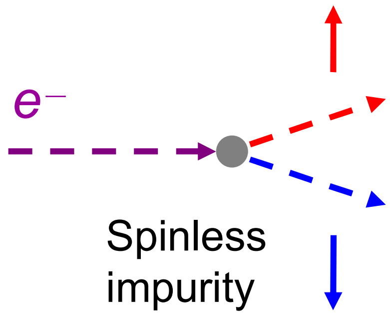
Spin Hall effect: extrinsic mechanism

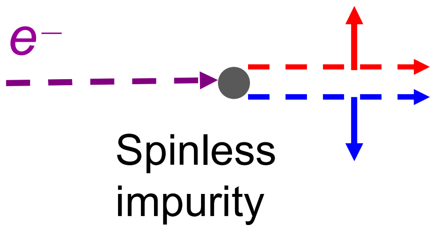
(Dyakonov and Perel, JETP 1971; J.E. Hirsch, PRL 1999.)

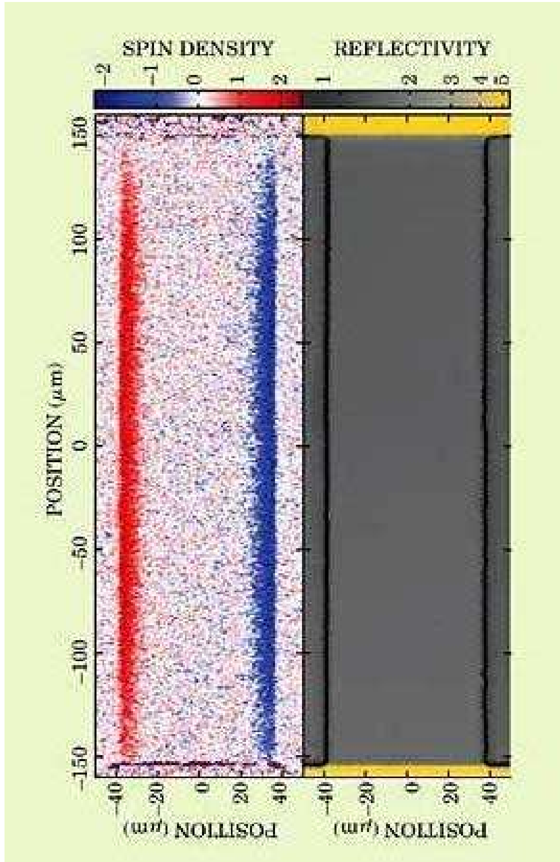
Due to SO interaction between electron and impurity

- Skew scattering (Smit, Physica 1955)



- Side jump (Berger, PRB 1970)





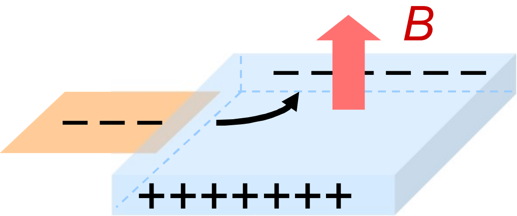
Local Kerr effect in strained n-type bulk InGaAs, 0.03% polarization

Kato et al, Science 2004

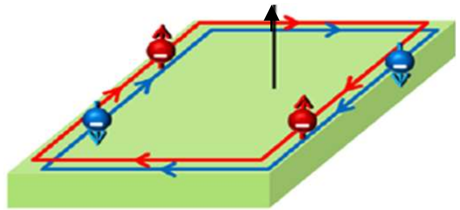
From quantum Hall effect to quantum spin Hall effect

w/o TRS

- Hall (1879)



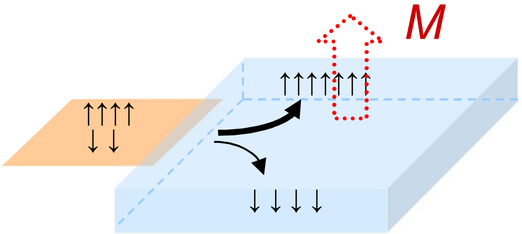
- QHE (1980)



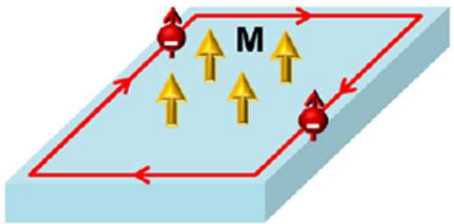
- MOSFET
- Heterojunction
- Graphene
- …

(2D only)

- AHE (1881)



- QAHE (2013)

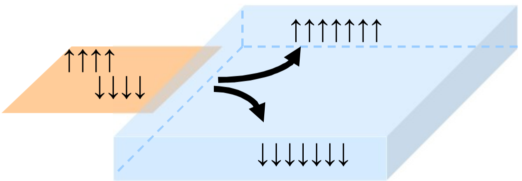


- Bi_2Te_3 doped with Cr etc
- $MnBi_2Te_4$
- …

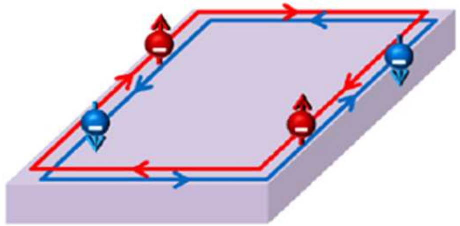
(2D only)

w/ TRS

- SHE (2004, intrinsic)



- QSHE (2007)

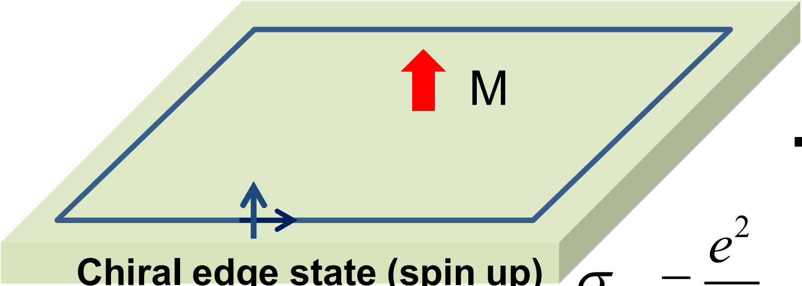


Topological insulator

- HgTe QW
- WTe_2
- …

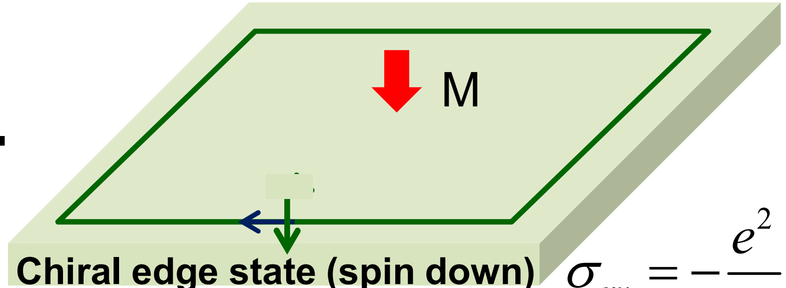
Chang and Li, J Phys 2016

Quantum spin Hall effect ~ two copies of QAHE



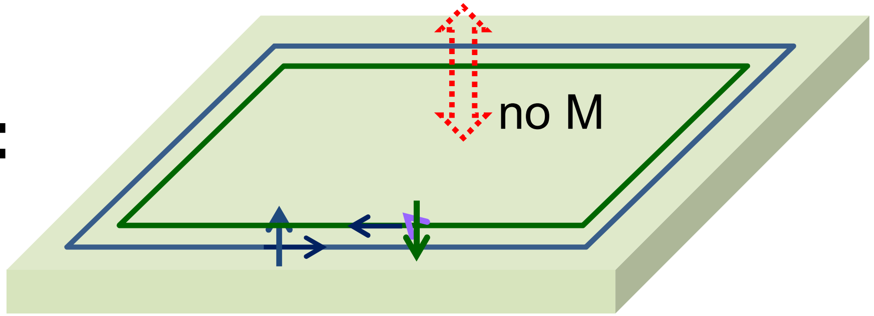
$$\sigma_{xy} = \frac{e^2}{h}$$

+



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

=



Helical edge state

$$\sigma_{xy} = 0$$

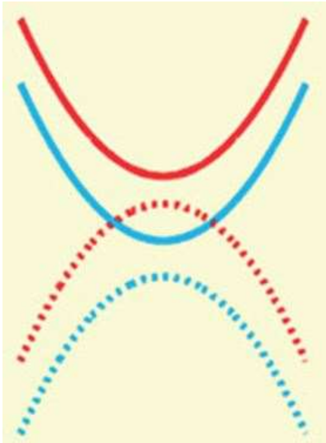
$$\text{but} \quad \sigma^s_{xy} = \frac{e}{2\pi} \quad \left(e \rightarrow \frac{\hbar}{2}\right)$$

- The QSH system has time-reversal symmetry
- After the spin-orbit coupling is added, the spin current is no longer quantized. But the edge states remain robust.

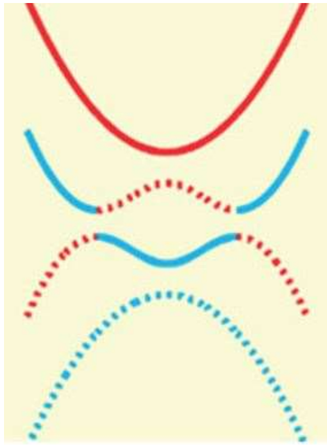
Band inversion and topology

QAH

Band inversion



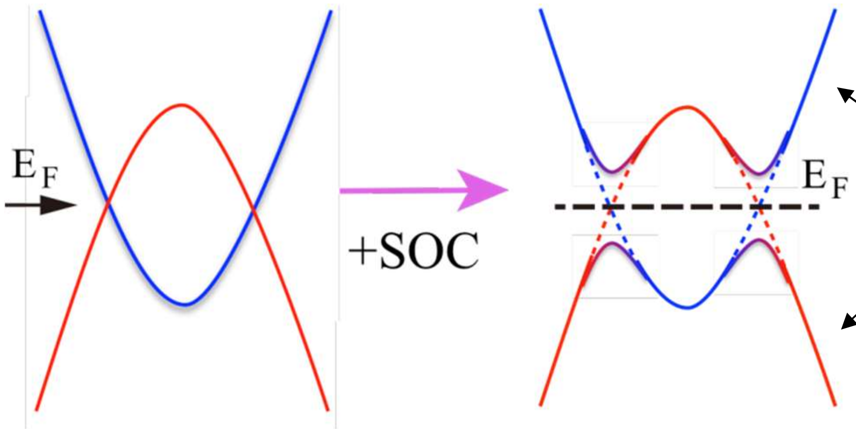
Turn on magnetization



Turn on SOC

QSH

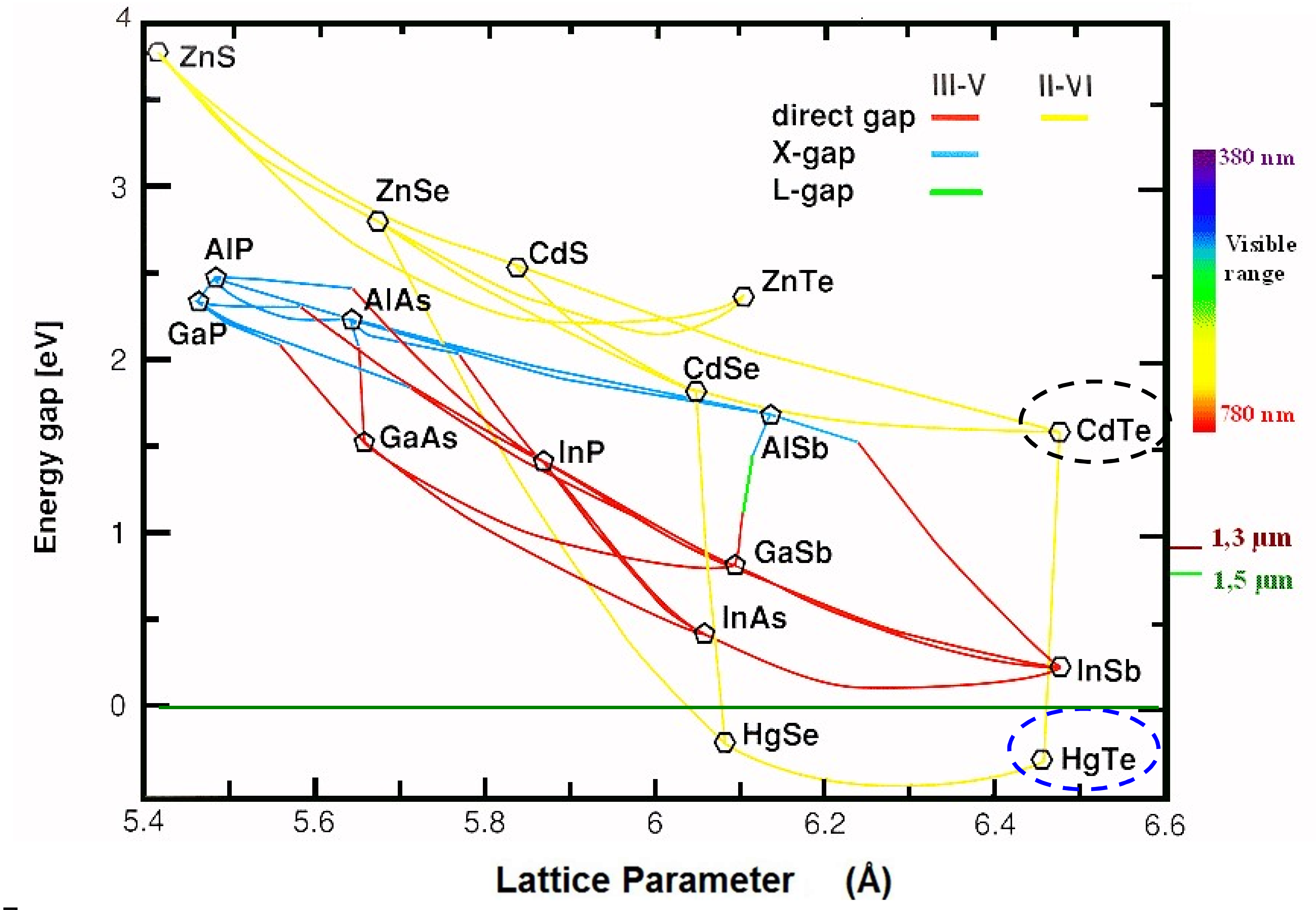
Band inversion (negative bandgap)



Bloch bands with opposite Berry curvatures

Inversion by nature (Time-Reversal Symm preserved)

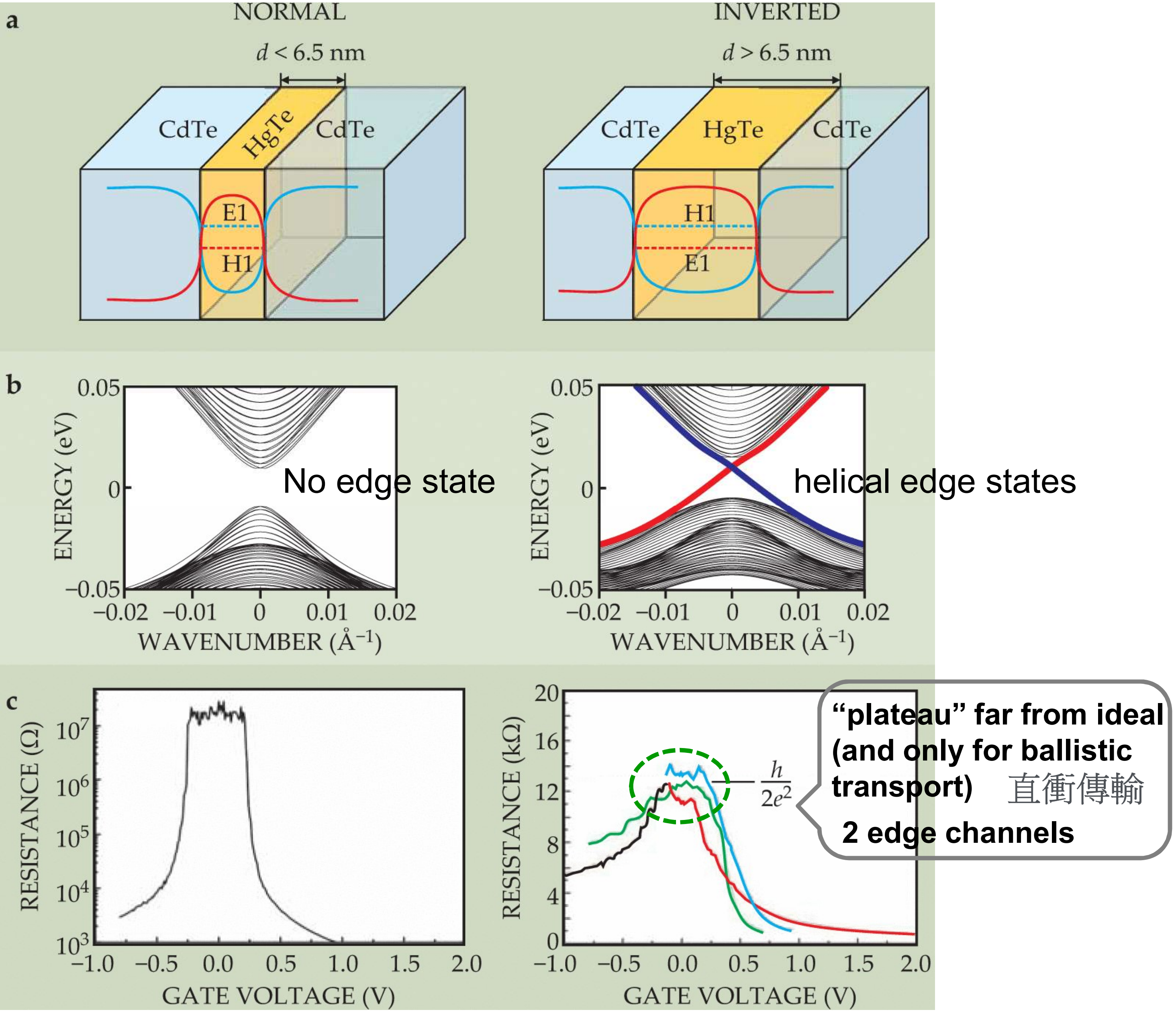
Looking for natural band inversion



(Konig et al, Science 2007)

Quantum Spin Hall Insulator State in HgTe Quantum Wells

E1 ~ s orbital
H1 ~ p orbital



Qi and Zhang, Phys Today 2010

Quantum spin Hall effect in two-dimensional transition metal dichalcogenides (TMD)

Science 2014

Xiaofeng Qian,[1*] Junwei Liu,[2*] Liang Fu,[2†] Ju Li[1†]

Energies for 3 forms from theoretical calculations

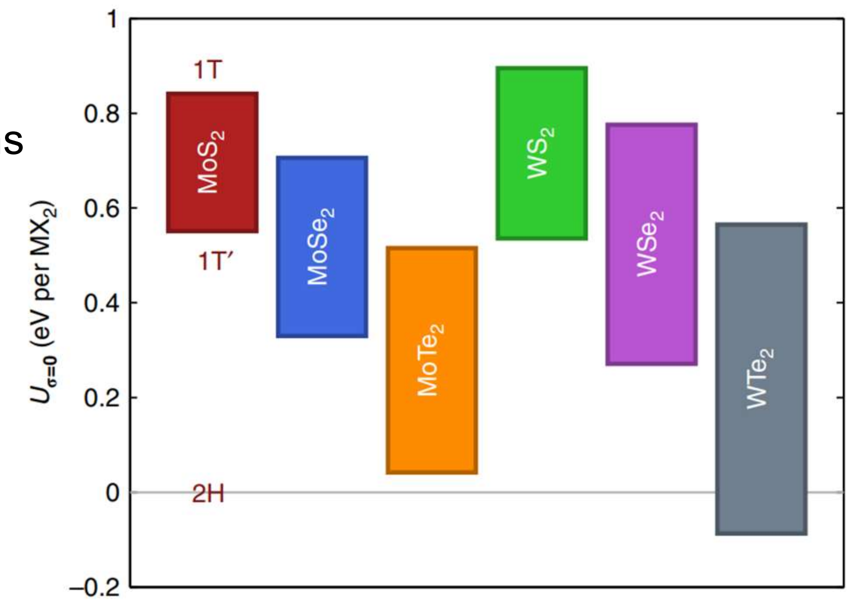
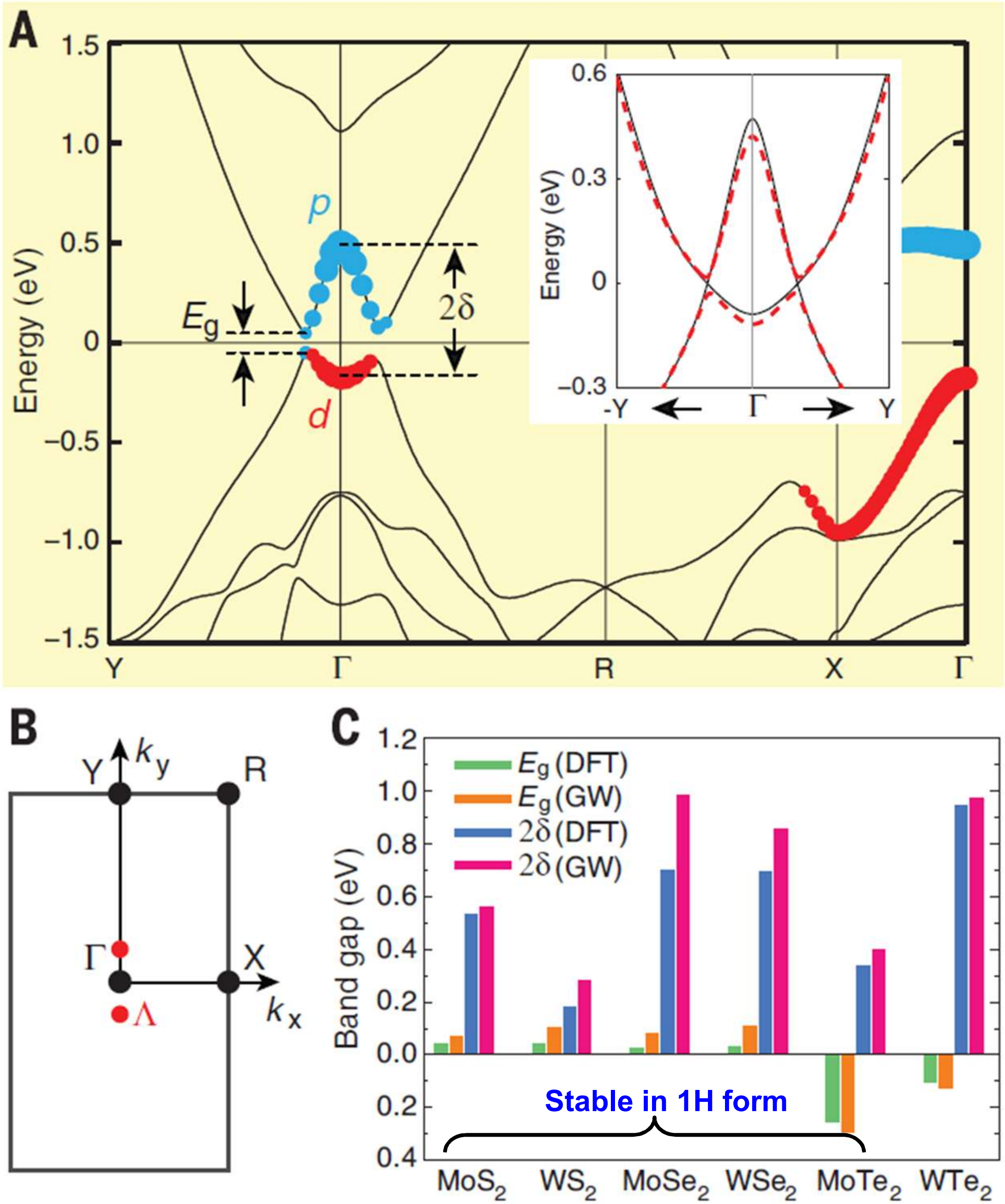


Figure 2 | Ground-state energy differences between monolayer phases of the six studied materials. The energy U is given per formula unit MX_2 for

Duerloo et al, Nat Comm 2014

Calculated electronic structures of 1T′-MX_2 (MoS_2)

Band inversion



w/o and w/ SOC

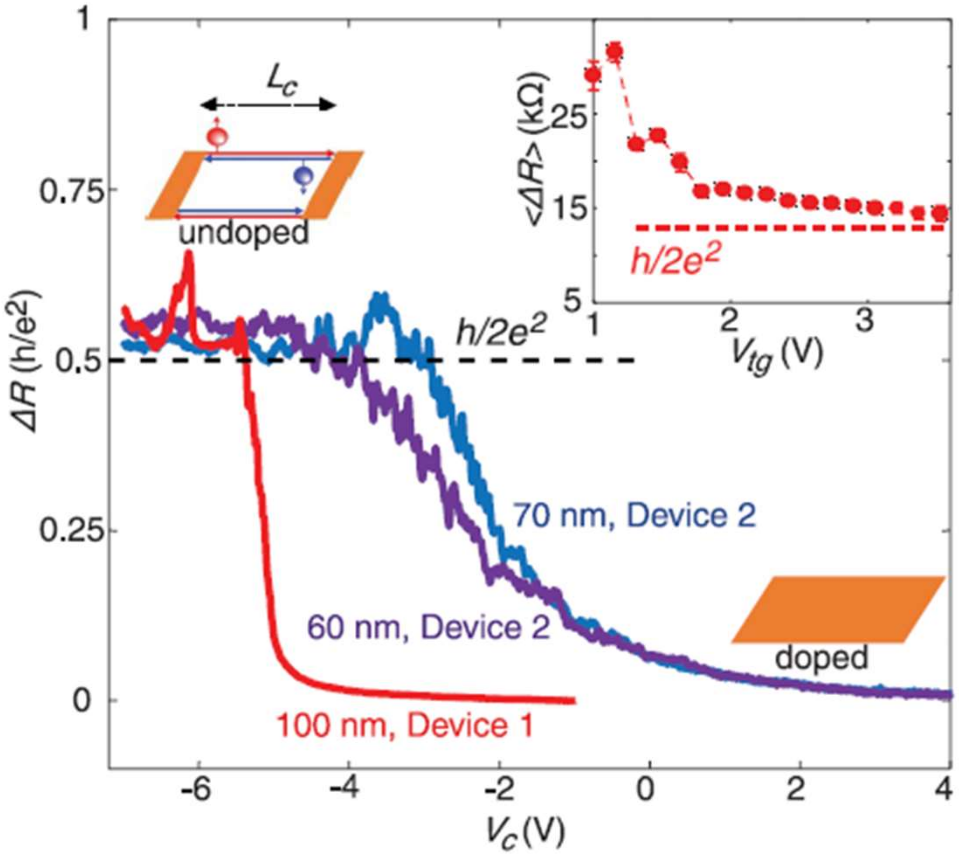
Qian, Science 2014

All have band inversion and are predicted to be QSHI in 1-T' form

Observation of the quantum spin Hall effect up to 100 kelvin in a monolayer crystal 1T'-WTe_2

Sanfeng Wu,[1*†] Valla Fatemi,[1*†] Quinn D. Gibson,[2] Kenji Watanabe,[3] Takashi Taniguchi,[3] Robert J. Cava,[2] Pablo Jarillo-Herrero[1†]

Science 2018



- "Plateau" exists only for ballistic transport
- Nothing is really quantized, except that there are "2" edge channels

The topology behind QSHI, aka 2D TI

(With TRS, the Chern number is zero.)

Topological insulator

A. Time-reversal symmetry
   1. Time-reversal-invariant momentum
   2. Spin-orbit interaction

B. Z_2 topological number
   1. Chern number
   2. Winding number
   3. Z_2 topological number again
   4. Lattice with inversion symmetry

C. Helical edge state

Time-reversal operator (spin ½)

$$\Theta = -i\sigma_y K = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} K$$

or $= e^{-is_y\pi/\hbar}K$

Rotates spin-up to spin-down

In general, for half-integer spin,

$$\Theta = e^{-iJ_y\pi/\hbar}K$$

⇒ $$\Theta^2 = -1$$

for integer spin, $\Theta^2 = +1$

- Spinor Bloch state under TR

$$\begin{pmatrix} \varphi_{\mathbf{k}\uparrow} \\ \varphi_{\mathbf{k}\downarrow} \end{pmatrix} \xrightarrow{TR} \Theta \begin{pmatrix} \varphi_{\mathbf{k}\uparrow} \\ \varphi_{\mathbf{k}\downarrow} \end{pmatrix} = \begin{pmatrix} -\varphi^*_{\mathbf{k}\downarrow} \\ +\varphi^*_{\mathbf{k}\uparrow} \end{pmatrix}$$

Kramer degeneracy

For a system with TRS and *half-integer* spin, if ψ is an energy eigenstate, then $\Theta\psi$ is also an energy eigenstate. Furthermore, these two states are degenerate and orthogonal to each other.

Pf. Since $H\Theta = \Theta H$, so if ψ is an eigenstate with energy ε, $H\psi = \varepsilon\psi$, then

$$H\Theta\psi = \Theta H\psi = \varepsilon\Theta\psi. \tag{1.58}$$

That is, $\Theta\psi$ is also an eigenstate with energy ε.
Furthermore, using the identity $\langle\beta|\alpha\rangle = \langle\tilde{\alpha}|\tilde{\beta}\rangle$, one has

$$\begin{aligned} \langle\psi|\Theta\psi\rangle &= \langle\Theta(\Theta\psi)|\Theta\psi\rangle && (1.59) \\ &= -\langle\psi|\Theta\psi\rangle, && (1.60) \end{aligned}$$

in which $\Theta^2 = -1$ has been used to get the second equation. Therefore, $\langle\psi|\Theta\psi\rangle = 0$. QED.

Spin-orbit coupling (SOC)

$$H_{so} = \lambda_{so}\boldsymbol{\sigma} \times \mathbf{p} \cdot \nabla V_L.$$

If weak, then $\psi_{n\mathbf{k}\pm} \simeq \psi_{n\mathbf{k}\uparrow/\downarrow}$

Spinor Bloch state with TRS

$$\Theta = i\sigma_y K,\ \Theta^2 = -1$$

$$\begin{cases} \Theta\psi_{n\mathbf{k}+} = -\psi_{n-\mathbf{k}-} \\ \Theta\psi_{n\mathbf{k}-} = +\psi_{n-\mathbf{k}+} \end{cases}$$

If the Bloch states are topologically non-trivial, then one needs to write

$$\begin{cases} \Theta\psi_{n\mathbf{k}+} = -e^{i\chi_{n-k}}\psi_{n-\mathbf{k}-}, \\ \Theta\psi_{n\mathbf{k}-} = +e^{i\chi_{nk}}\psi_{n-\mathbf{k}+}. \end{cases} \tag{1.6}$$

It's possible *not* to have such a phase (in the so-called **TR-smooth gauge**). However, this would result in points of gauge singularity within the BZ.

[Spin-Orbit Coupling included]

- With both TRS and SIS (aka PT symmetry)

$$\varepsilon_{n\mathbf{k}s} = \varepsilon_{n-\mathbf{k}-s} = \varepsilon_{n\mathbf{k}-s}$$

(global 2-fold degeneracy)

- With TRS, without SIS

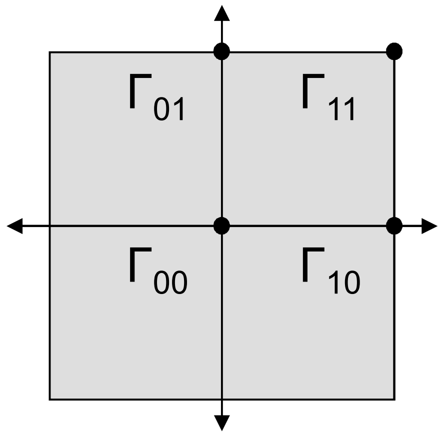
$$\varepsilon_{n-\mathbf{k}s} \neq \varepsilon_{n\mathbf{k}s}$$

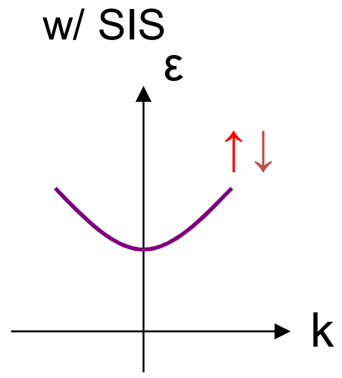
Except at
time-reversal-invariant
momentum (TRIM)

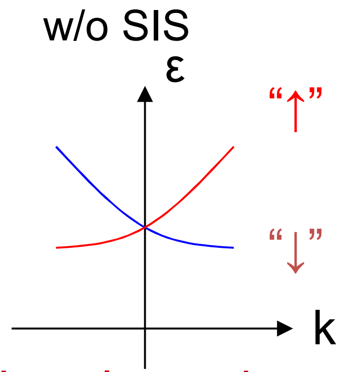
$$\mathbf{k} = -\mathbf{k} + \mathbf{G}$$

At TRIM

$$\varepsilon_{n\mathbf{k}s} = \varepsilon_{n-\mathbf{k}-s} = \varepsilon_{n,-\mathbf{k}+\mathbf{G},-s} = \varepsilon_{n\mathbf{k}-s}$$







Level crossing at TRIM

There are several ways to characterize the topology of a QSHI

Here we mention three:

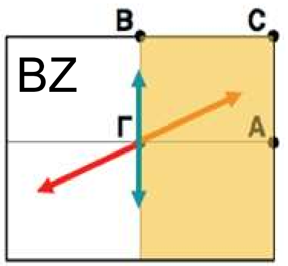
1. Chern number of effective BZ (Moore and Balent)
2. Winding number of gauge transformation (Fu and Kane)
3. Cumultaive parities at TRIM

   (see, e.g., Favata and Marrazzo, Electronic Structure 2023)

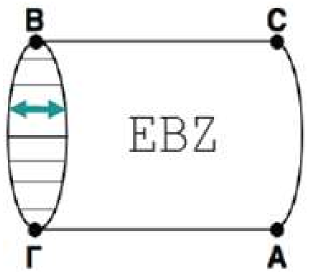
1 Topology in 2D TI

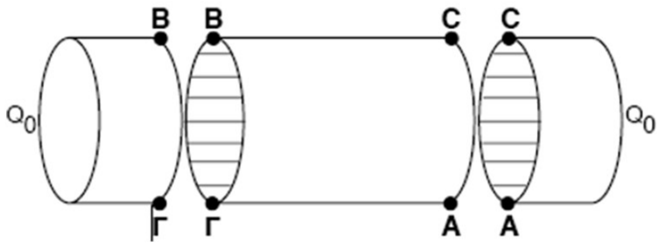
Moore and Balent, PRB 07

Consider lattice fermion with time reversal symmetry (TRS)



A time-reversal invariant plane





- Without B field, Chern number $C_1 = 0$
- Bloch states at *k*, -*k* are not independent,

independent states live in EBZ.

- EBZ is a cylinder, not a closed torus.

∴ No obvious quantization.

→ Solution: add caps to close the EBZ

- C_1 of the closed surface may depend on caps
- C_1 mod 2 is independent of caps, thus is an

intrinsic property of the EBZ

→ 2 types of insulator, the "0-type", and the "1-type"

The topology is protected by TRS

2 Topology in 2D TI (Fu and Kane 2006)

Consider a Kramer pair,

adopt TR-smooth gauge,

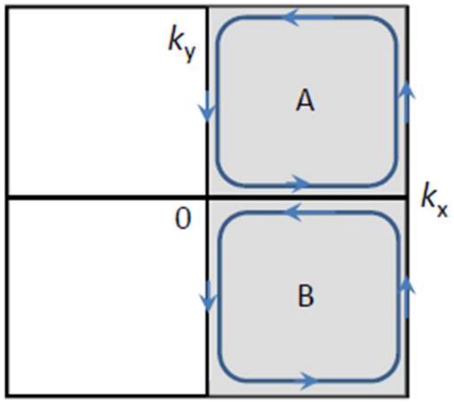
$$\begin{cases} \Theta\psi_{n\mathbf{k}+} = -\psi_{n-\mathbf{k}-} \\ \Theta\psi_{n\mathbf{k}-} = +\psi_{n-\mathbf{k}+} \end{cases}$$

→ There are singularities inside the BZ

(Non-Abelian)
Berry connection

$$\mathbf{A}^n_{\alpha\beta}(\mathbf{k}) = i\langle u_{n\mathbf{k}\alpha}|\frac{\partial}{\partial\mathbf{k}}|u_{n\mathbf{k}\beta}\rangle$$

2 patches of gauge



Gauge transformation

$$|u_{\mathbf{k}\alpha}\rangle_B = U_{\alpha\beta}|u_{\mathbf{k}\beta}\rangle_A$$

U(2) matrix

$$\Rightarrow \quad \mathsf{A}^B_\ell = \mathsf{U}^\dagger \mathsf{A}^A_\ell \mathsf{U} + i\mathsf{U}^\dagger\frac{\partial}{\partial k_\ell}\mathsf{U}$$

Winding number of the phase of gauge-transition

$$w = \frac{1}{2\pi i}\oint_{\partial A} d\mathbf{k}\cdot \mathrm{tr}\left(\mathsf{U}^\dagger\frac{\partial}{\partial\mathbf{k}}\mathsf{U}\right)$$

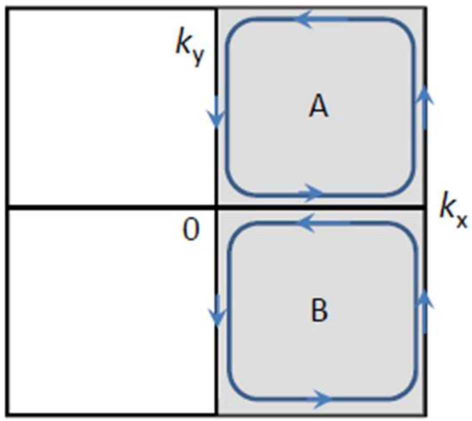
$$\Rightarrow \quad w = \frac{1}{2\pi}\oint_{\partial A} d\mathbf{k}\cdot\left(\mathbf{A}^A - \mathbf{A}^B\right)$$

$$\oint_{\partial A} d\mathbf{k} \cdot \mathbf{A}^A = \int_A d^2k \; F_z^A$$

The same cannot be done for $|u^B_{\mathbf{k}\alpha}\rangle$, since it is *not* smoothly defined in A. Instead, we write

$$\begin{aligned} \oint_{\partial A} d\mathbf{k} \cdot \mathbf{A}^B &= \oint_{\partial EBZ} d\mathbf{k} \cdot \mathbf{A}^B - \oint_{\partial B} d\mathbf{k} \cdot \mathbf{A}^B \\ &= \oint_{\partial EBZ} d\mathbf{k} \cdot \mathbf{A}^B - \int_B d^2k \; F_z^B \end{aligned}$$

$$\Rightarrow \quad w = \frac{1}{2\pi}\left(\int_{EBZ} d^2k \; F_z - \underbrace{\oint_{\partial EBZ} d\mathbf{k} \cdot \mathbf{A}}_{\text{mod-2 gauge invariant}}\right)$$

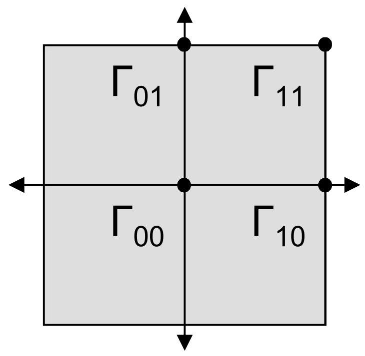


$\sim$ Gauss-Bonnet theorem

$$\chi = \frac{1}{2\pi}\left(\int_M da \; G + \int_{\partial M} ds \; k_g\right)$$

3 If there is inversion symm, (Fu and Kane 2006)

then Bloch state at TRIM Γ_i has a definite parity



same for this pair

- Parity eigenvalue

$$\Pi\psi_{n\Lambda_i\alpha}(\mathbf{r}) = \zeta_{n\Lambda_i}\psi_{n\Lambda_i\alpha}(\mathbf{r})$$

$$\zeta_{n\Lambda_i} = 1 \text{ or } -1$$

- Cumulative parity at Γ_i

$$\delta_i = \prod_{n\in\text{filled}} \zeta_n(\Lambda_i)$$

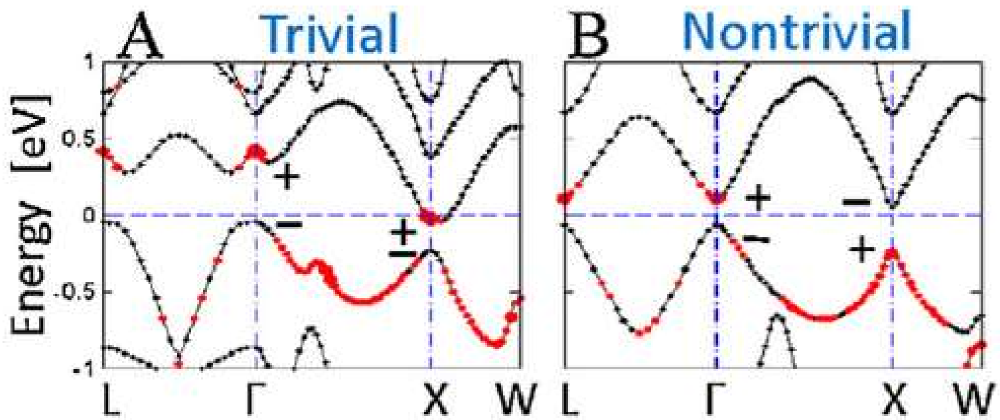
- Z_2 topological number

$$(-1)^\nu \equiv \delta_1\delta_2\delta_3\delta_4 = +1$$ (normal phase)

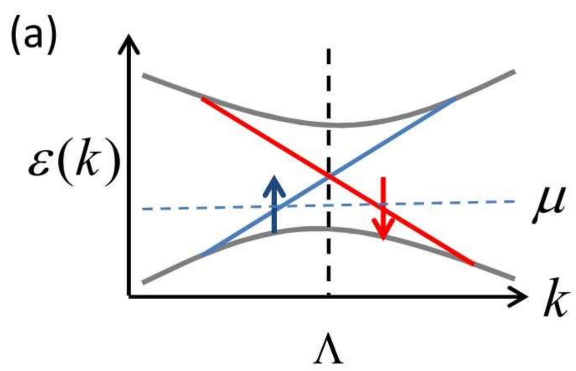
$$(-1)^\nu \equiv \delta_1\delta_2\delta_3\delta_4 = -1$$ (topo phase)

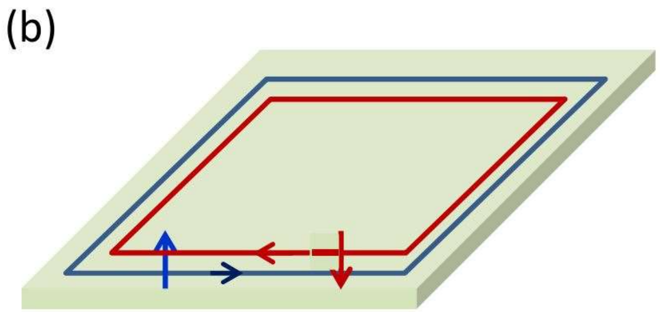
→ $\nu = 0,1$

- Band inversion, parity change, and topological transition



Edge states of 2D TI



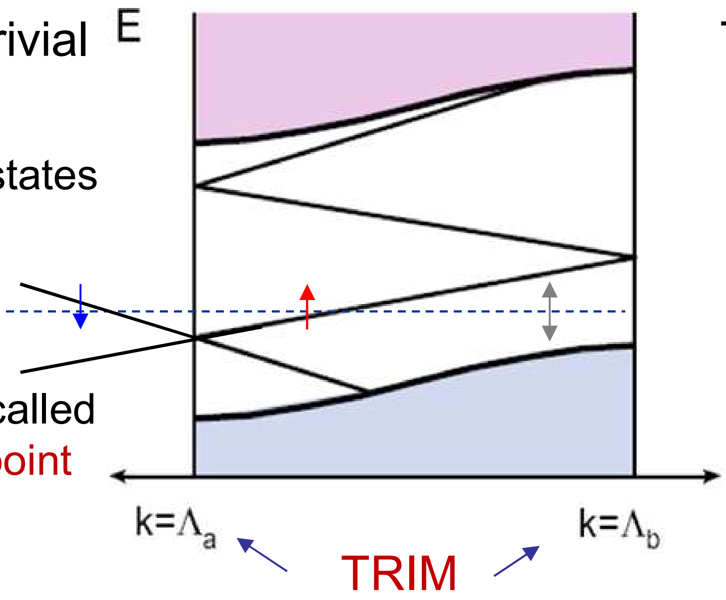


Non-trivial

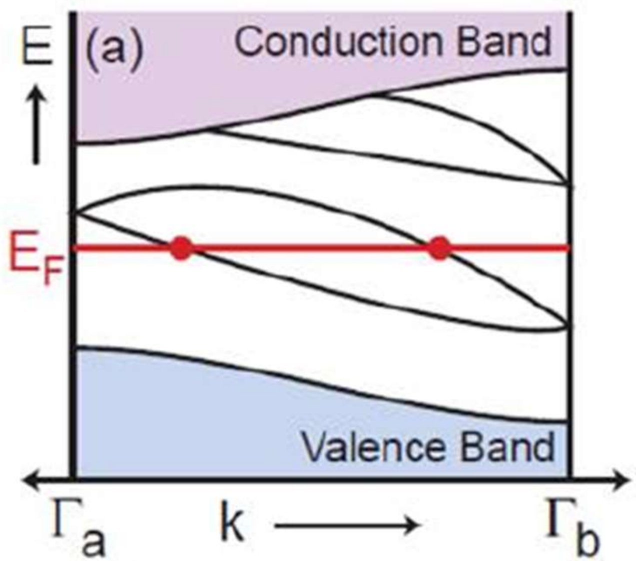
Edge states

Fermi level

Often called Dirac point



Trivial



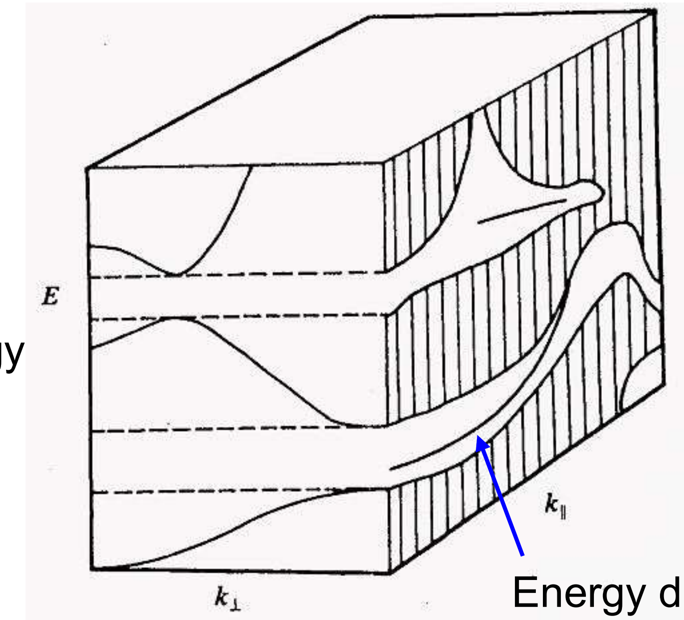
- odd # of Dirac points
- robust surface state

- even # of Dirac points
- fragile surface state

3D Topological insulator

A. Fermi circle of the surface state
B. Weak topological indices
C. Bulk-edge correspondence
D. Topological crystalline insulator and beyond

Surface Brillouin zone



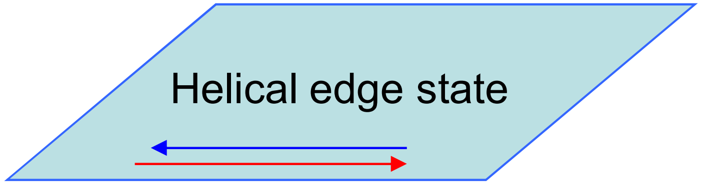
Projected bulk bands

Bulk energy bands

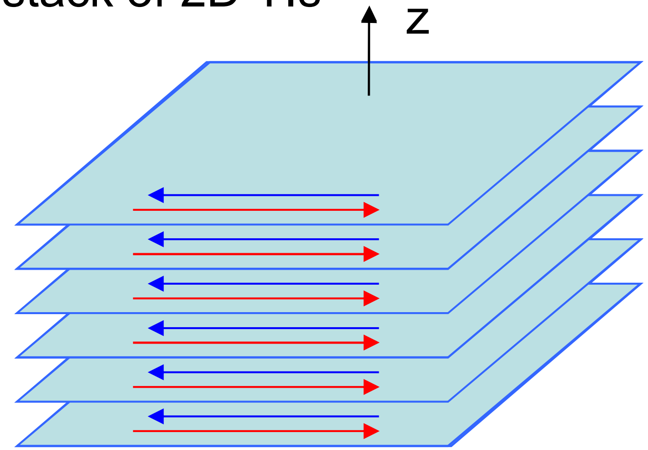
Energy dispersion of edge state

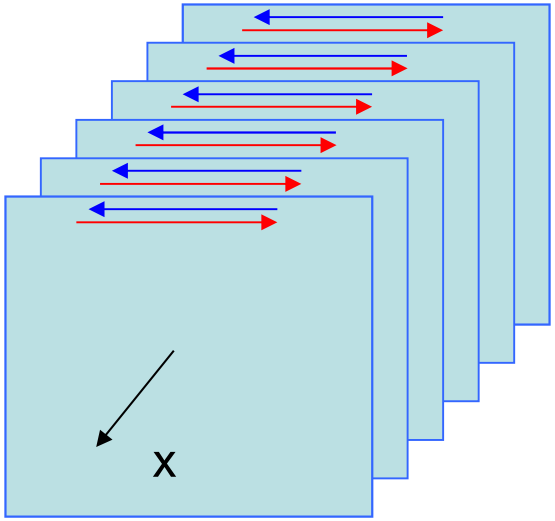
From 2D TI to 3D TI

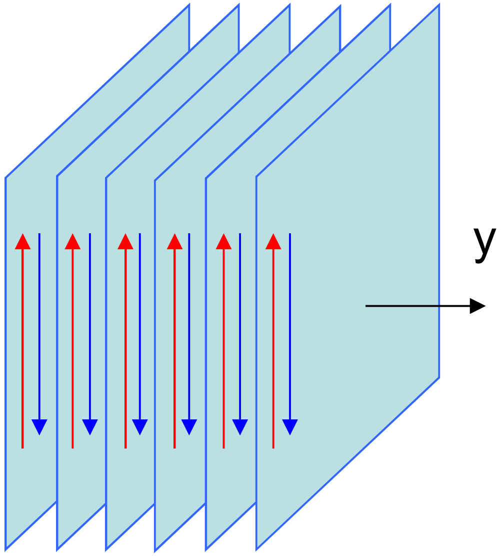
Real space



A stack of 2D TIs



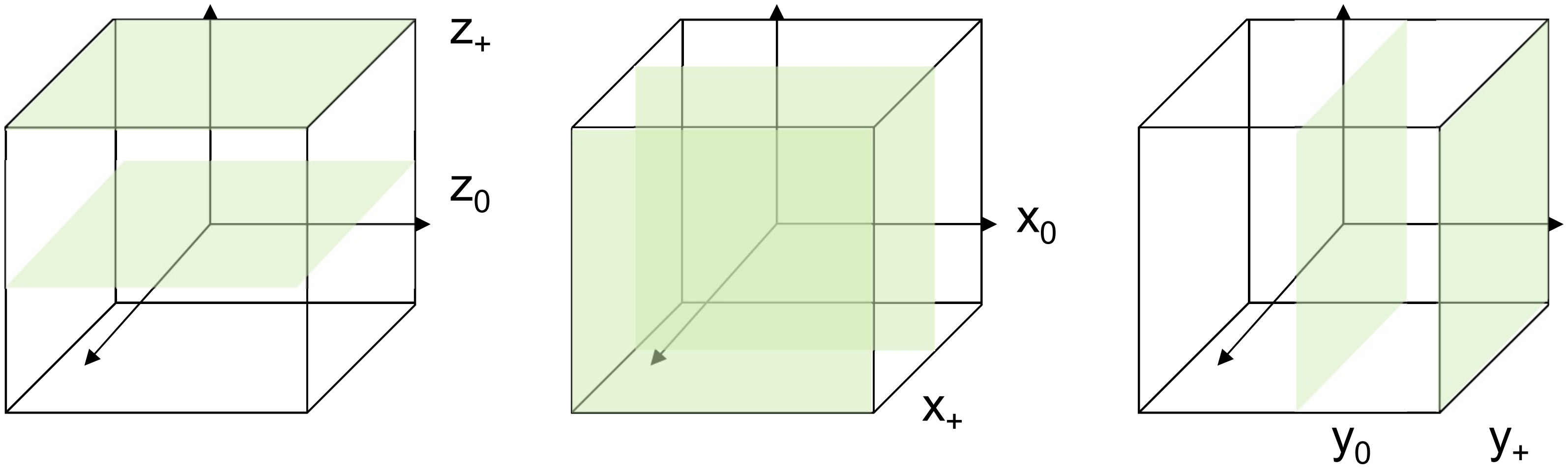




3 TI indices

Momentum space

Each time-reversal invariant plane has a Z_2 index



$$(-1)^{\nu} \equiv \delta_1\delta_2\delta_3\delta_4 = z_0$$

$$(-1)^{\nu'} \equiv \delta_5\delta_6\delta_7\delta_8 = z_+ \qquad \text{etc}$$

➡ Six Z_2 indices: $(x_0, y_0, z_0, x_+, y_+, z_+)$

However,

$$x_0 x_+ = y_0 y_+ = z_0 z_+ = \delta_1 \delta_2 \delta_3 \delta_4 \delta_5 \delta_6 \delta_7 \delta_8$$

2 independent relations

So only 4 independent Z_2 numbers

can choose, e.g., $(z_0 z_+; x_+, y_+, z_+)$

or $(\nu_0; \nu_1, \nu_2, \nu_3)$

strong; weak

Fu, Kane, and Mele PRL 07

Moore and Balents PRB 07

Roy, PRB 09

For example,

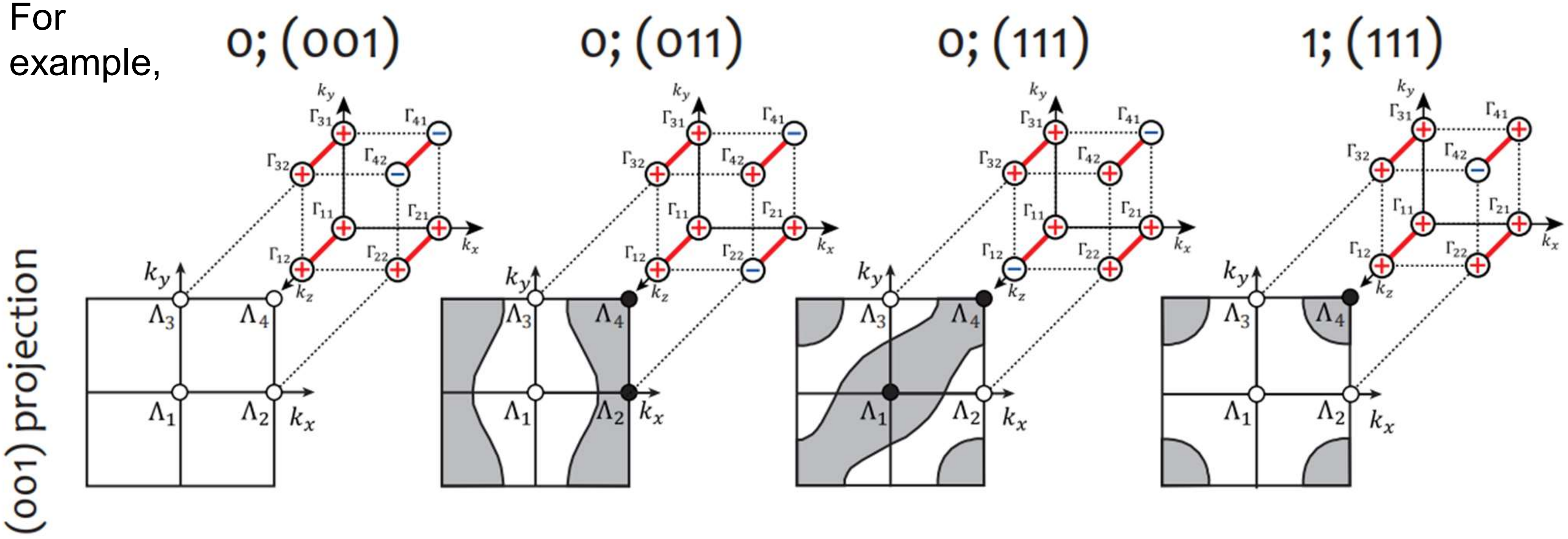
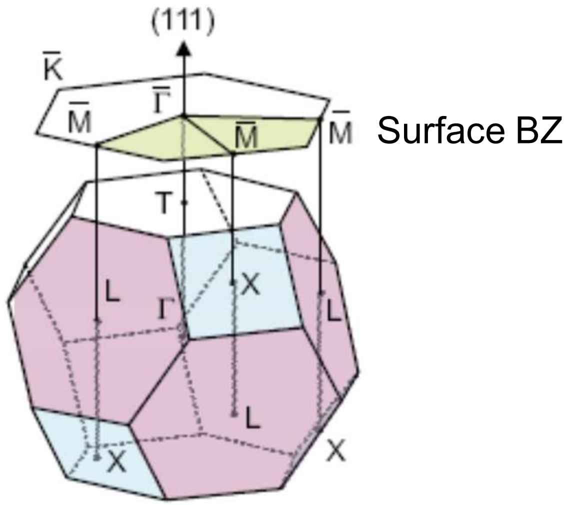


Fig. from Eschbach, 2016

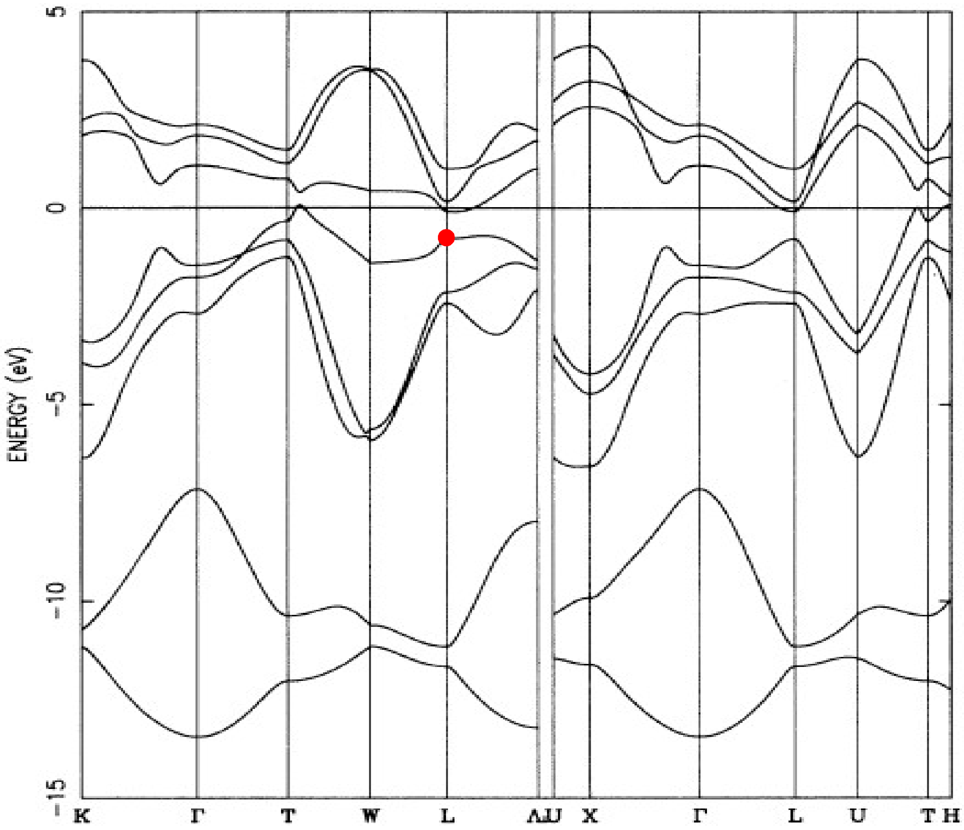
~ 2D TIs stacked along $\vec{M}_\nu = \left(\nu_1 \vec{b}_1 + \nu_2 \vec{b}_2 + \nu_3 \vec{b}_3\right)/2$

$Bi_{1-x}Sb_x$ as a strong TI
(Fu and Kane, PRB 2007)

$$\delta_i \equiv \prod_{n \text{ filled}} \xi_{2n}(\Gamma_i)$$



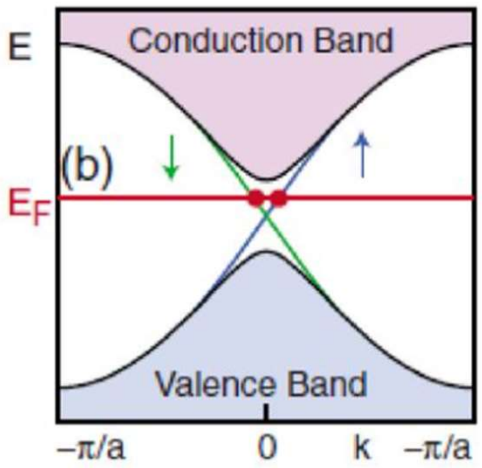
Band structure of Sb (Liu and Allen PRB95)



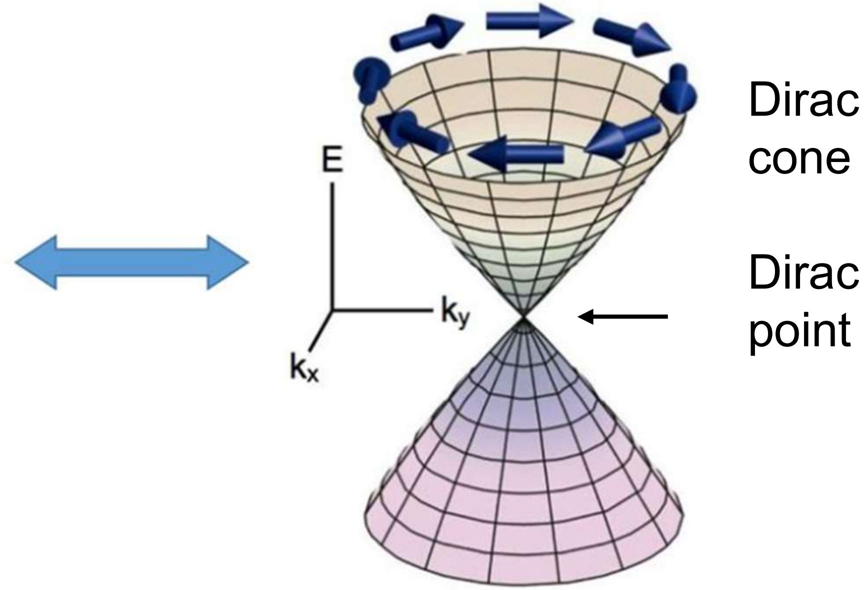
Bismuth	parities
$\Gamma_6^+\ \Gamma_6^-\ \Gamma_6^+\ \Gamma_6^+\ \Gamma_{45}^+$	−
$L_s\ L_a\ L_s\ L_a\ L_a$	−
$X_a\ X_s\ X_s\ X_a\ X_a$	−
$T_6^-\ T_6^+\ T_6^-\ T_6^+\ T_{45}^+$	−
Z_2 class	(0;000)
Antimony	
$\Gamma_6^+\ \Gamma_6^-\ \Gamma_6^+\ \Gamma_6^+\ \Gamma_{45}^+$	−
$L_s\ L_a\ L_s\ L_a\ L_s$	+
$X_a\ X_s\ X_s\ X_a\ X_a$	−
$T_6^-\ T_6^+\ T_6^-\ T_6^+\ T_{45}^+$	−
Z_2 class	(1;111)

5 filled bands

Spin-momentum locking of the Dirac cone at TRIM

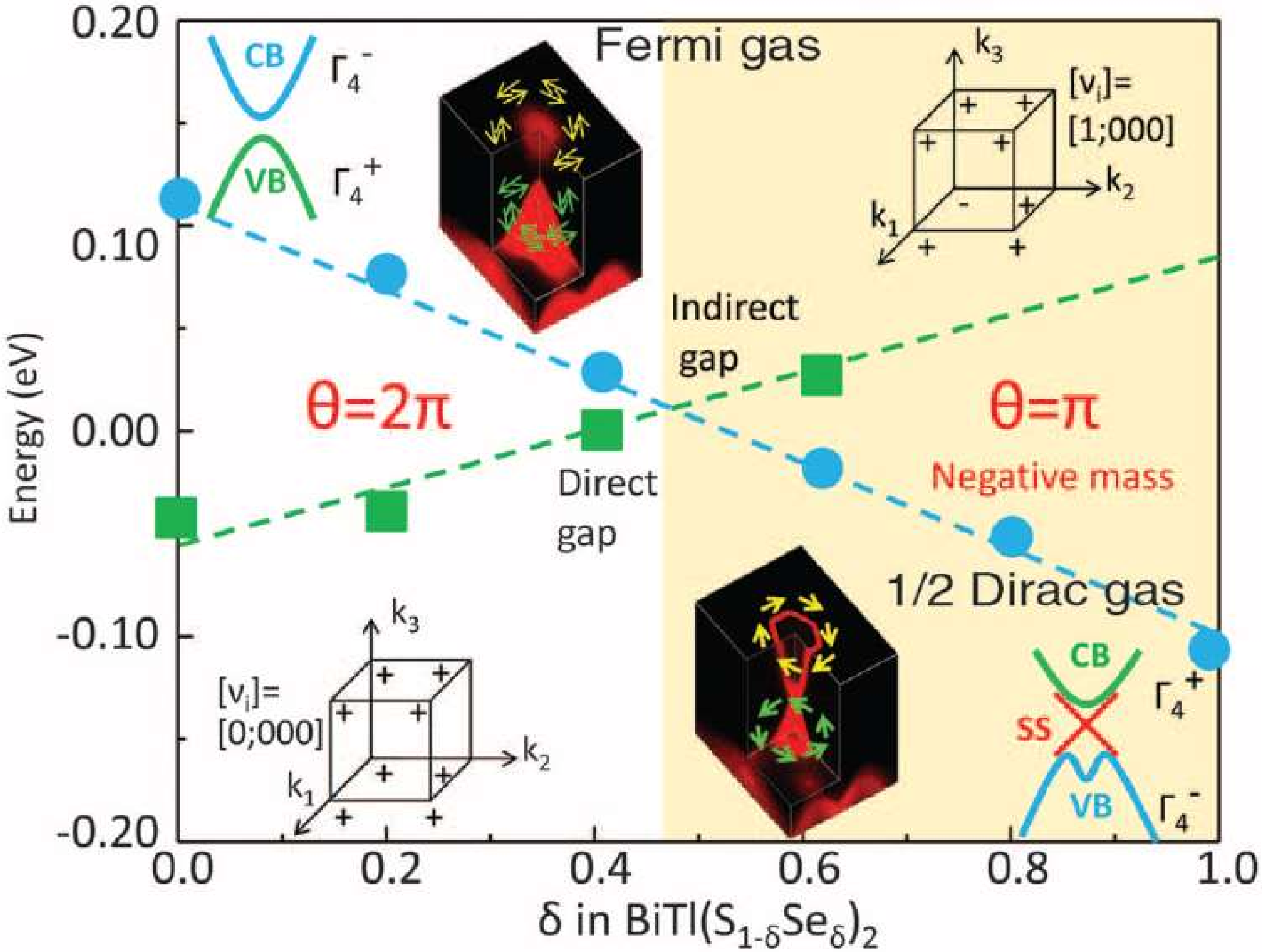


TRIM

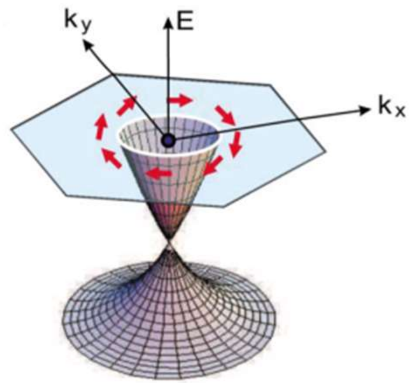


Spin-resolved ARPES

Band inversion, parity change, emergence of SS, and spin-momentum locking

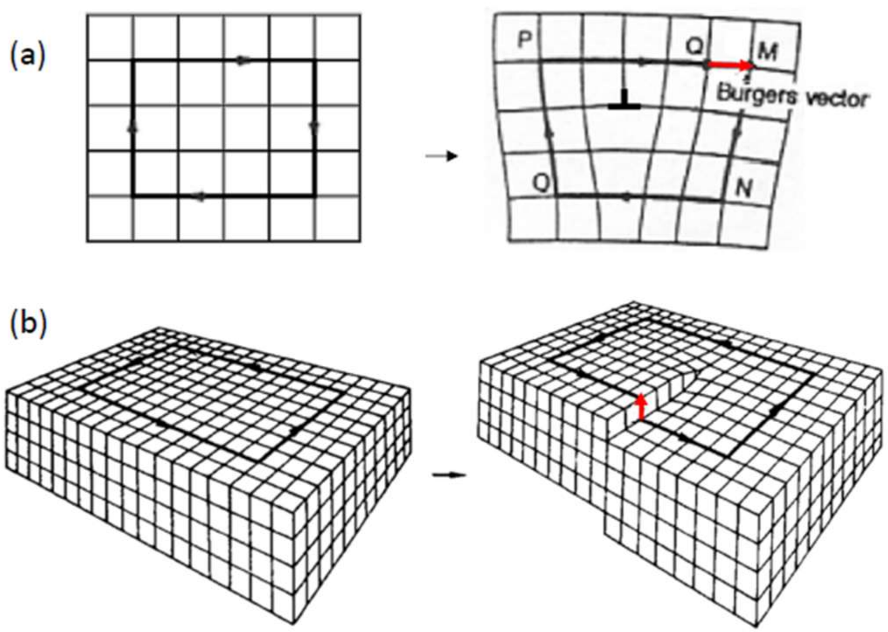


$$H_{SS} = \alpha(\vec{k} \times \vec{\sigma})_z$$



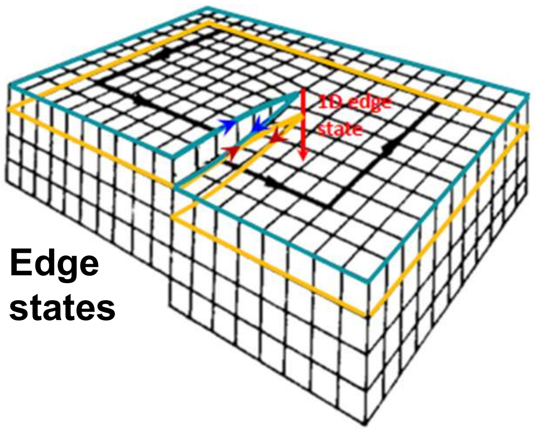
S.Y. Xu et al Science 2011

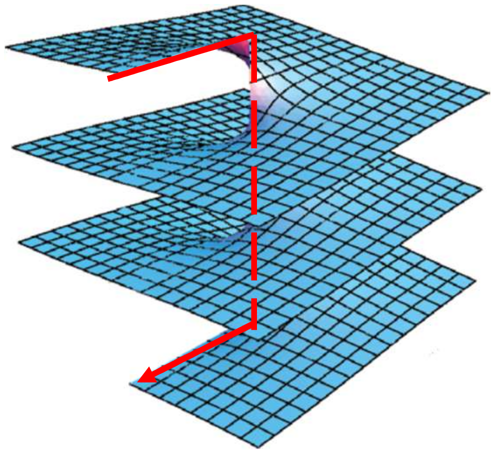
Weak TI index and defect



Two types of dislocation:

- Edge dislocation
- Screw dislocation





Electronic state along 1D defect

- robust against disorder
- chiral quantum wire

Ran Y et al, Nature Phys 2009

Topological insulators are protected by time-reversal symmetry.

Similar topology can also be protected by crystalline symmetries.

They are called topological crystalline insulator (TCI)

PRL **106,** 106802 (2011) PHYSICAL REVIEW LETTERS week ending 11 MARCH 2011

Topological Crystalline Insulators

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(Received 5 October 2010; revised manuscript received 31 December 2010; published 8 March 2011)

Again they would have robust surface states, but

- Electron spin, SOC are no longer essential
- Can have even number of Dirac points
- The dispersion near a DP can be quadratic … etc

https://www.youtube.com/watch?v=dTKhkRuCg8E nature

Topological quantum chemistry

Barry Bradlyn[1*], L. Elcoro[2*], Jennifer Cano[1*], M. G. Vergniory[3,4,5*], Zhijun Wang[6*], C. Felser[7], M. I. Aroyo[2] & B. Andrei Bernevig[3,6,8,9]

2017

nature COMMUNICATIONS

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DOI: 10.1038/s41467-017-00133-2 OPEN

Symmetry-based indicators of band topology in the 230 space groups

2017

Hoi Chun Po[1,2], Ashvin Vishwanath[1,2] & Haruki Watanabe[3]

ARTICLE

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https://doi.org/10.1038/s41467-021-26241-8 OPEN

Magnetic topological quantum chemistry

Luis Elcoro[1,9], Benjamin J. Wieder[2,3,4,9✉], Zhida Song[4], Yuanfeng Xu[5], Barry Bradlyn[6] & B. Andrei Bernevig[4,7,8,10✉]

2021

Higher order TI (protected by crystal symm)

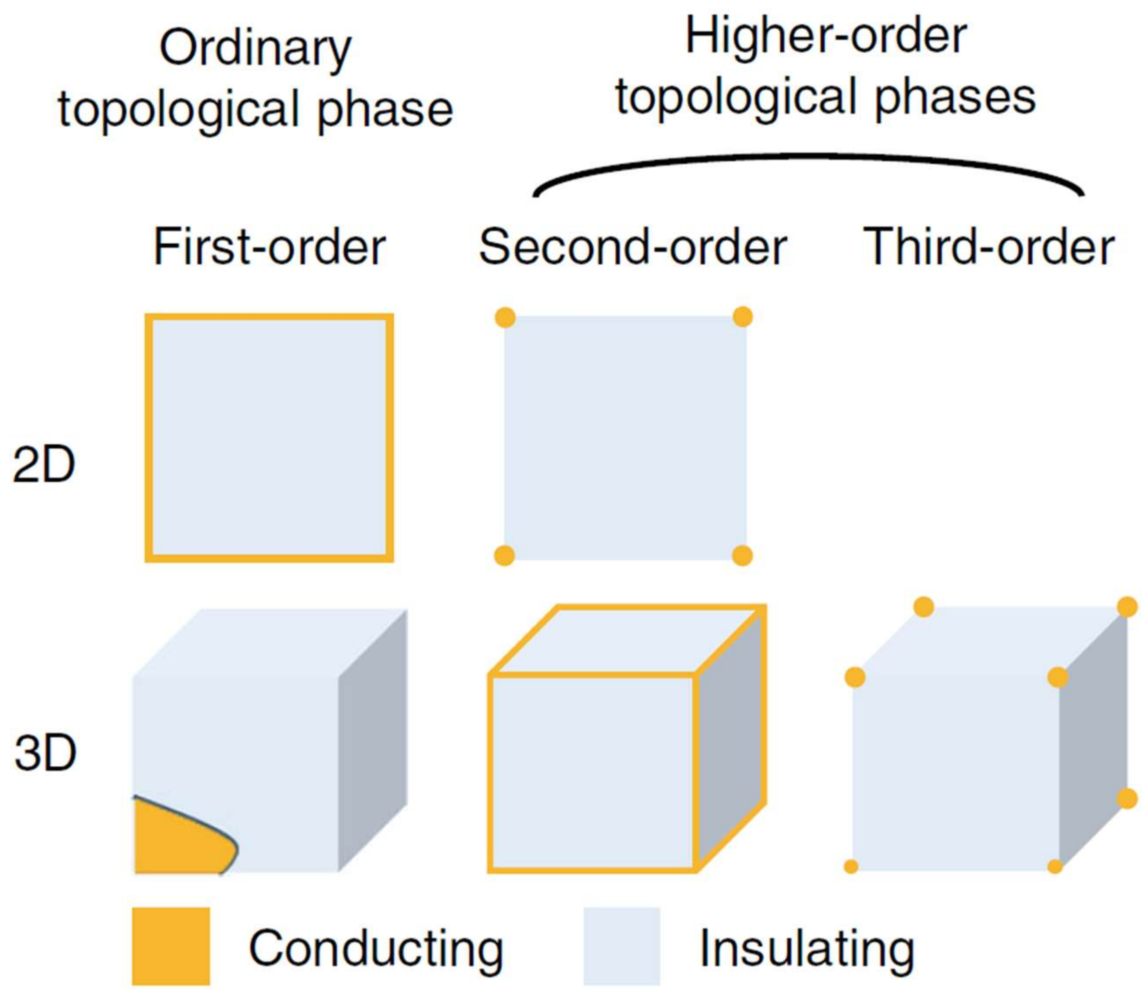

Fig from Kim et al, in Light: Science & Applications (2020)