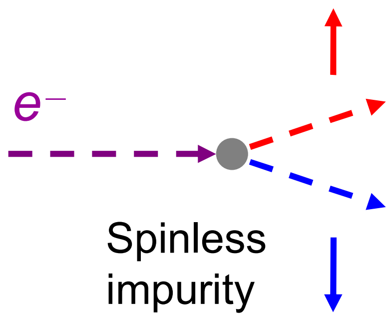
Spin Hall effect: extrinsic mechanism

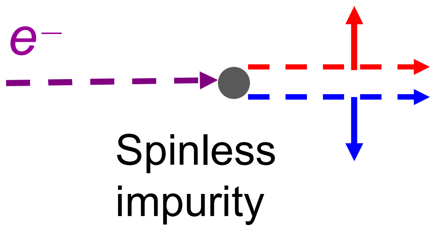
(Dyakonov and Perel, JETP 1971; J.E. Hirsch, PRL 1999.)

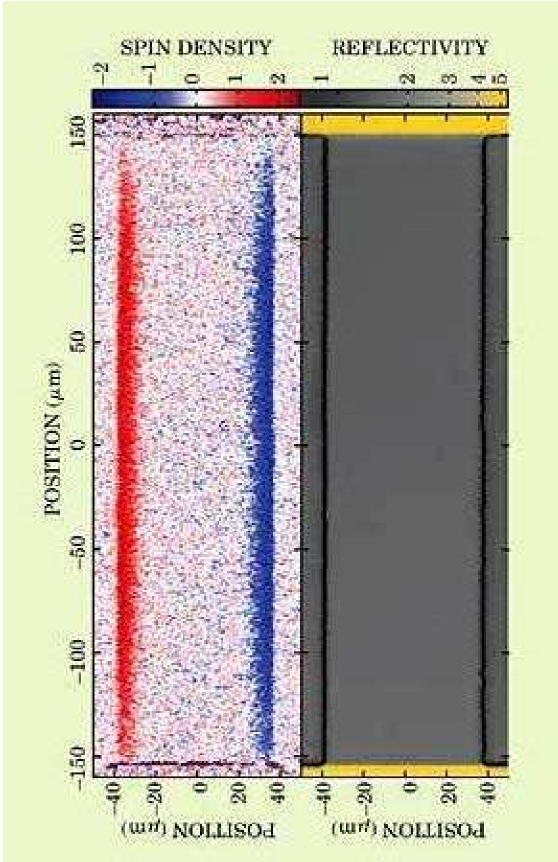
Due to SO interaction between electron and impurity

- Skew scattering (Smit, Physica 1955)



- Side jump (Berger, PRB 1970)





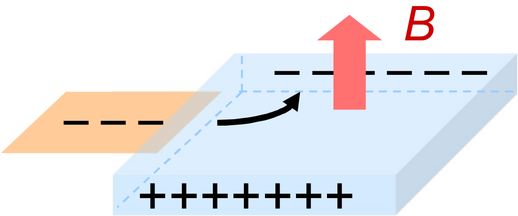
Local Kerr effect in strained n-type bulk InGaAs, 0.03% polarization

Kato et al, Science 2004

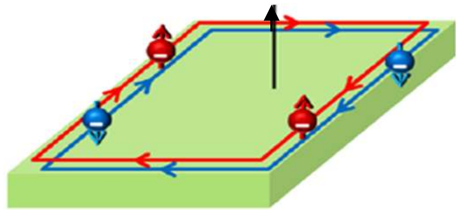
From quantum Hall effect to quantum spin Hall effect

w/o TRS

- Hall (1879)



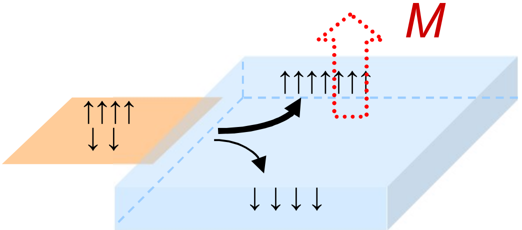
- QHE (1980)



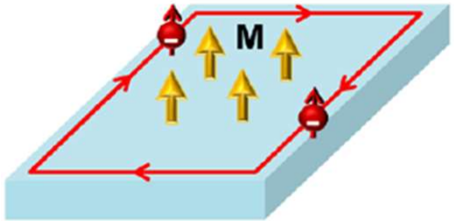
- MOSFET
- Heterojunction
- Graphene
- …

(2D only)

- AHE (1881)



- QAHE (2013)

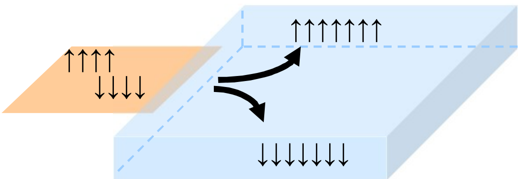


- Bi_2Te_3 doped with Cr etc
- $MnBi_2Te_4$
- …

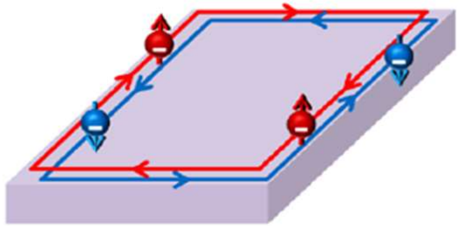
(2D only)

w/ TRS

- SHE (2004, intrinsic)



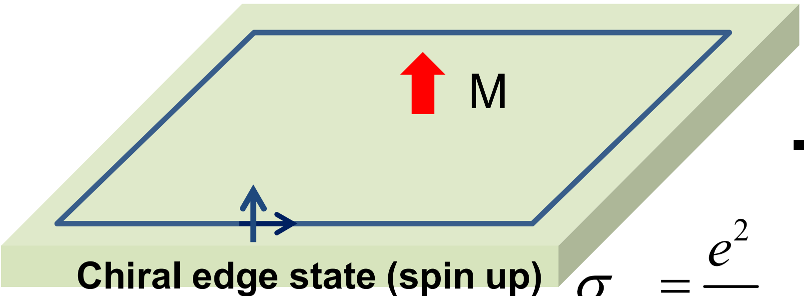
- QSHE (2007) ➡ **Topological insulator**



- HgTe QW
- WTe_2
- …

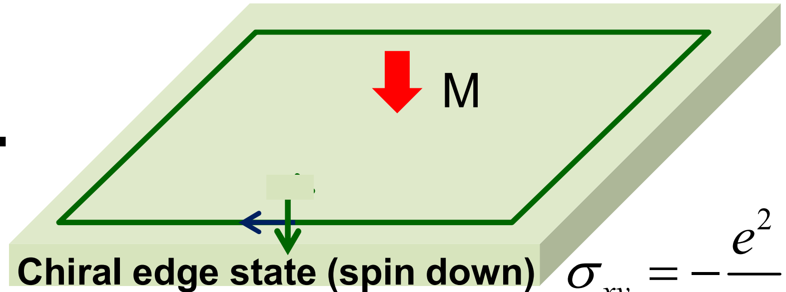
Chang and Li, J Phys 2016

Quantum spin Hall effect ~ two copies of QAHE



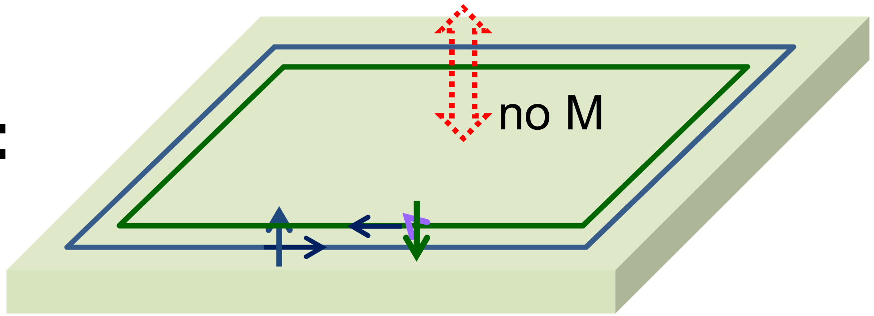
$$\sigma_{xy} = \frac{e^2}{h}$$

+



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

=



Helical edge state

$$\sigma_{xy} = 0$$

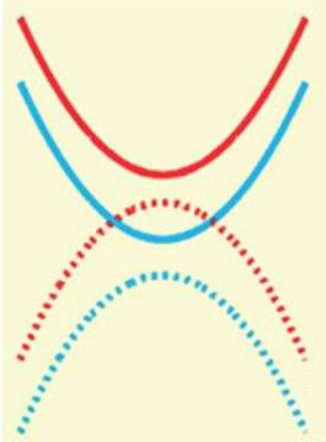
$$\text{but} \quad \sigma^s_{xy} = \frac{e}{2\pi} \quad \left(e \to \frac{\hbar}{2} \right)$$

- 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.

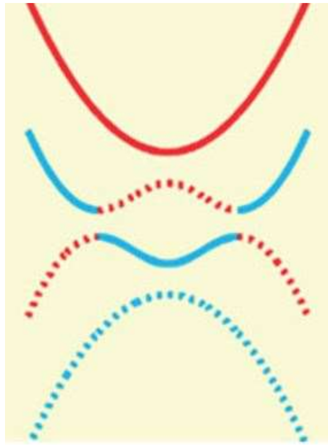
Band inversion and topology

QAH

Band
inversion



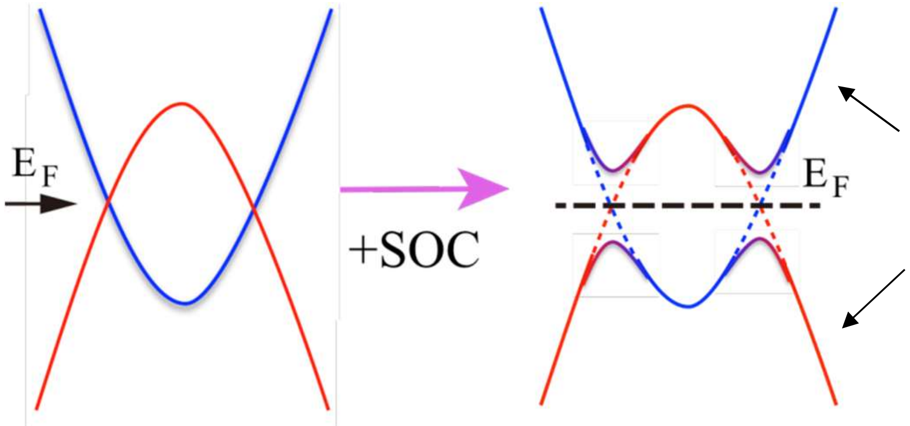
Turn on magnetization



Turn on SOC

QSH

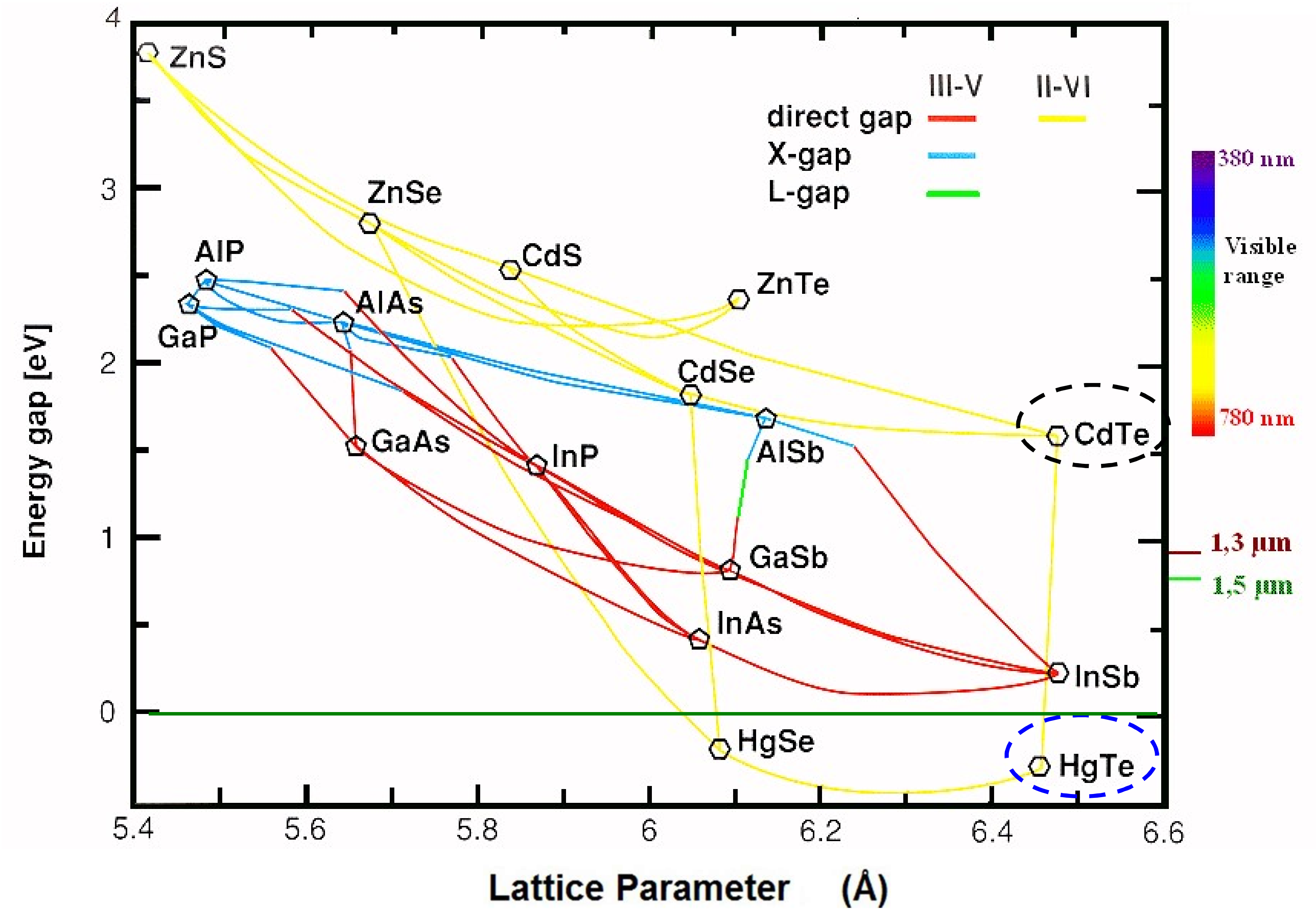
Band
inversion
(negative
bandgap)



Bloch bands with
opposite Berry
curvatures

Inversion by nature
(Time-Reversal Symm
preserved)

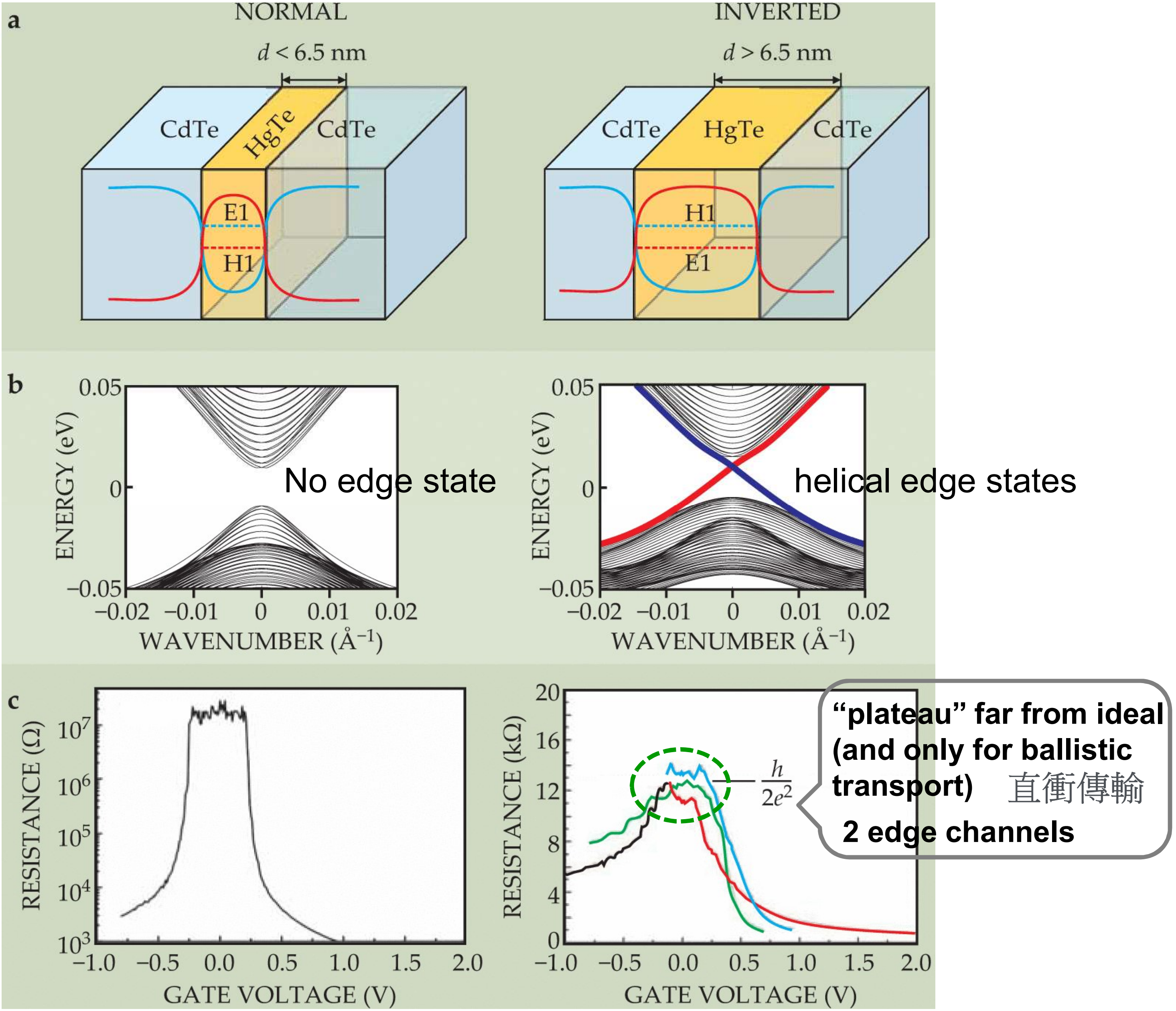
Looking for natural band inversion



(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

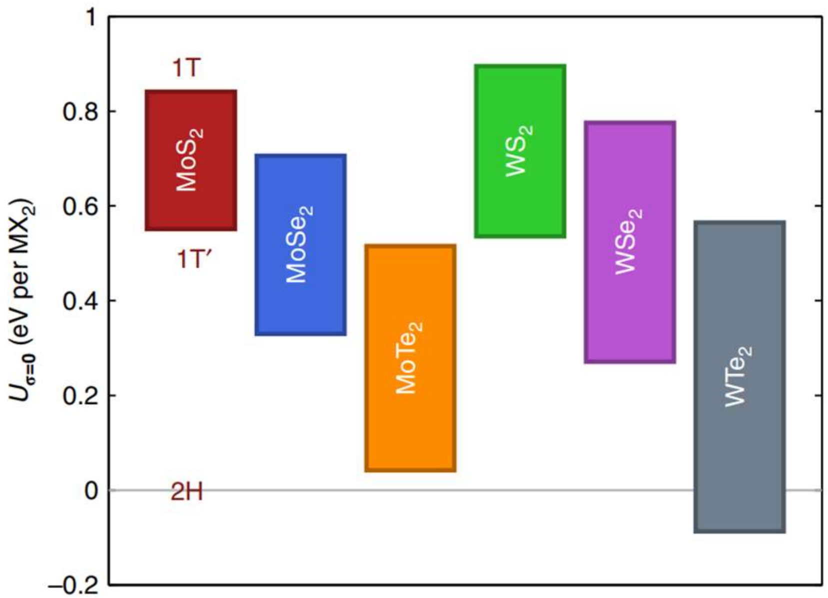
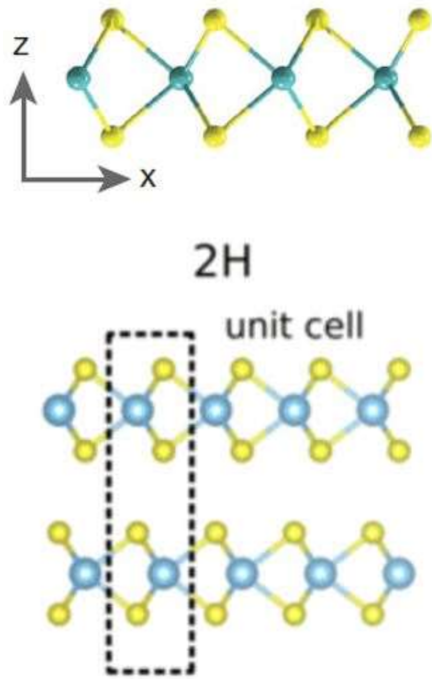


Figure 2 | Ground-state energy differences between monolayer phases of the six studied materials. The energy U is given per formula unit MX_2 for

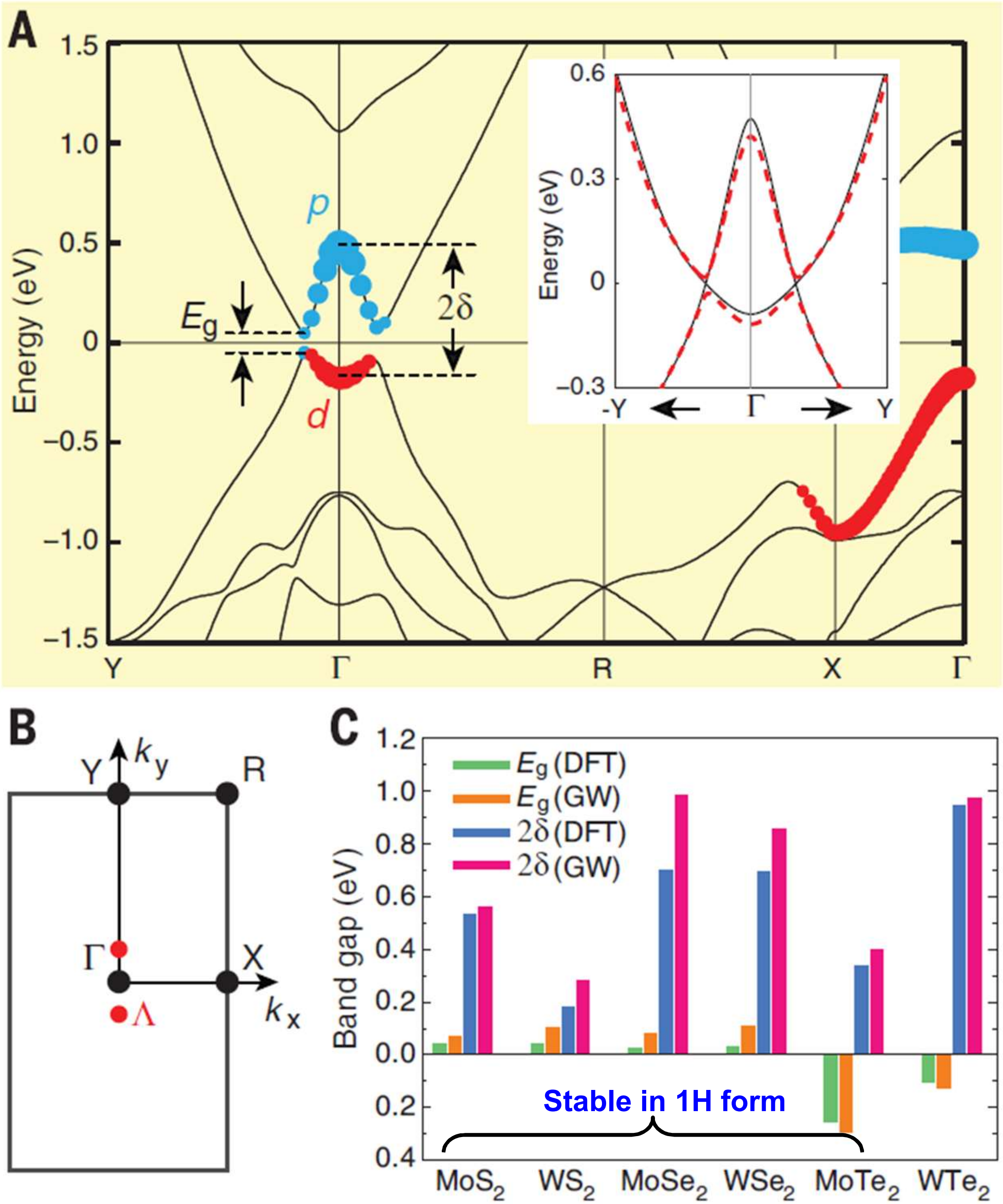
1H



Duerloo et al, Nat Comm 2014

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

Band inversion



w/o and w/ SOC

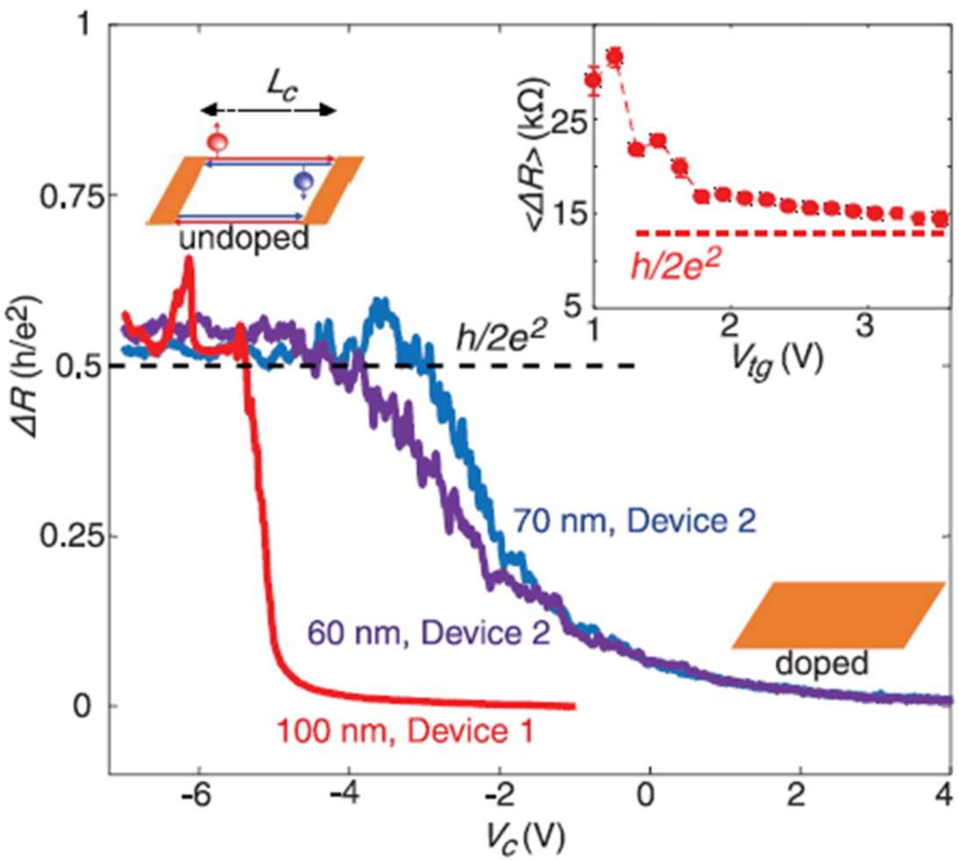
Qian, Science 2014

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

With electron spin, the Bloch states become spinors

$$\psi_{n\vec{k}} = \begin{pmatrix} \varphi_{n\vec{k}\uparrow} \\ \varphi_{n\vec{k}\downarrow} \end{pmatrix}$$

- Without SOC (or with S_zL_z coupling only), the energy eigenstates are

$$\psi_{n\vec{k}\uparrow} = \varphi_{n\vec{k}\uparrow} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\psi_{n\vec{k}\downarrow} = \varphi_{n\vec{k}\downarrow} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

- Without SOC, $H_{so} = \lambda_{so}\boldsymbol{\sigma} \times \mathbf{p} \cdot \nabla V_L$

the energy eigenstates are $\psi_{n\vec{k}\pm}$

If SOC is weak, then

$$\psi_{n\mathbf{k}\pm} \simeq \psi_{n\mathbf{k}\uparrow/\downarrow}$$

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,

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

$\Rightarrow$ $\Theta^2 = -1$

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

- Spinor Bloch state under TR

$$\begin{pmatrix} \varphi_{n\vec{k}\uparrow} \\ \varphi_{n\vec{k}\downarrow} \end{pmatrix} \rightarrow \Theta \begin{pmatrix} \varphi_{n\vec{k}\uparrow} \\ \varphi_{n\vec{k}\downarrow} \end{pmatrix} = \begin{pmatrix} -\varphi^*_{n-\vec{k}\downarrow} \\ +\varphi^*_{n-\vec{k}\uparrow} \end{pmatrix}$$

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.

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

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

(global 2-fold degeneracy)

- With TRS, without SIS

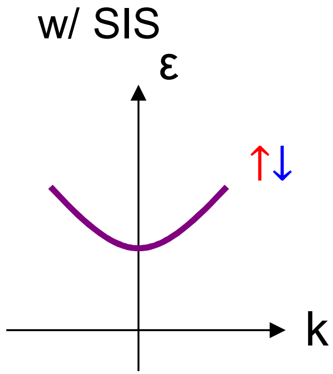
$$\varepsilon_{n-\mathbf{k}s} \neq \varepsilon_{n\mathbf{k}s}$$

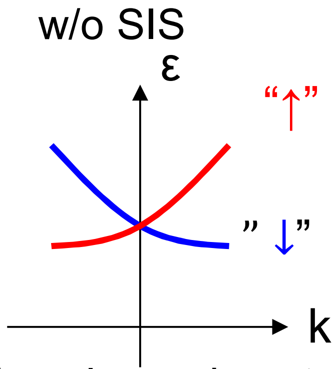
Except at time-reversal-invariant momentum (TRIM)

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

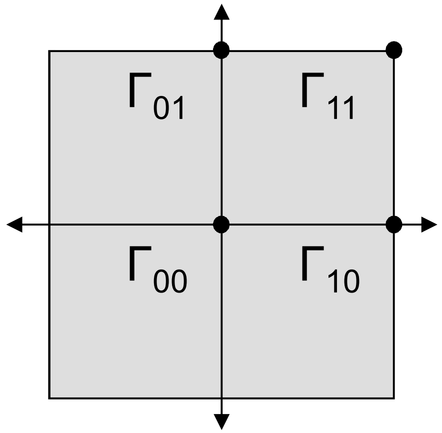
At TRIM

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





Level crossing at TRIM



TRIM

Different ways to characterize the topology of a QSHI (2D TI)

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

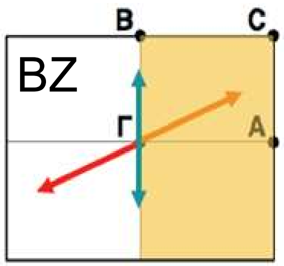
   (see, e.g., Favata and Marrazzo, Electronic Structure 2023)

Quantum spin Hall effect intro, by C. Kane

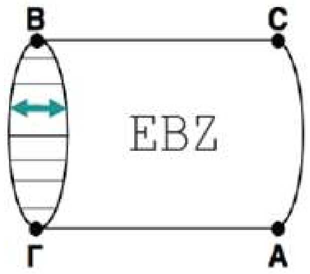
Quantum spin Hall effect summary, by C. Kane

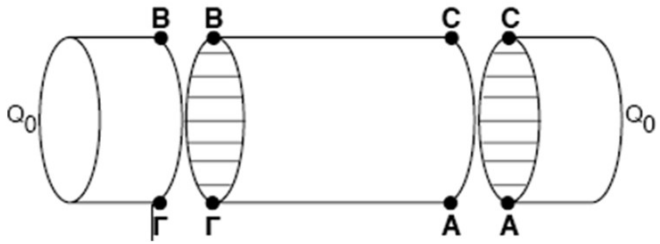
1 Topology in 2D TI (Moore and Balent, PRB 07)

Consider lattice fermions with time reversal symmetry



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, but 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,

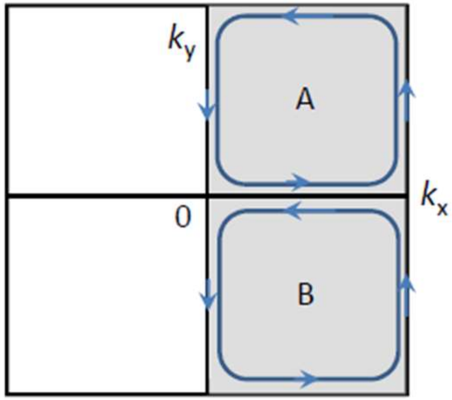
adopt TR-smooth gauge,

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

→ 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



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

- Gauge transformation

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

U(2) matrix

- Winding number of the phase of gauge-transition

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

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

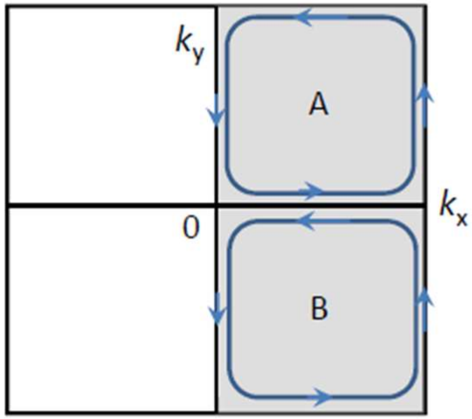
$$\oint_{\partial A} d\mathbf{k} \cdot \mathbf{A}^A = \int_A d^2k \; F_z^A$$

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

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

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

mod-2 gauge invariant

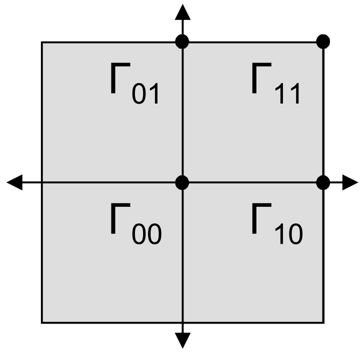


Cf: Gauss-Bonnet theorem for a 2D surface with edge

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

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

then a Bloch state at TRIM Γ_i have definite parities



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

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

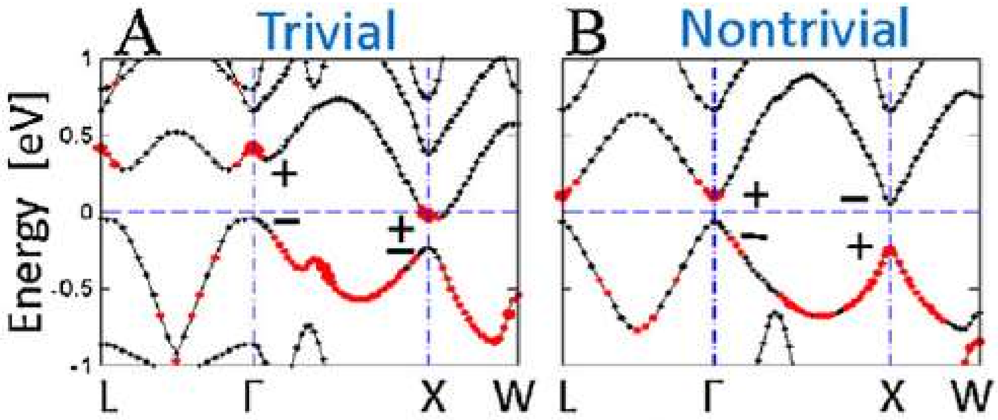
- Z_2 topological number

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

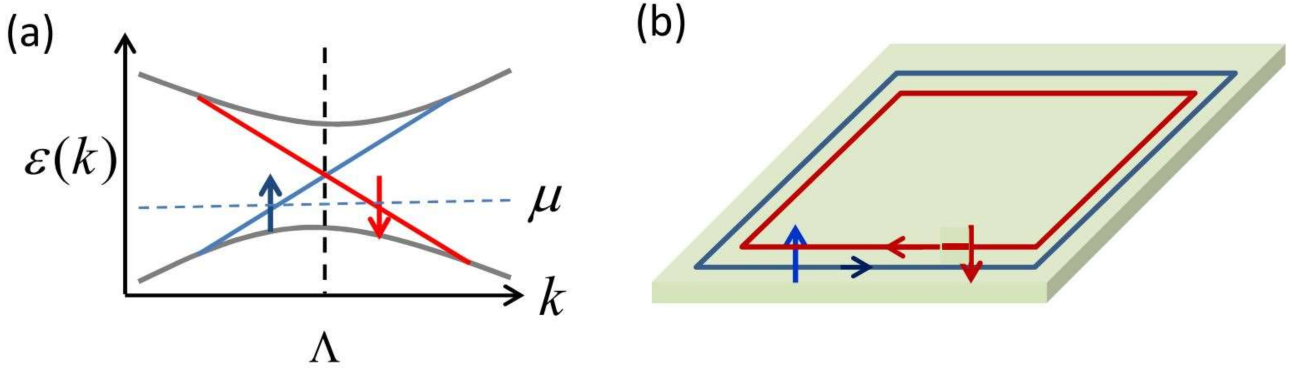
$$(-1)^\nu \equiv \delta_1\delta_2\delta_3\delta_4 = -1$$ (topo phase)

$\Rightarrow$ $\nu = 0{,}1$

- Parity change, and topological transition

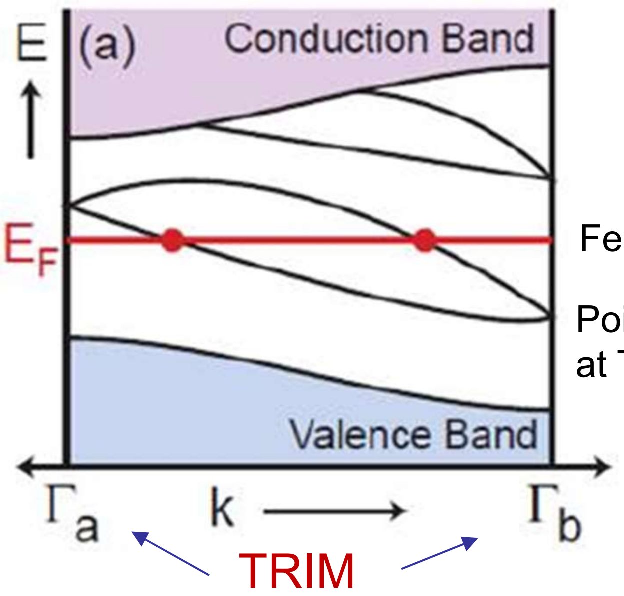


Helical edge states of 2D TI, spin-momentum locking



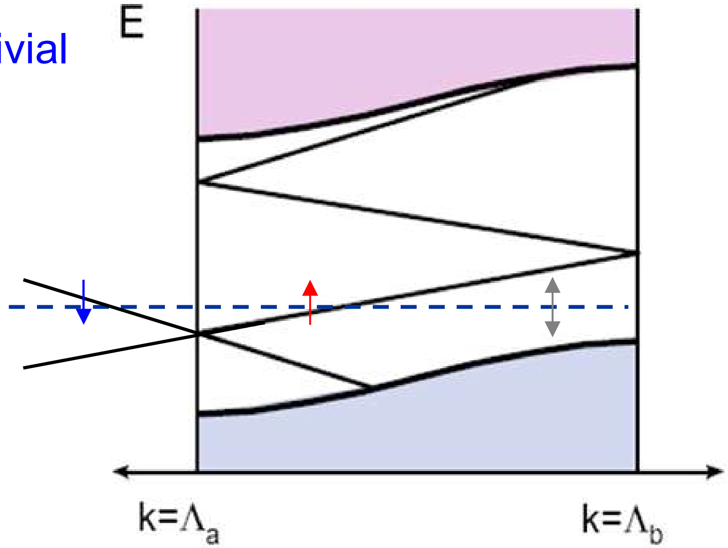
Trivial insulator vs nontrivial insulator

Trivial



fragile surface state

Non-trivial



robust edge channels, but
spin transport is not quantized.

3D Topological insulator

A. Fermi circle of the surface state

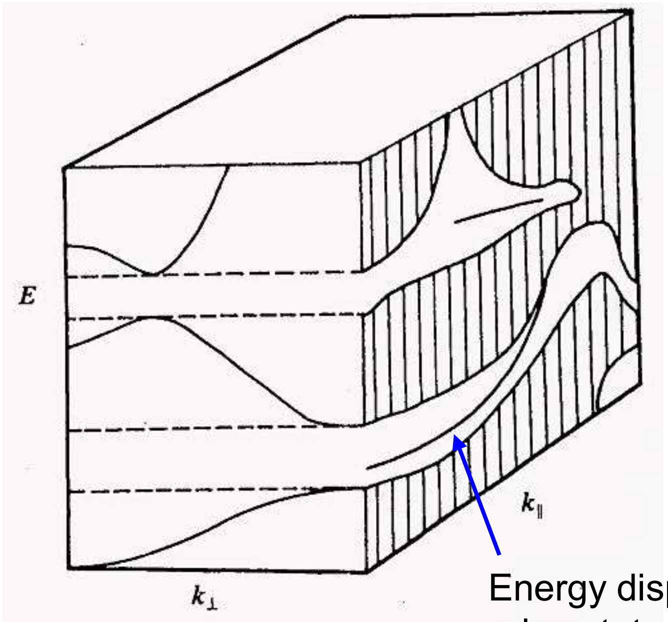
B. Weak topological indices

C. Bulk-edge correspondence

D. Topological crystalline insulator and beyond

The energy bands in 2D BZ projected to 1D surface BZ (similarly, 3D to 2D)

Bulk energy bands

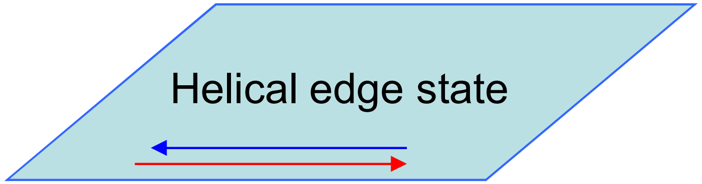


Projected bulk bands

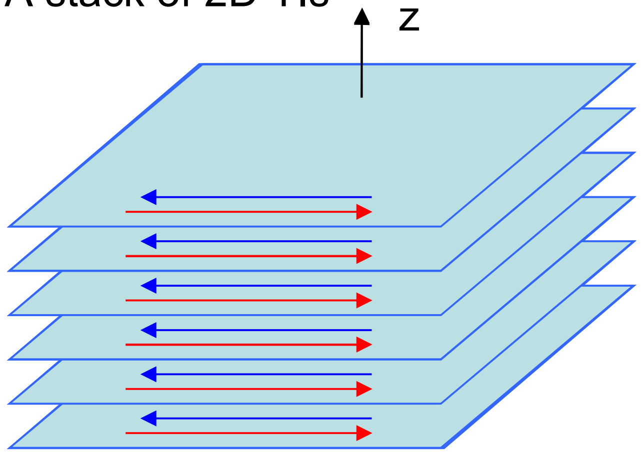
Energy dispersion of edge state

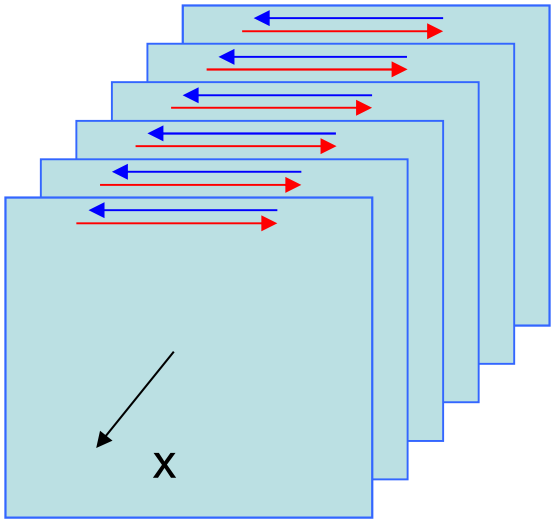
From 2D TI to 3D TI

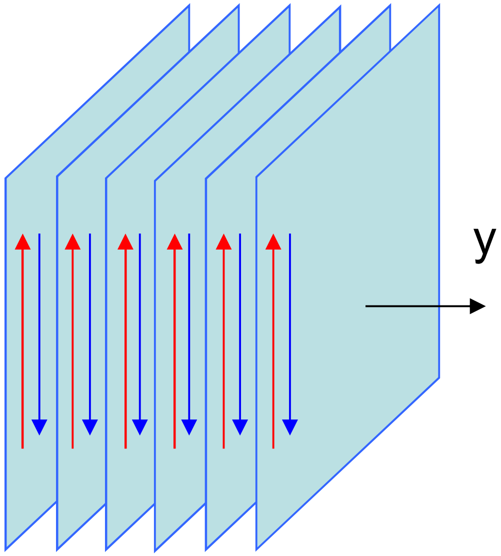
Real space



A stack of 2D TIs





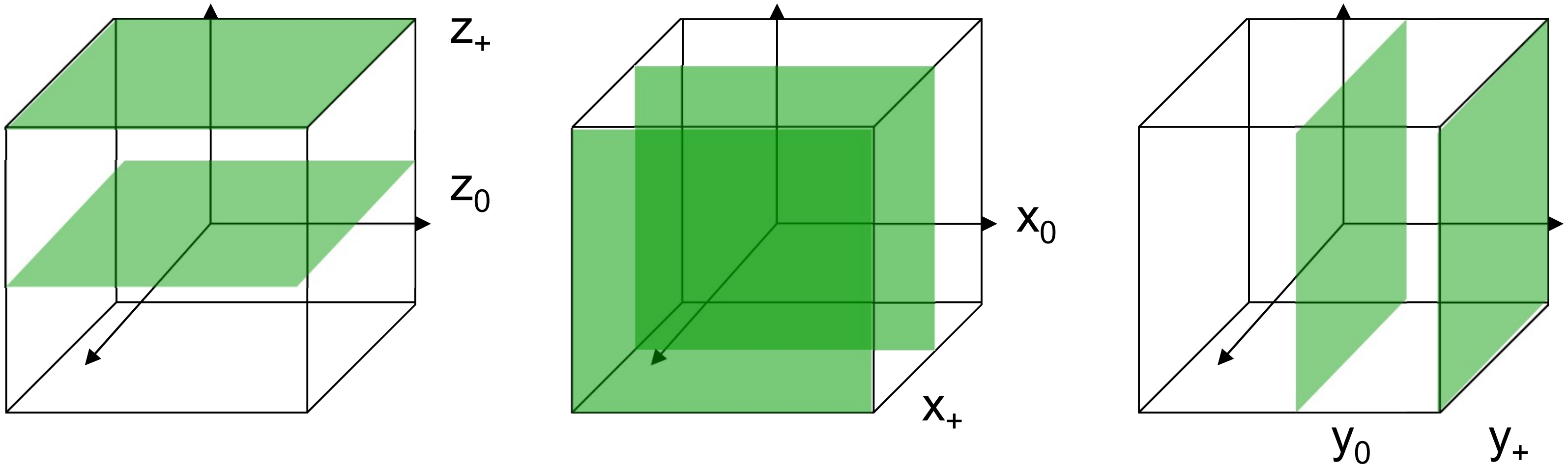


3 TI indices

Momentum space

According to the Moore-Balent argument,

each time-reversal invariant plane has a Z_2 index



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

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

➡ 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

➡ only 4 independent Z_2 numbers

Fu, Kane, and Mele PRL 07
Moore and Balents PRB 07
Roy, PRB 09

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

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

strong; weak

For example,

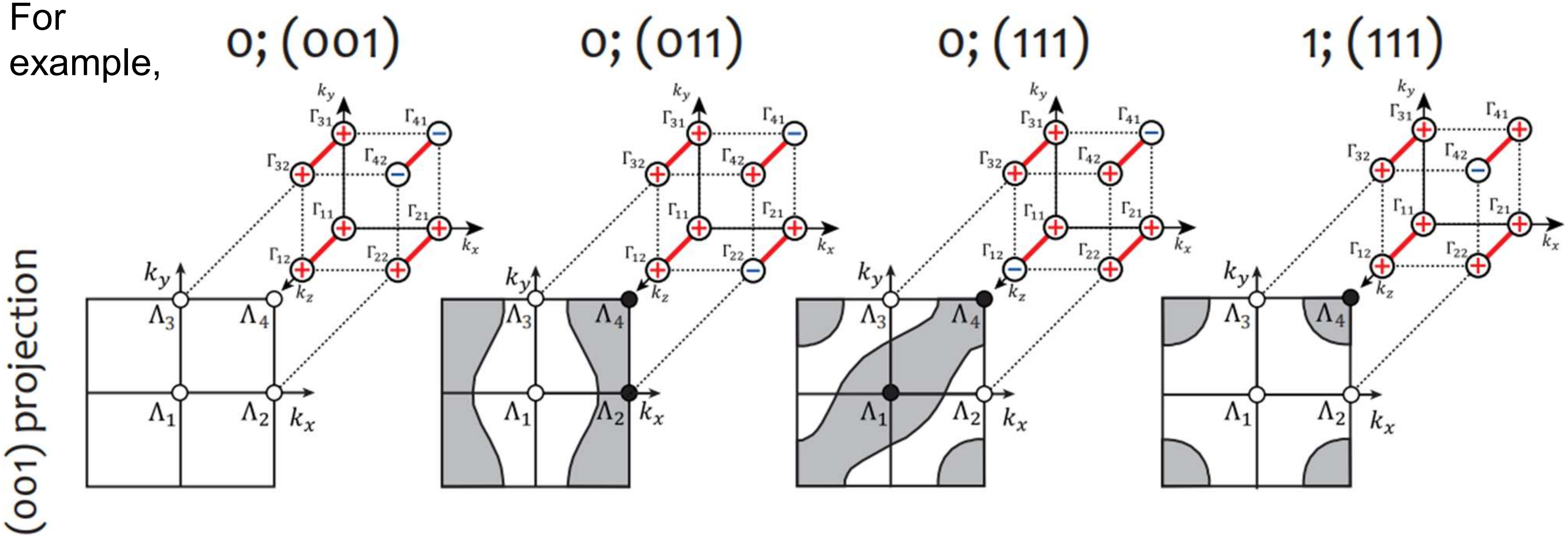
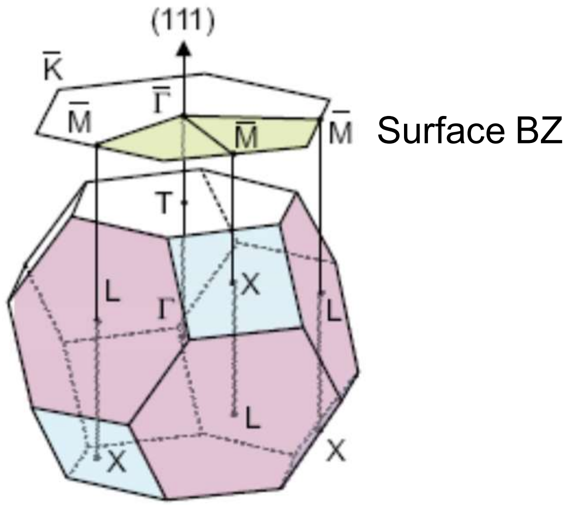


Fig. from Eschbach, 2016

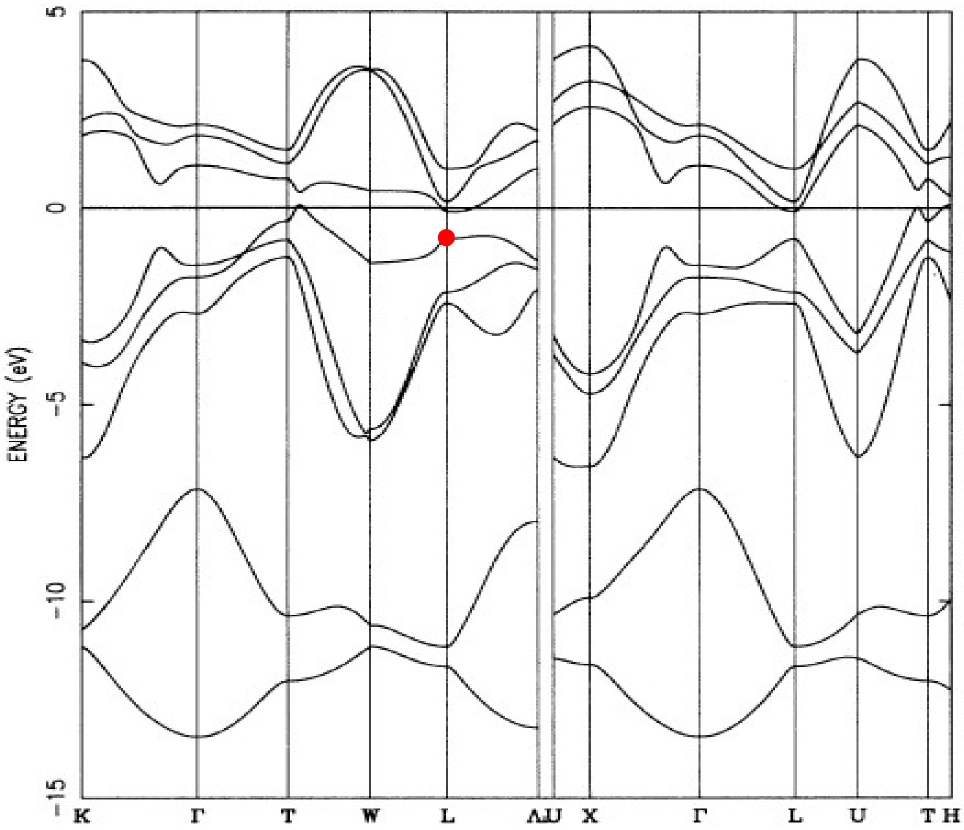
~ 2D TIs stacked along $\vec{M}_\nu = \left(\nu_1 \vec{b}_1 + \nu_2 \vec{b}_2 + \nu_3 \vec{b}_3\right)/2$

$Bi_{1-x}Sb_x$ 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)

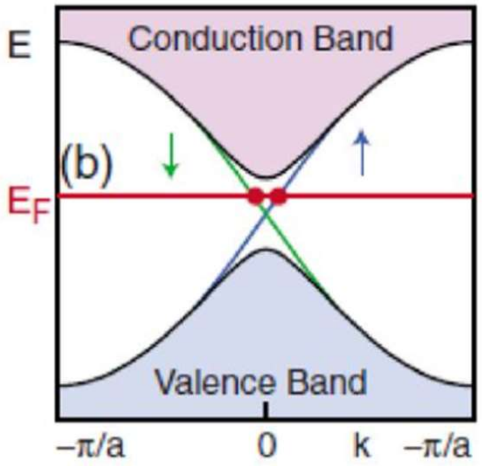


Bismuth	parities
$\Gamma_6^+ \Gamma_6^- \Gamma_6^+ \Gamma_6^+ \Gamma_{45}^+$	$-$
$L_s\ L_a\ L_s\ L_a\ L_a$	$-$
$X_a\ X_s\ X_s\ X_a\ X_a$	$-$
$T_6^- T_6^+ T_6^- T_6^+ T_{45}^-$	$-$
Z_2 class	(0;000)
Antimony	
$\Gamma_6^+ \Gamma_6^- \Gamma_6^+ \Gamma_6^+ \Gamma_{45}^+$	$-$
$L_s\ L_a\ L_s\ L_a\ L_s$	$+$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

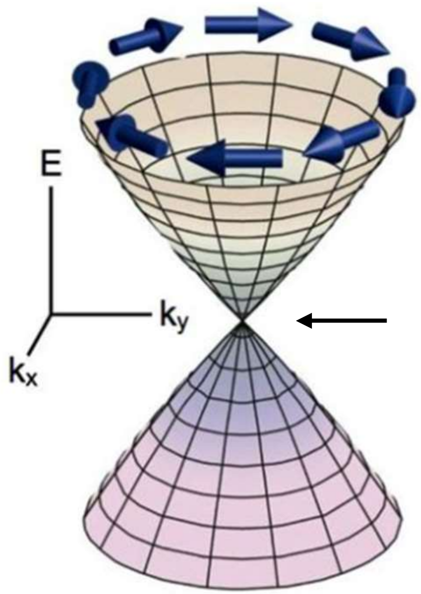
5 filled bands

Spin-momentum locking

Dirac cone of surface state at TRIM



TRIM



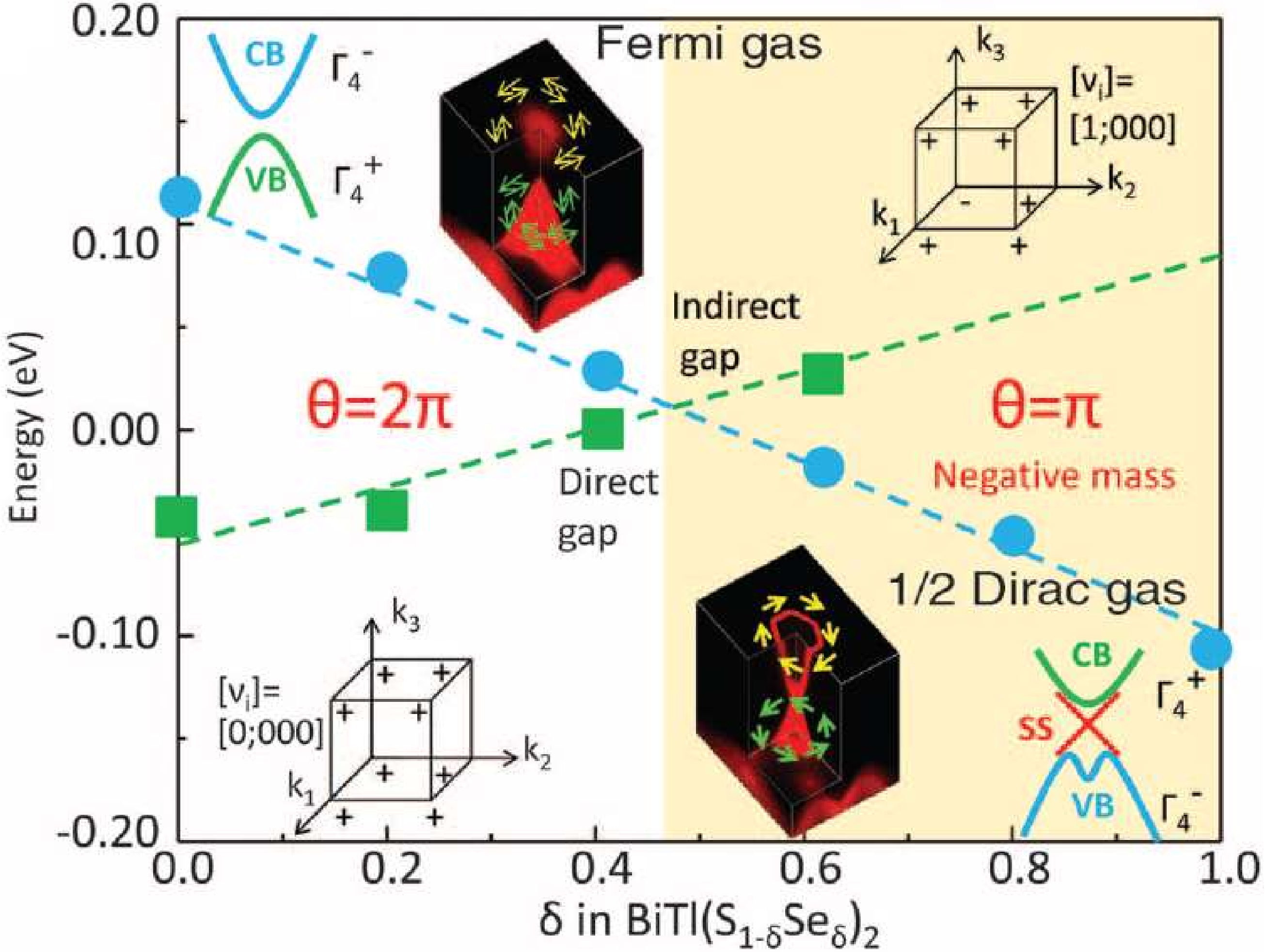
Dirac cone

Dirac point

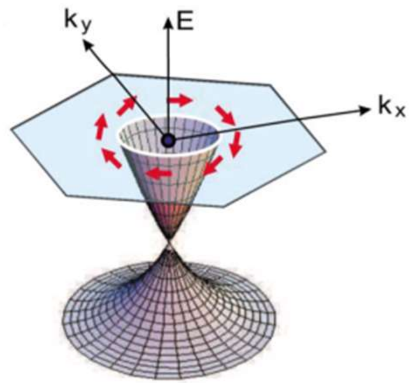
Spin-resolved ARPES

Band inversion, parity change, emergence of SS, and

spin-momentum locking

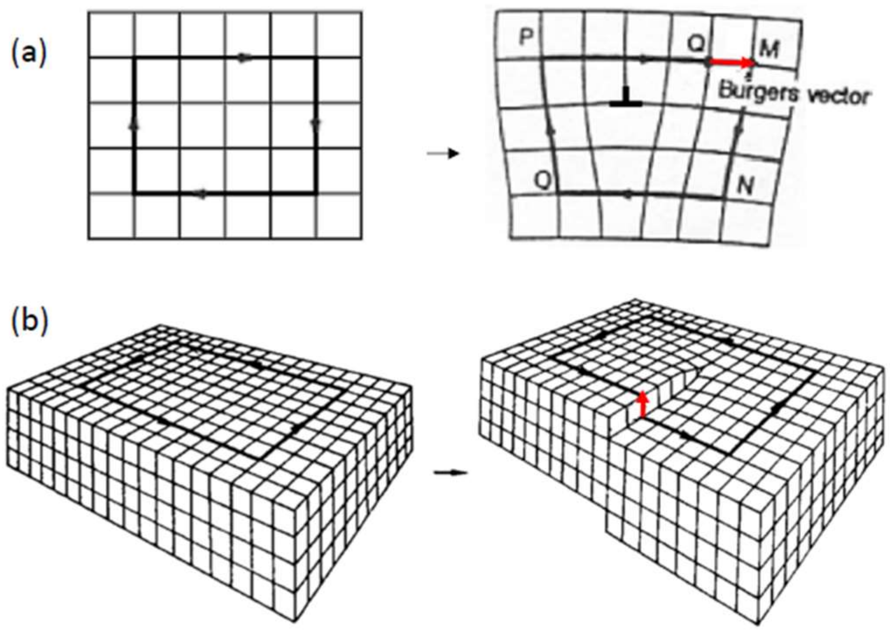


$$H_{SS} = \alpha(\vec{k} \times \vec{\sigma})_z$$



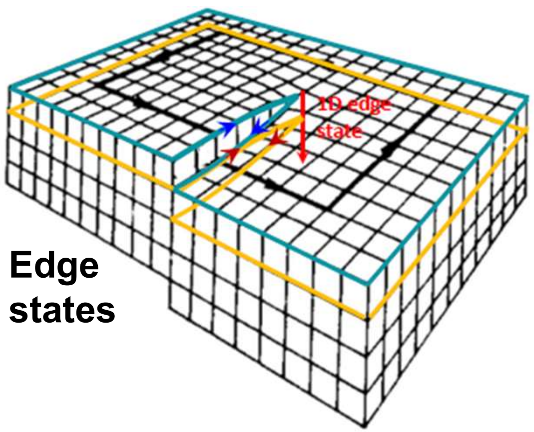
S.Y. Xu et al Science 2011

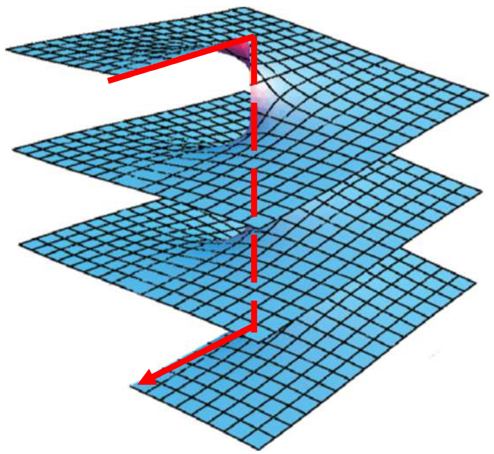
Weak TI index and defect



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

Liang Fu

Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA

(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
- 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)

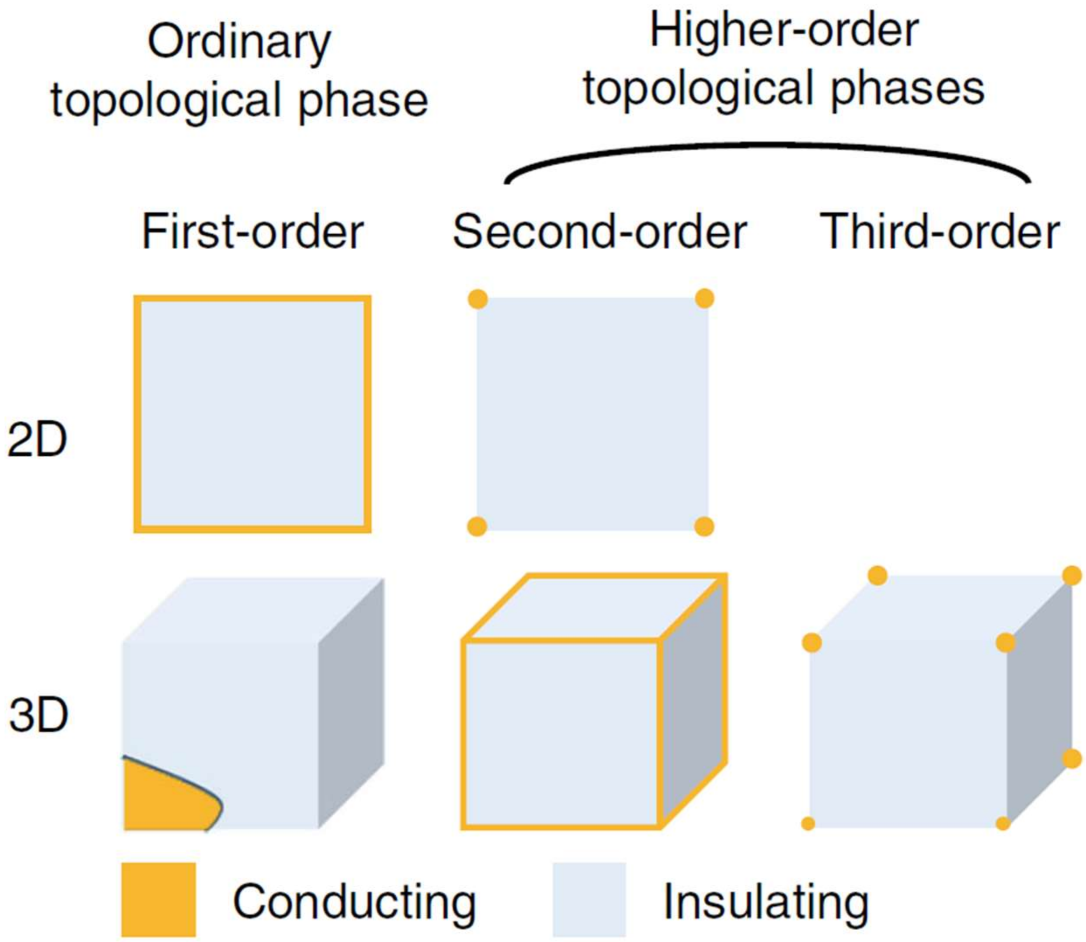

Fig from Kim et al, in Light: Science & Applications (2020)