5$

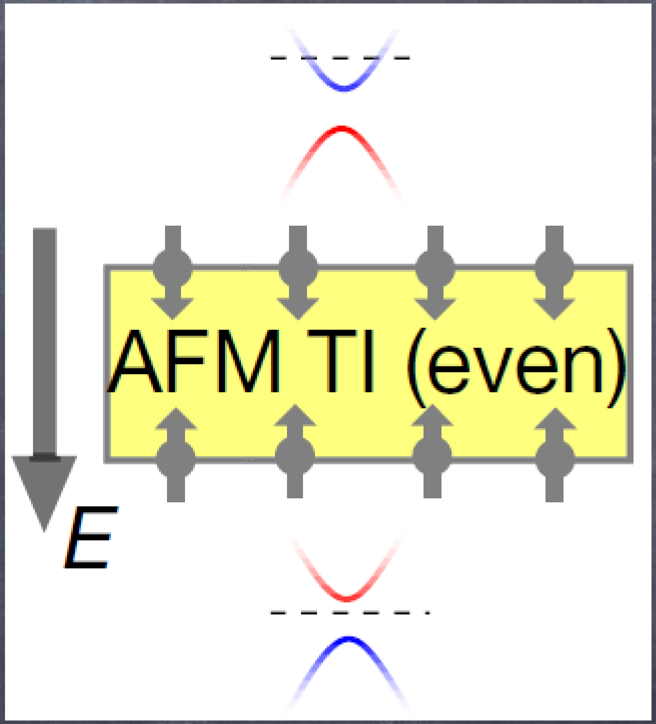

$\sigma_{xy}^{top} = 0.5$
$\sigma_{xy}^{bottom} = 0.5$
Chern insulator
$\sigma_{xy}^{tot} = 1$

Nature 595, 521 (2021)

Layer Hall effect
(AFM-TI, $MnBi_2Te_4$)



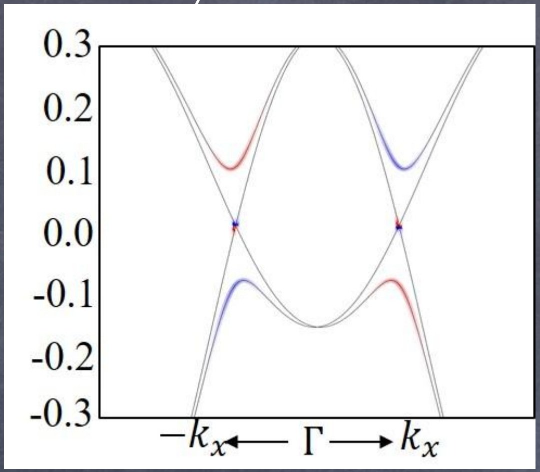


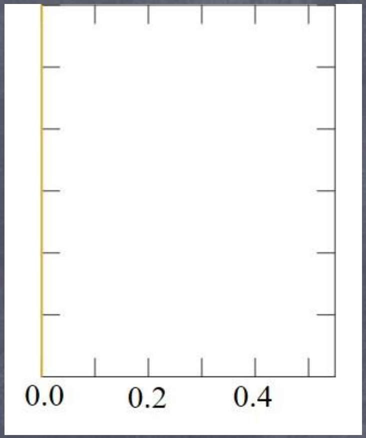


Parity anomaly

$c_7 = 0.0$

Bi/SnSe





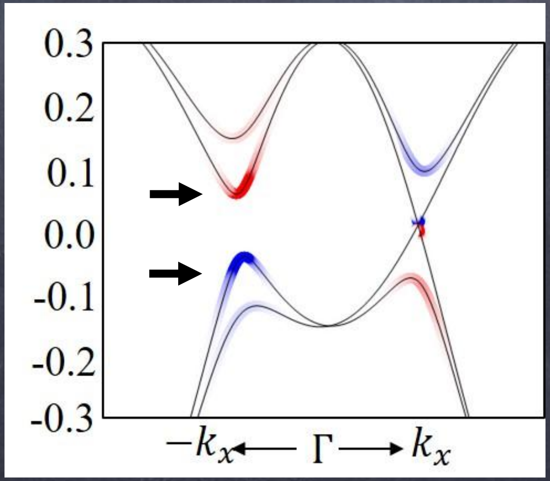
$\sigma_{xy} = 0$

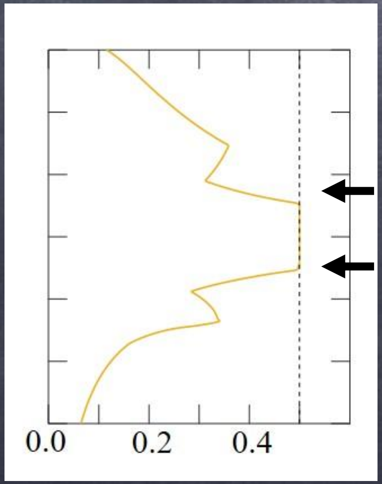
Berry curvature Ω_z

$c_7 = 0.015$

$\sigma_{xy}(e^2/h)$

Bi/SnSe+FL





$\sigma_{xy} = \frac{1}{2}\frac{e^2}{h}$

Topology: non-conserved quantity

YT Yao et al., PRB109, 155143 (2024)

S_z conserve

$$H_0 = \begin{array}{c} \\ \\ \end{array}\begin{array}{cc} |\uparrow\rangle & |\downarrow\rangle \\ \begin{pmatrix} H_{QAH}^{+} & 0 \\ 0 & H_{QAH}^{-} \end{pmatrix} & \end{array}\begin{array}{l} \text{Basis} \\ |\uparrow\rangle \\ |\downarrow\rangle \end{array}$$

H_{QAH} Haldane Hamiltonian (2x2 matrix)

Spin-up Chern number

$$H_{QAH}^{+} \Rightarrow \sum_{m=occ} \int_{BZ} d^2k\, \Omega_m^{\uparrow}(k) = C_s^{\uparrow} = 1$$

Spin-down Chern number

$$H_{QAH}^{-} \Rightarrow \sum_{m=occ} \int_{BZ} d^2k\, \Omega_m^{\downarrow}(k) = C_s^{\downarrow} = -1$$

Spin Chern number (C_s) : $C_s = \dfrac{(C_s^{\uparrow} - C_s^{\downarrow})}{2} = 1$

S_z non-conserve

$$H_M = \begin{array}{cc} |\uparrow\rangle & |\downarrow\rangle \\ \begin{pmatrix} H_{QAH}^{+} & -H_R \\ H_R & H_{QAH}^{-} \end{pmatrix} & \end{array}\begin{array}{l} \text{Basis} \\ |\uparrow\rangle \\ |\downarrow\rangle \end{array}$$

Rashba SOC

H_{QAH} Haldane Hamiltonian

$|\uparrow\rangle_{VB}$ and $|\downarrow\rangle_{VB}$ mixed

How do we define topological invariants?

To separate the mixed non-conserved degrees of freedom in the valence band

Feature Spectrum Topology

Ref: E. Prodan PRB 80, 125327 (2009)
Ref: H. Lin arXiv:2310.14832v1 (2023)
YT Yao et al., PRB109, 155143 (2024)

Feature operator

$$\widehat{\mathbb{F}}_O|\tilde{\phi}_{mk}\rangle = (P\hat{O}P)|\tilde{\phi}_{mk}\rangle = O_{mk}|\tilde{\phi}_{mk}\rangle$$

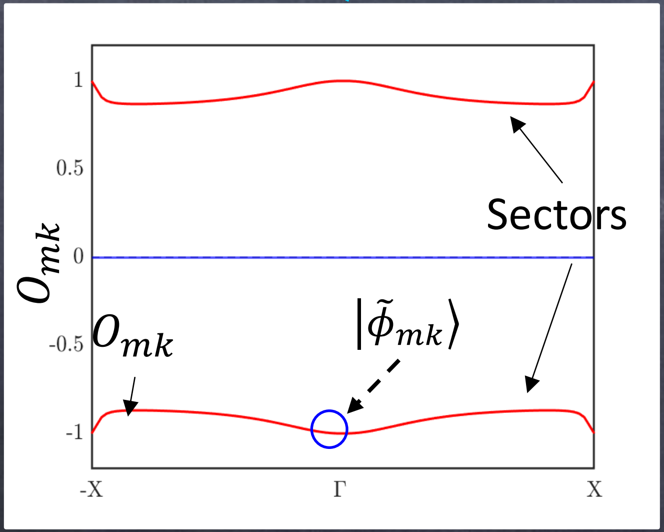
$\hat{O}$ = operator, e.g. $\hat{S}_z$, $\hat{L}_z \cdots$ Projector: $P = \sum_{n\in occ.} |u_{nk}\rangle\langle u_{nk}|$

Bloch wavefunction of valence bands

Feature eigenvalue $= O_{mk}$

Feature Bloch state $= |\tilde{u}_{mk}\rangle = P|\tilde{\phi}_{mk}\rangle = \sum_{n\in occ.} \langle u_{nk}|\tilde{\phi}_{mk}\rangle\, |u_{nk}\rangle$

Feature spectrum



Topological invariant :
Feature Chern number

Feature Spectrum Topology ($\hat{S}_z$)

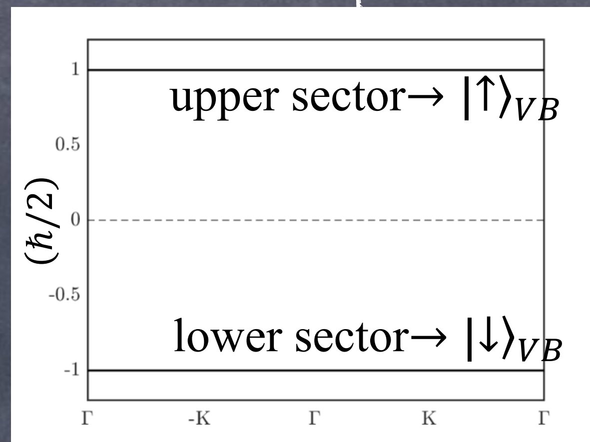
YT Yao et al., PRB109, 155143 (2024)

Feature operator: $\widehat{\mathbb{F}}_O = P\hat{O}P \Rightarrow \widehat{\mathbb{F}}_{S_z} = P\hat{S}_zP$

S_z conserve

$$\begin{array}{cccc} & |\uparrow\rangle & |\downarrow\rangle & \text{Basis} \\ H_0 = & \left(\begin{array}{c} H_{QAH}^{+} \\ 0 \end{array}\right. & \left.\begin{array}{c} 0 \\ H_{QAH}^{-} \end{array}\right) & \begin{array}{c} |\uparrow\rangle \\ |\downarrow\rangle \end{array} \end{array}$$

Feature spectrum



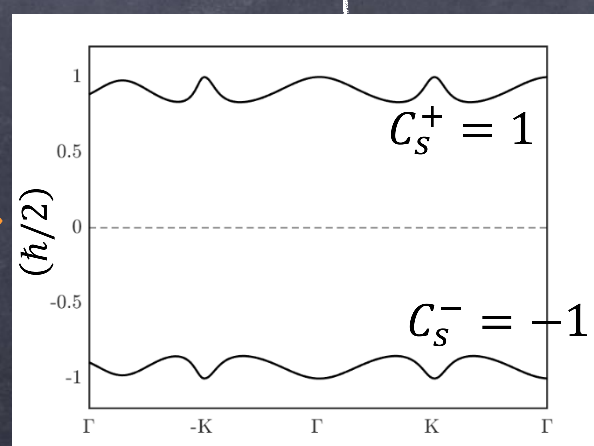
Eigenvalue of S_z (S_z conserve)

$$\hat{S}_z|\psi_{nk}\rangle = \pm\frac{\hbar}{2}|\psi_{nk}\rangle$$

S_z non-conserve

$$\begin{array}{cccc} & |\uparrow\rangle & |\downarrow\rangle & \text{Basis} \\ H_M = & \left(\begin{array}{c} H_{QAH}^{+} \\ H_R \end{array}\right. & \left.\begin{array}{c} -H_R \\ H_{QAH}^{-} \end{array}\right) & \begin{array}{c} |\uparrow\rangle \\ |\downarrow\rangle \end{array} \end{array}$$

Feature spectrum



Feature Chern number

$$C_s = \frac{(C_s^+ - C_s^-)}{2} = 1$$

Feature-energy duality

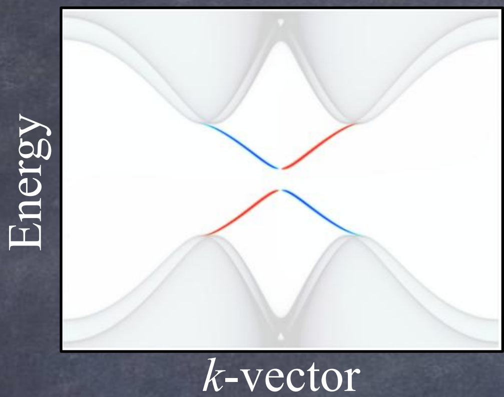
PRB109, 155143 (2024)

Band (w/o $\mathcal{T}$)

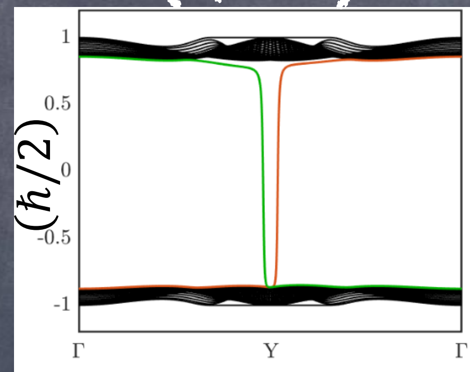
# of gapless edge states

Feature (w/o $\mathcal{T}$)

# of gapless edge states



0

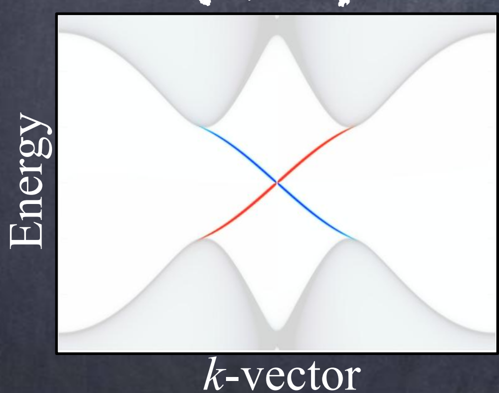


1

Spin Chern number

or

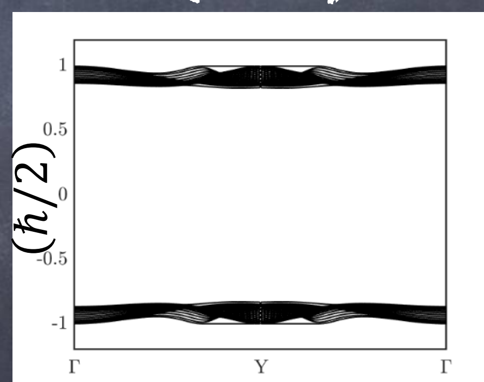
(w/ $\mathcal{T}$)



1

$+$

(w/ $\mathcal{T}$)



0

$=$

$$\begin{cases} C_s = 1 \\ C_s = 1 \end{cases}$$

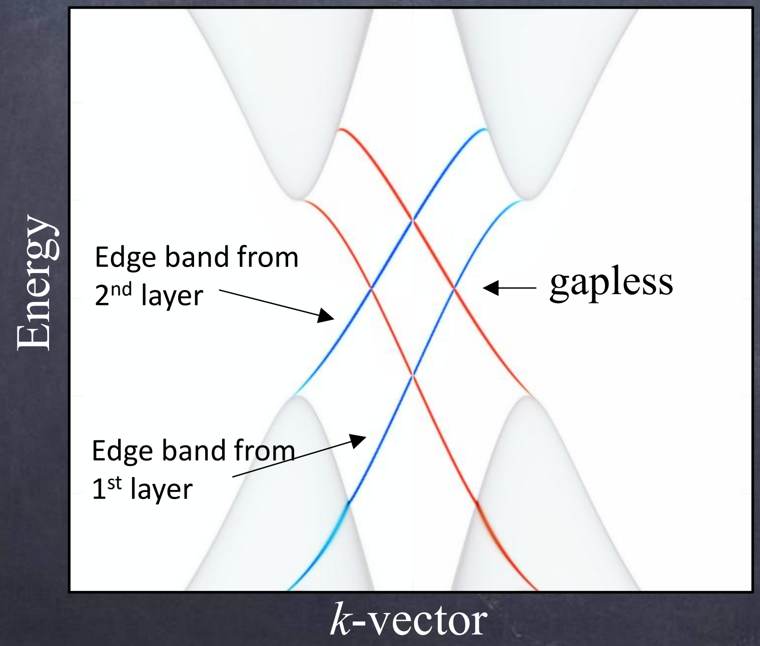
Feature-energy duality: Total number of gapless edge states on the band structure, combined with the non-trivial edge states in the feature spectrum, equals the spin Chern number of QSHI.

Bilayer Kane-Mele model

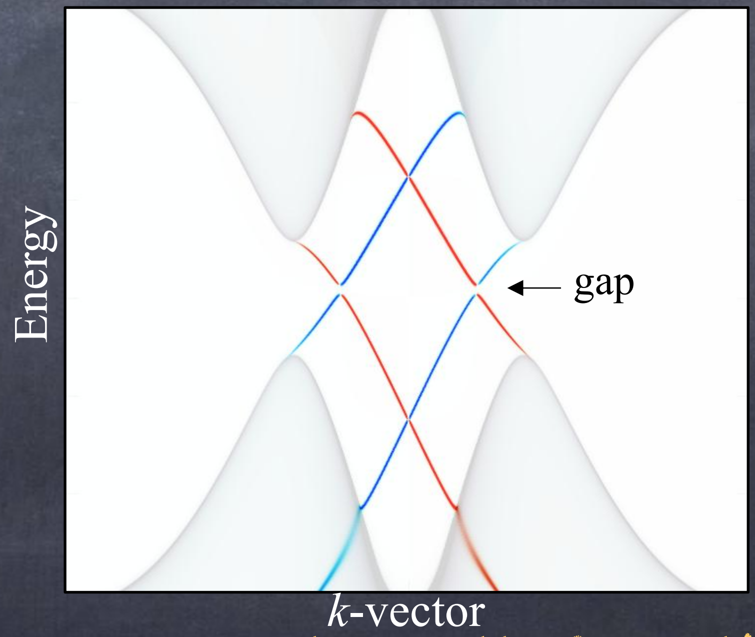
PRB109, 155143 (2024)

Bilayer Kane-Mele model (with interlayer coupling)

$$H_{Bilayer} = \underbrace{H_0}_{\text{Original Kane-Mele}} + \underbrace{t_l \sum_{il\alpha} \mu_i c^\dagger_{il\alpha} c_{i(l+1)\alpha}}_{\text{Interlayer coupling}} + t_o \sum_{il\alpha} \xi_l c^\dagger_{il\alpha} c_{il\alpha}$$



Interlayer coupling

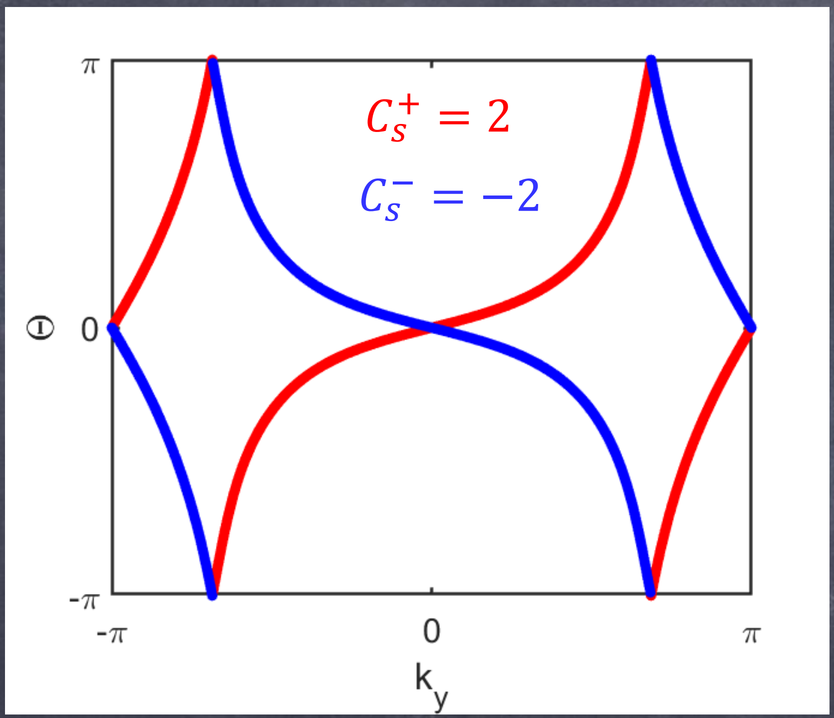


$\mathbb{Z}_2 = 0$, Topologically trivial!

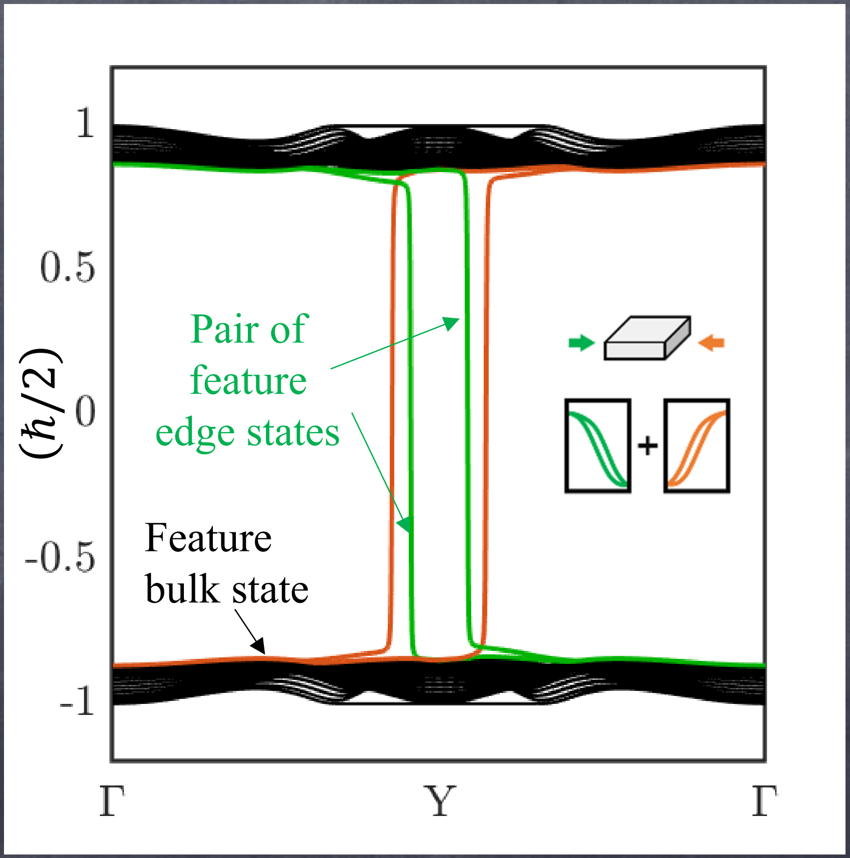
Feature Spectrum Topology

PRB109, 155143 (2024)

Wilson loop



Edge feature bands



Spin Chern number

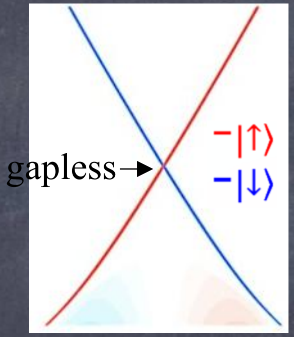
$$C_s = \frac{(C_s^+ - C_s^-)}{2} = 2$$

Material realization Bi_4Br_4

PRB109, 155143 (2024)

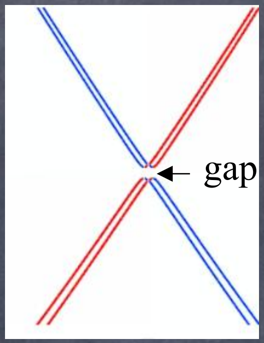
Monolayer Bi_4Br_4	Bilayer Bi_4Br_4	Trilayer Bi_4Br_4
$C_s = 1, \mathbb{Z}_2 = 1$	$C_s = 2, \mathbb{Z}_2 = 0$	$C_s = 3, \mathbb{Z}_2 = 1$

Bands



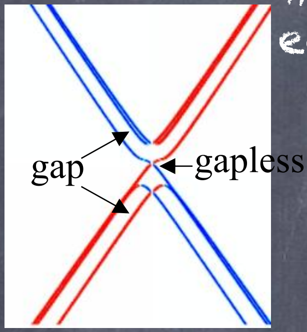
\# of gapless edge states

1



\# of gapless edge states

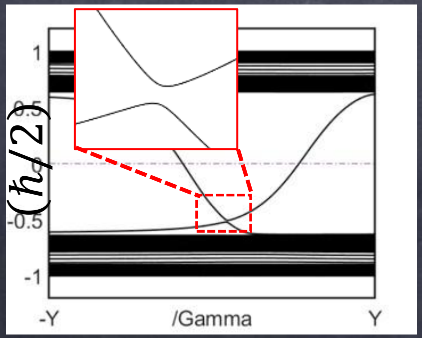
0



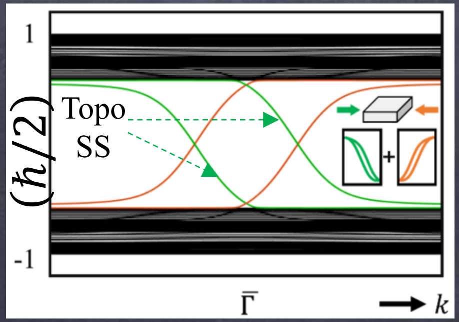
\# of gapless edge states

1

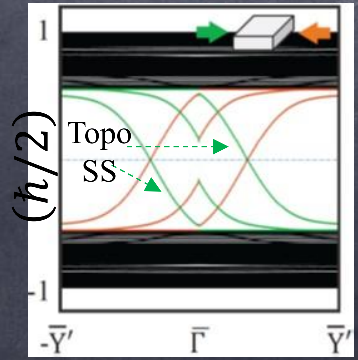
Feature



0



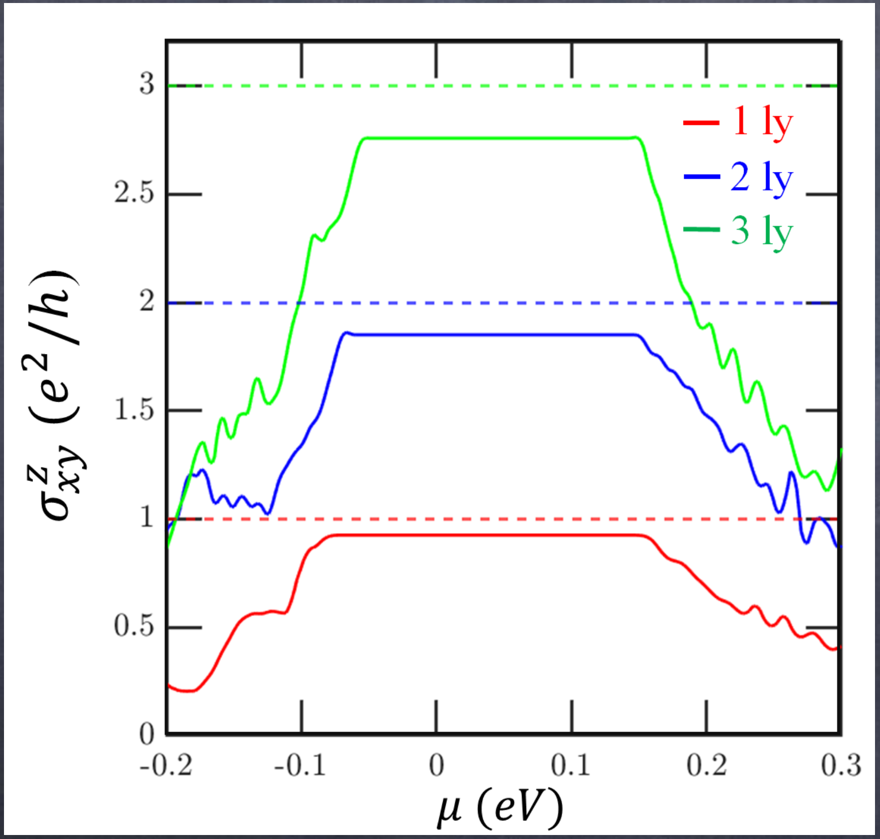
2



2

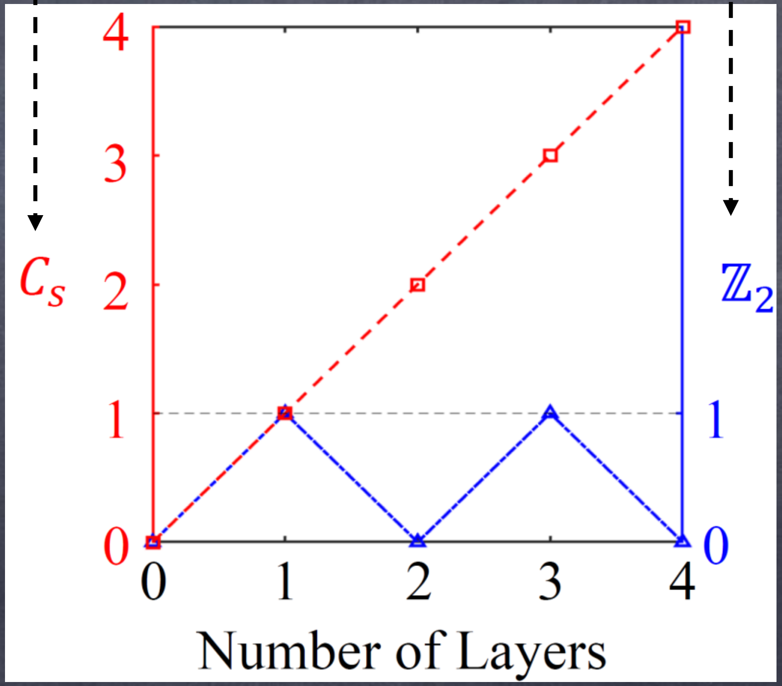
Material realization Bi_4Br_4

Spin Hall conductivity (layered Bi_4Br_4) based on standard Kubo formula



From feature eigenstates

From Bloch wavefun



Feature (orbital) Chern number

YT Yao et al., Rep. Prog. Phys. 89, 018001 (2026)

Spherical harmonics $Y_{l,m}$

$p_x \propto Y_{1,1} + Y_{1,-1}$

$p_y \propto i(Y_{1,1} - Y_{1,-1})$

$p_z \propto Y_{1,0}$

Feature operator:

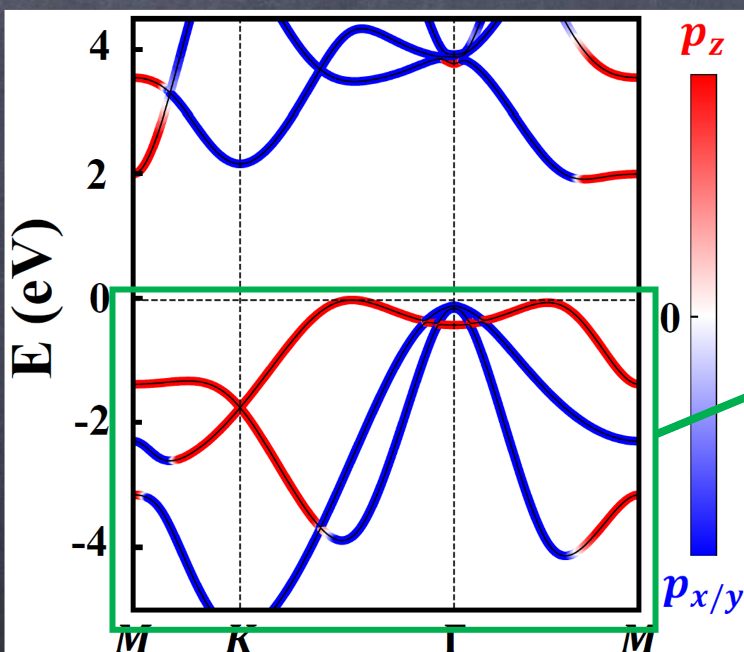
$$\hat{\mathbb{F}}_{L_z} = P\hat{L}_z P$$

Eigenvalue of L_z (L_z conserve)

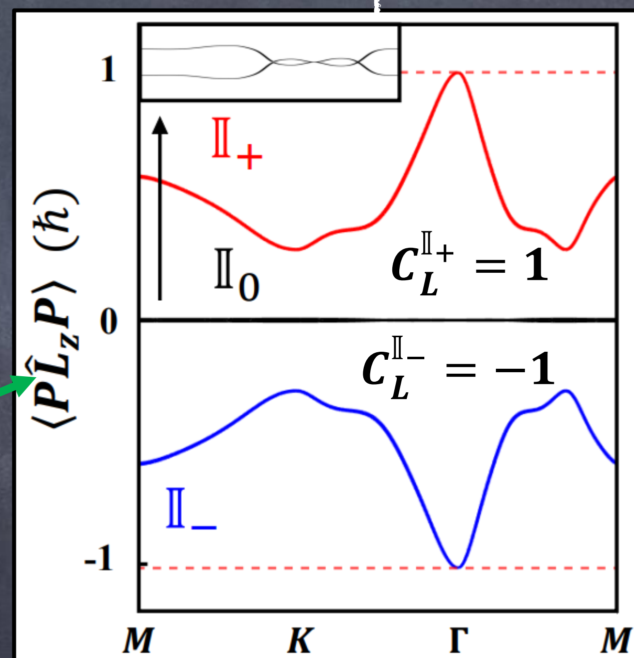
$$\hat{L}_z|\psi_{nk}\rangle = m\hbar|\psi_{nk}\rangle$$

$$m = 1, 0, -1$$

Band structure



Feature spectrum

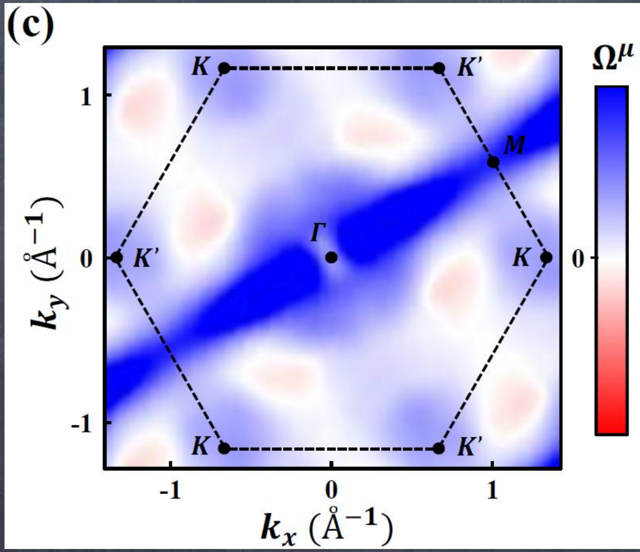


Feature (orbital) Chern number:

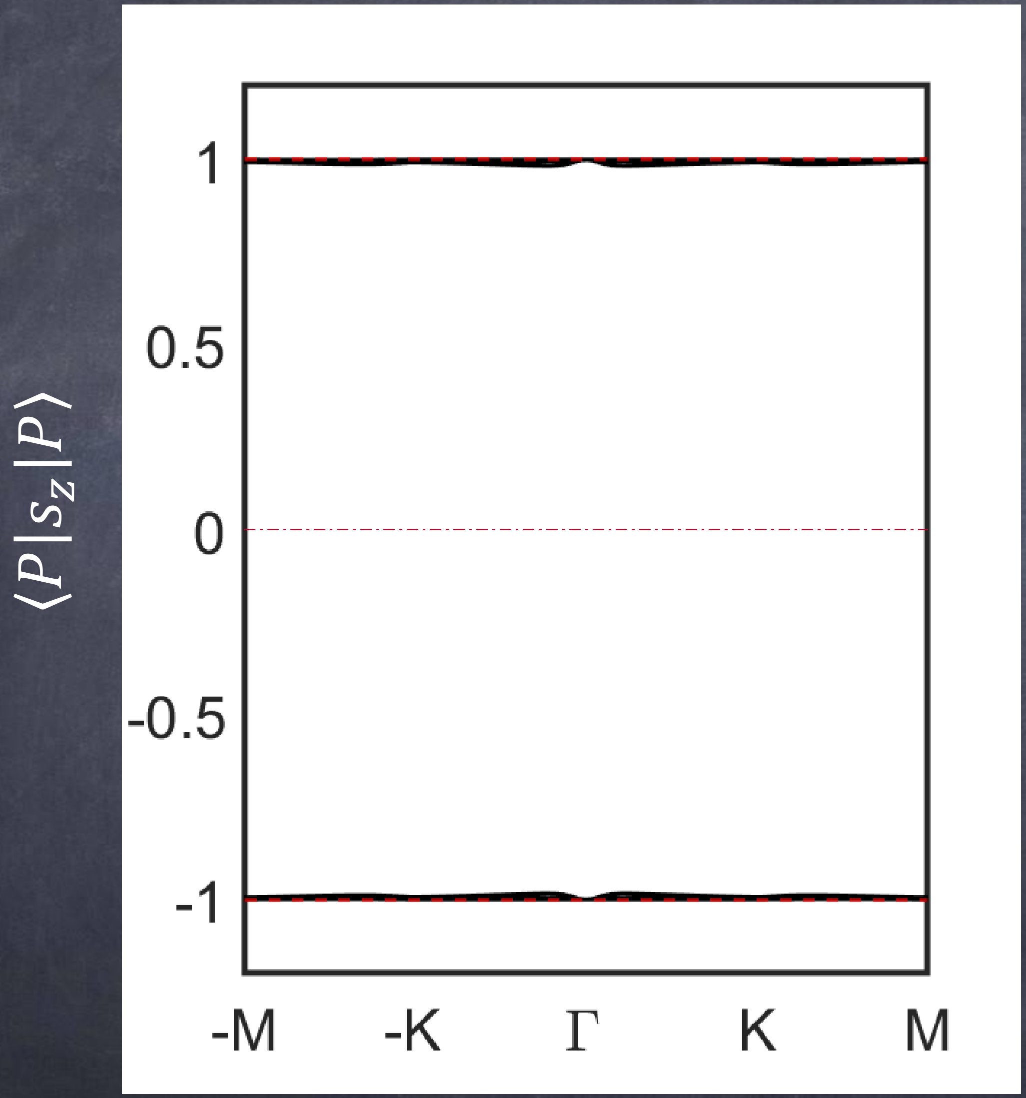
$$C_L = \frac{C_L^{\mathbb{I}+} - C_L^{\mathbb{I}-}}{2} = 1$$

Berry curvature $\Omega = i\mathrm{Tr}\left(P\left[\partial_{k_x}P, \partial_{k_y}P\right]\right)$, $P = \sum_{n\in occ} |u_{nk}\rangle\langle u_{nk}|$

Feature Berry curvature $\tilde{\Omega} = i\mathrm{Tr}\left(\tilde{P}\left[\partial_{k_x}\tilde{P}, \partial_{k_y}\tilde{P}\right]\right)$, $\tilde{P} = \sum_{m} |\tilde{u}_{mk}\rangle\langle \tilde{u}_{mk}|$

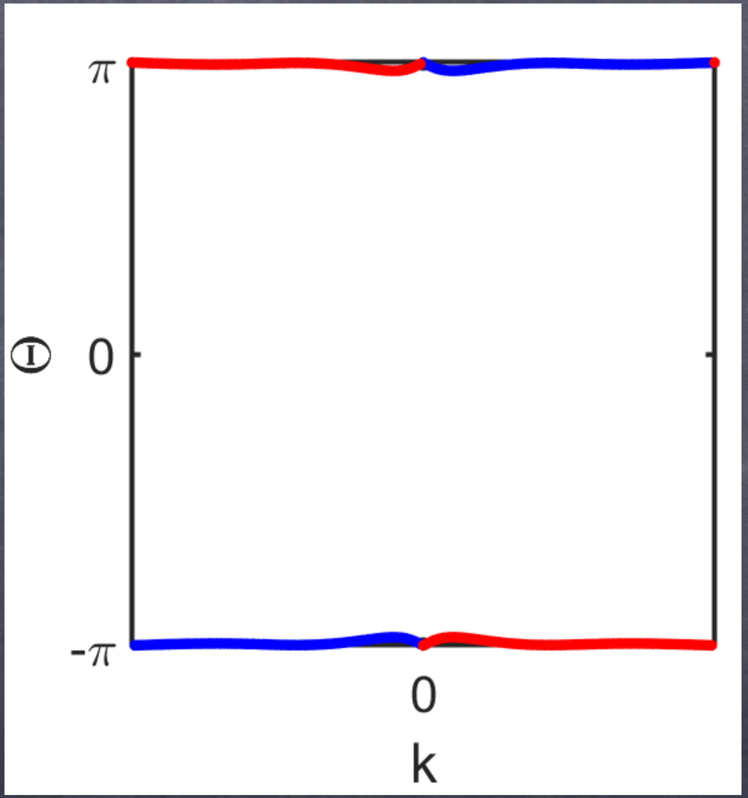


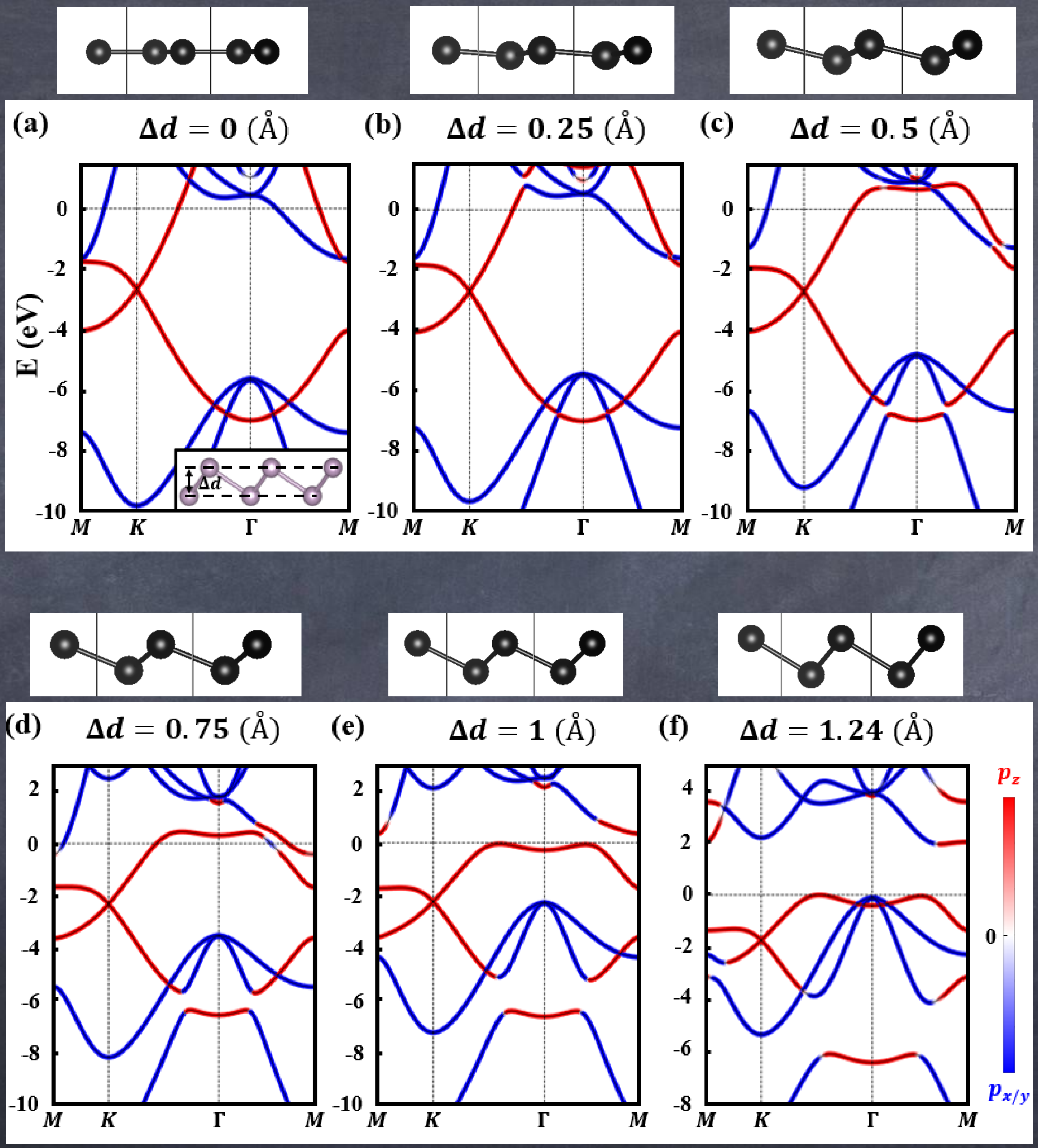
$\langle s_z \rangle$ Feature Band



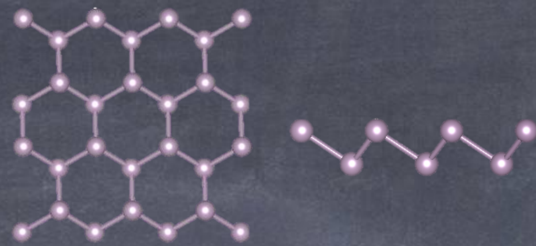
s_z Wilson's Loop

$C_s = 0$

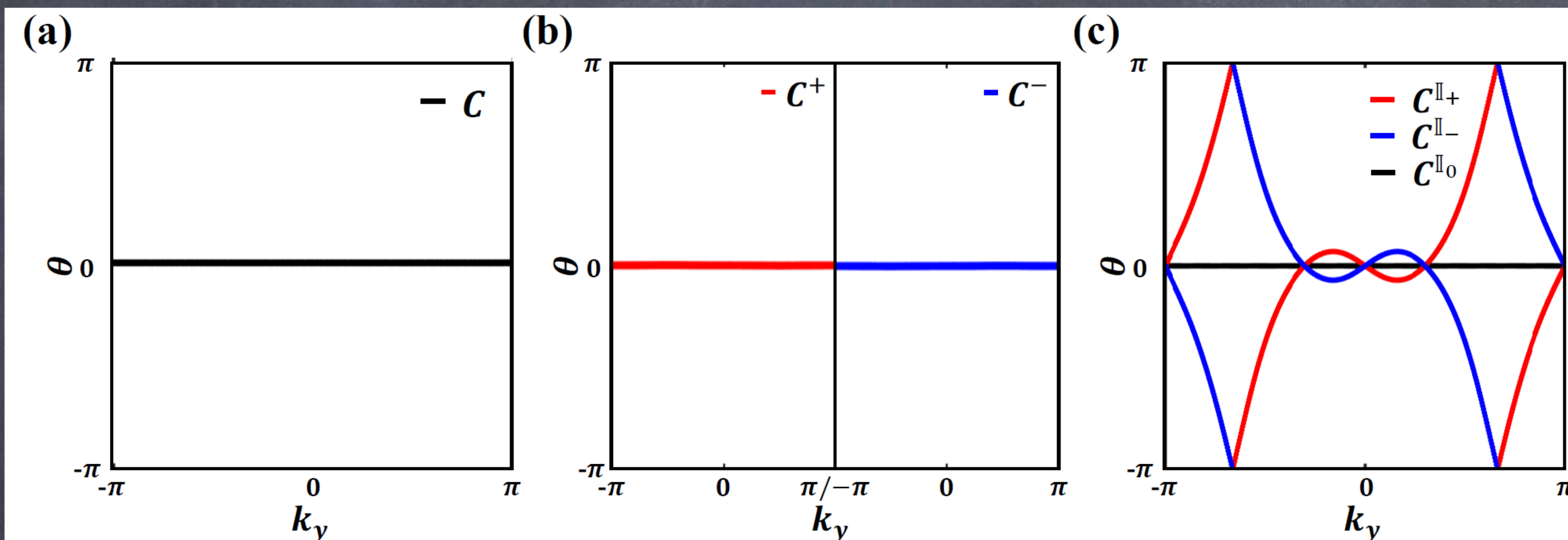



(a) $\Delta d = 0$ (Å)
(b) $\Delta d = 0.25$ (Å)
(c) $\Delta d = 0.5$ (Å)
(d) $\Delta d = 0.75$ (Å)
(e) $\Delta d = 1$ (Å)
(f) $\Delta d = 1.24$ (Å)
E (eV)
Δd
M K Γ M
p_z
$p_{x/y}$

Phosphorene:



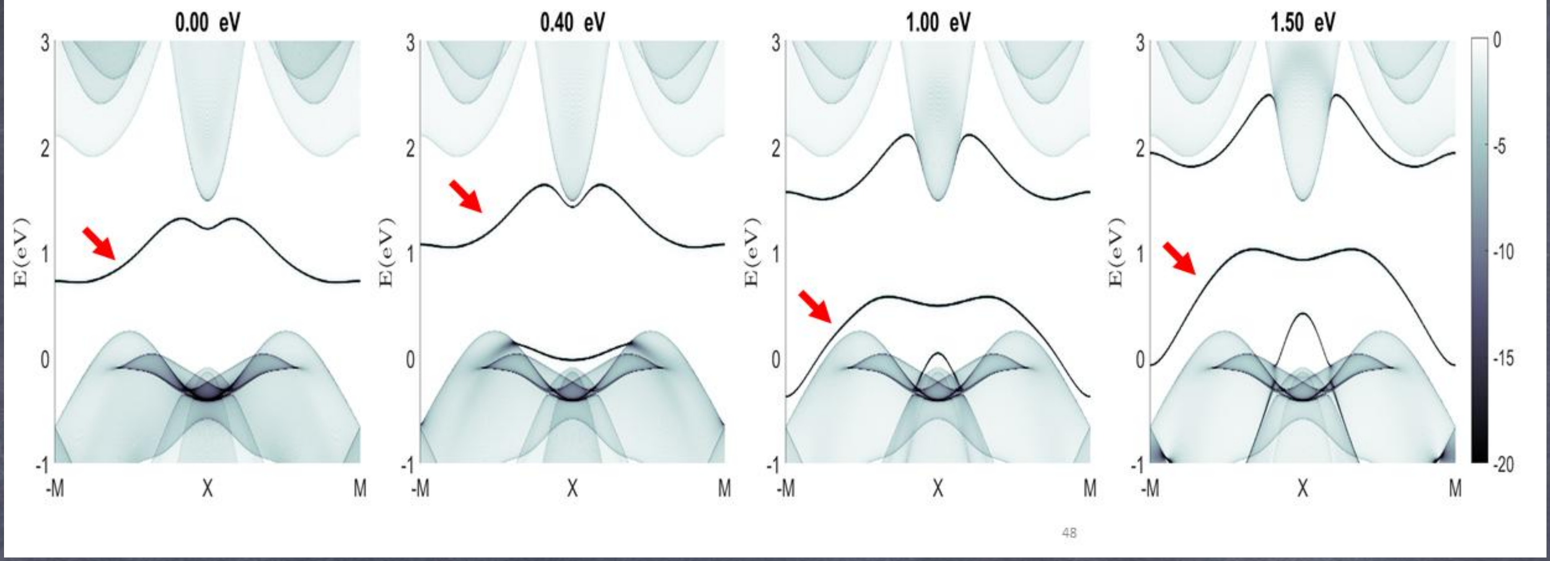
Chern number | Spin Chern number | Orbital Chern number



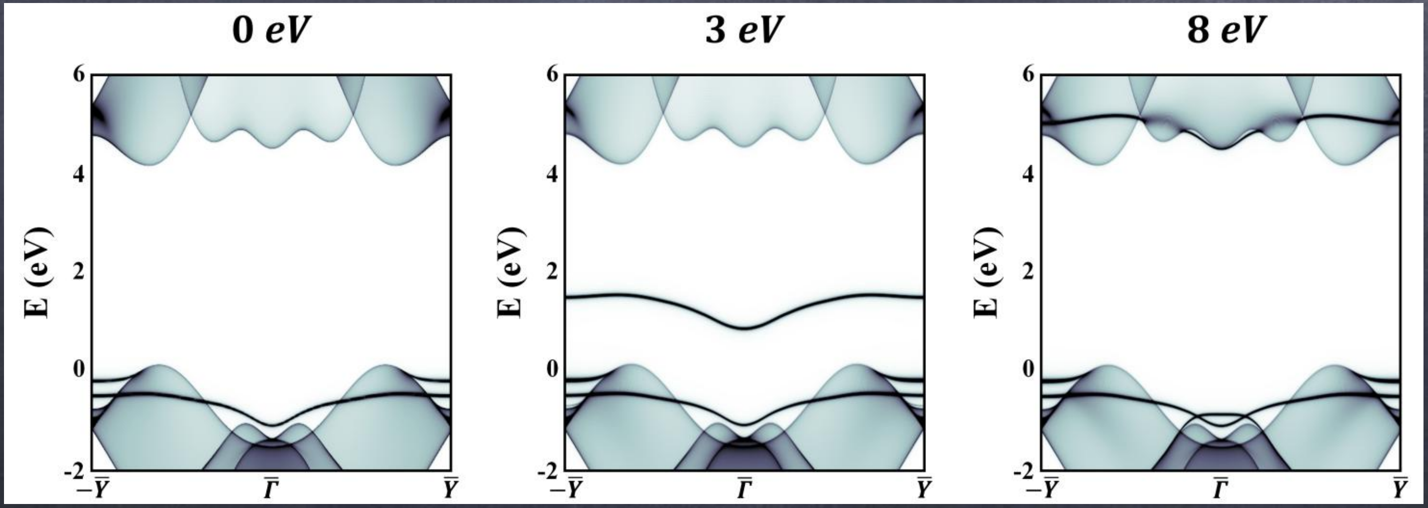
Wilson loop method

$$[\mathcal{W}^{\mu}(k_2)]_{m,n} = \left[\mathcal{W}^{\mu}_{\mathbf{k},\mathbf{G}_1}\right]_{m,n} = \langle \tilde{u}^{\mu}_{m,\mathbf{k}+\mathbf{G}_1} | \prod_{\mathbf{q}}^{\mathbf{k}+\mathbf{G}_1 \leftarrow \mathbf{k}} [P^{\mu}(\mathbf{q})] | \tilde{u}^{\mu}_{n,\mathbf{k}} \rangle$$

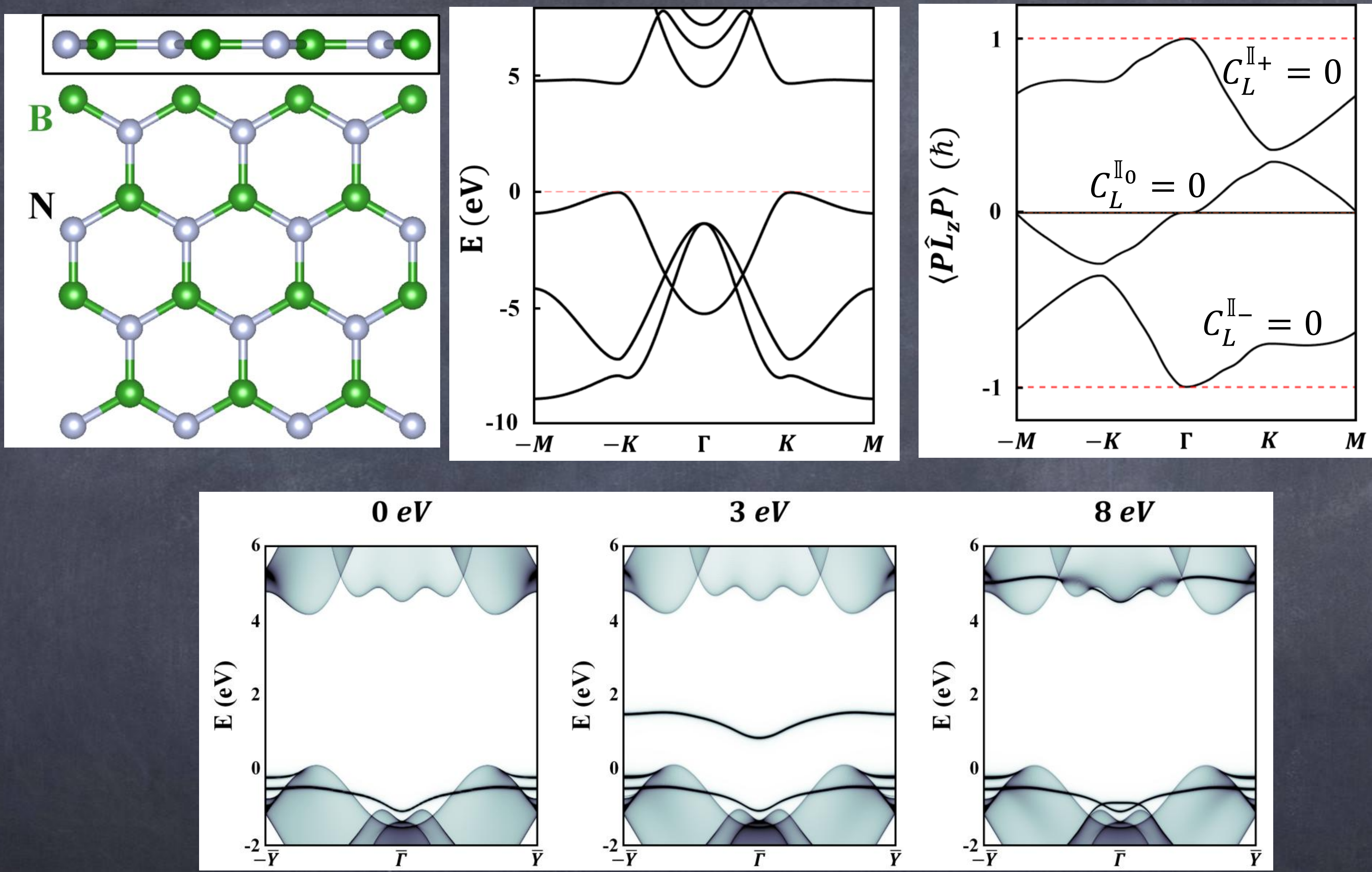
Phosphorene (Orbital Chern insulator)

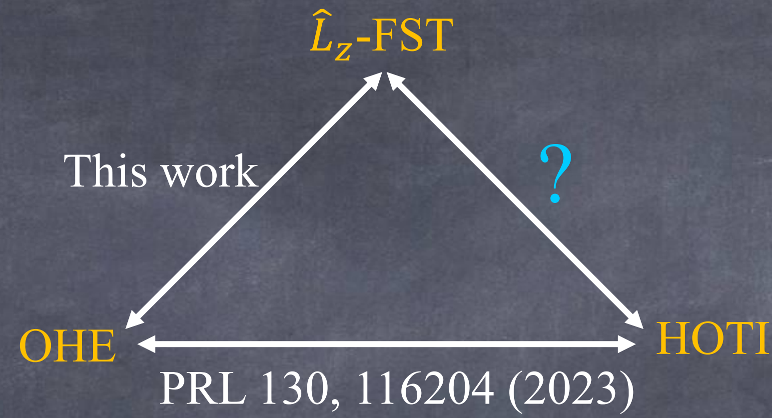


h-BN (true insulator)

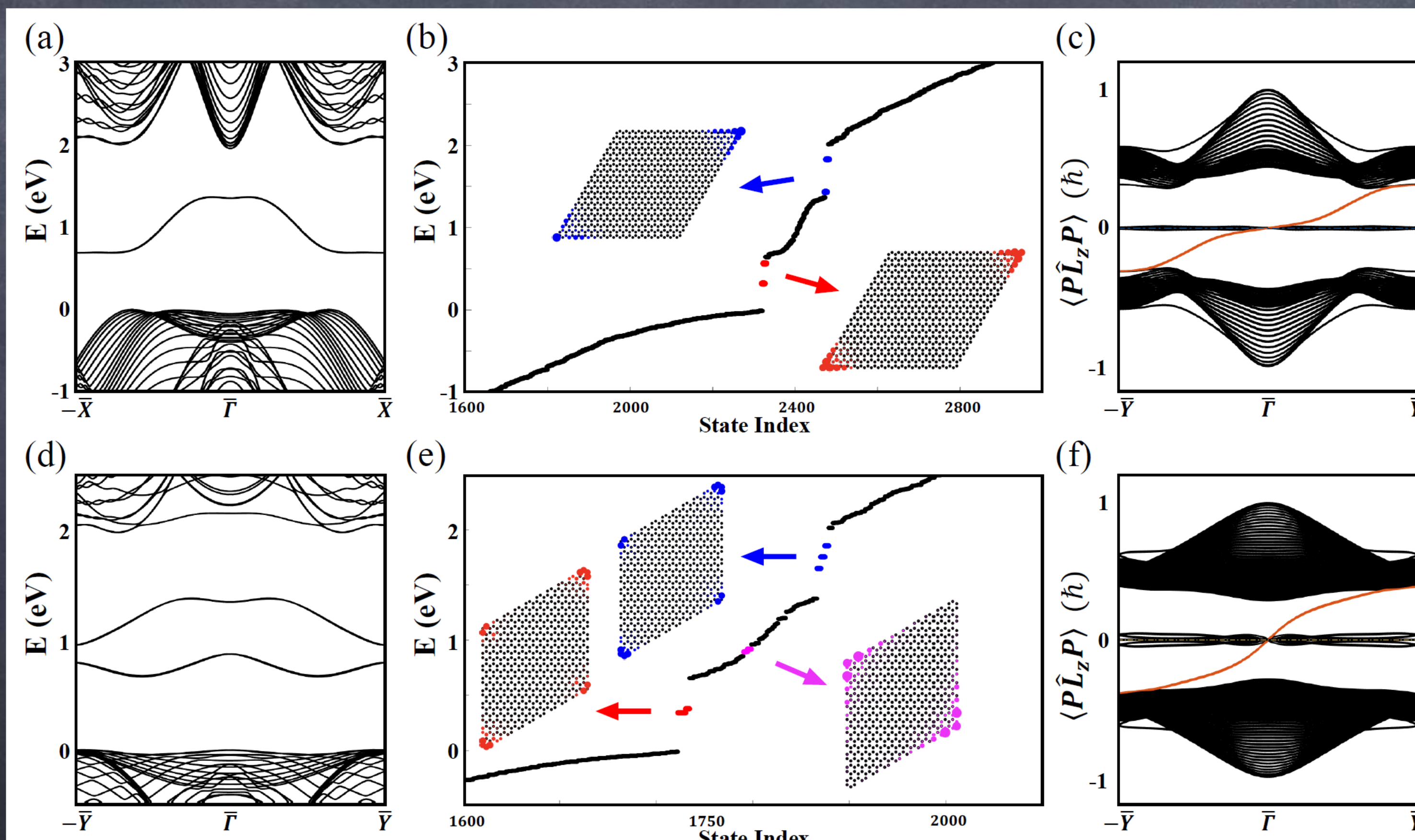


h-BN (true insulator)





$\hat{L}_z$-FST
This work
?
OHE
HOTI
PRL 130, 116204 (2023)

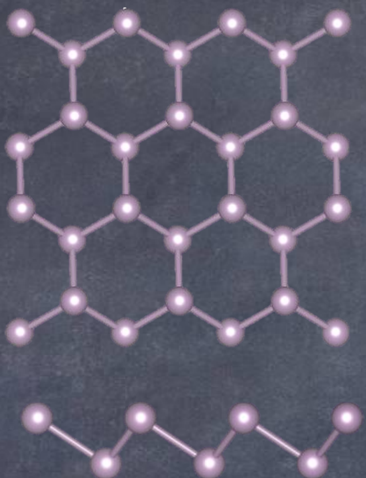


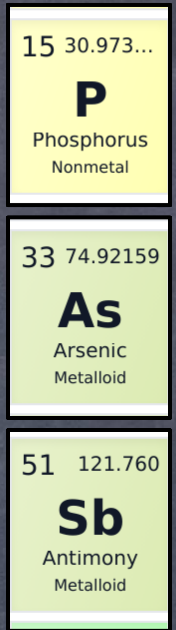
(a)
(b)
(c)
(d)
(e)
(f)
E (eV)
State Index
$\langle P\hat{L}_zP\rangle$ ($\hbar$)
$-\bar{X}$
$\bar{\Gamma}$
$\bar{X}$
$-\bar{Y}$
$\bar{Y}$
1600
2000
2400
2800
1750

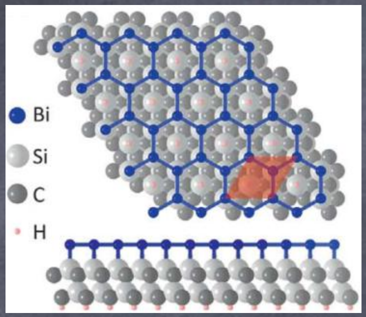
Candidate materials

YT Yao et al.,
Rep. Prog. Phys. 89, 018001 (2026)

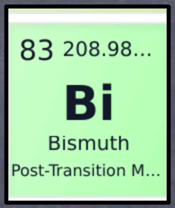
Hexagonal lattice

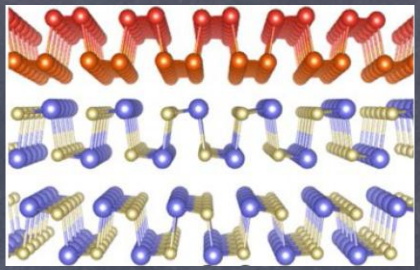






Spin Chern insulator

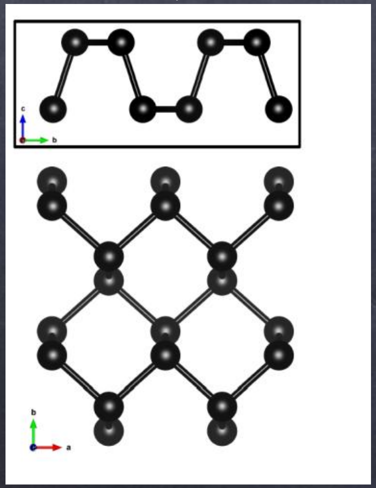


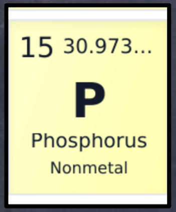


2D Weyl semimetal

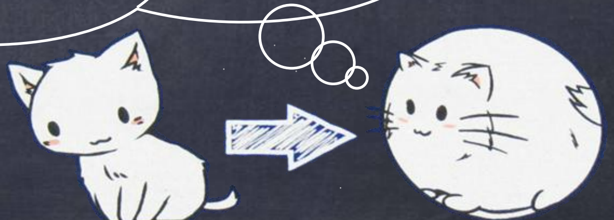
Nat. Commun. 15, 6001 (2024)

Black Phosphorene



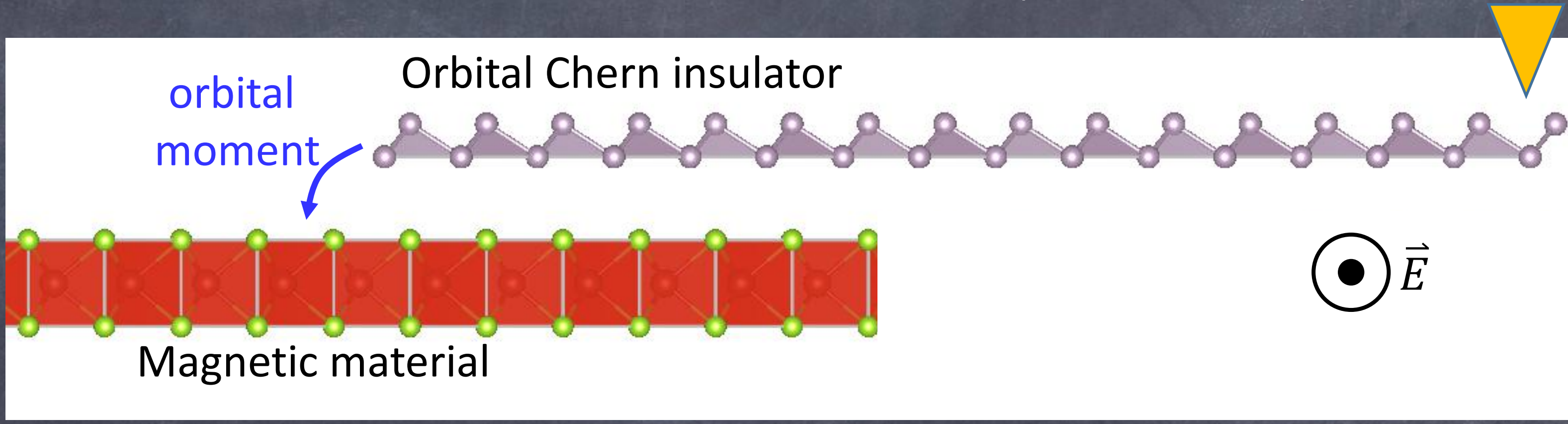


The feature spectrum topology is a general-purpose framework, not just group 5A, and can be used with various materials.



Possible measurement?

NV center
or
scanning near-field optical microscopy
(SNOM+MOKE)



1. The orbital torque in the magnetic material
2. Directly measure the boundary orbital magnetization