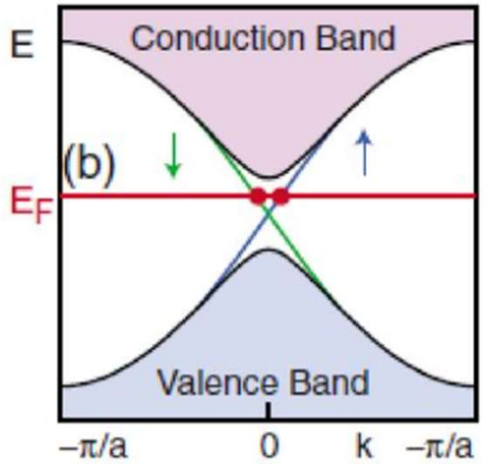
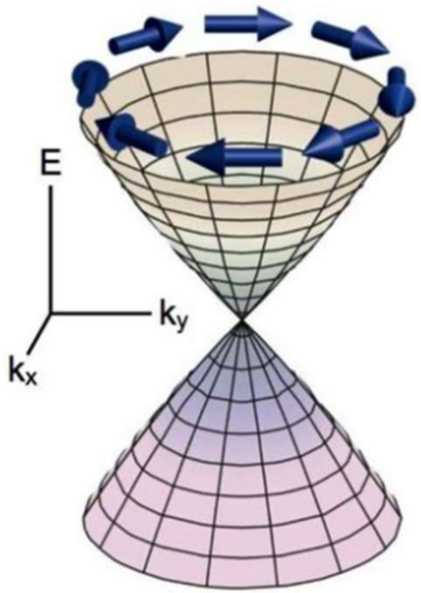
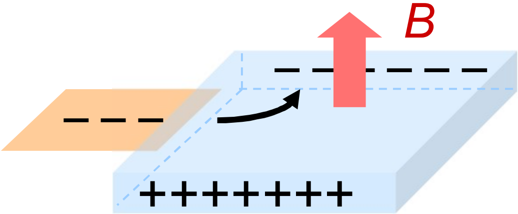
Introduction to topological insulator



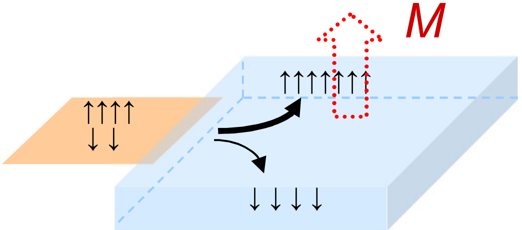


w/o TRS

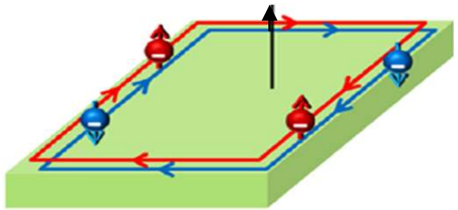
- Hall (1879)



- AHE (1881)



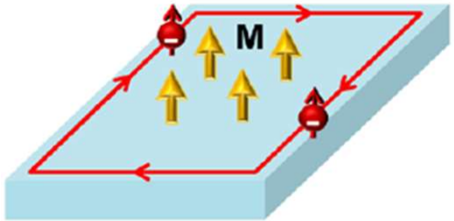
- QHE (1980)



- MOSFET
- Heterojunction
- Graphene
- …

(2D only)

- QAHE (2013)

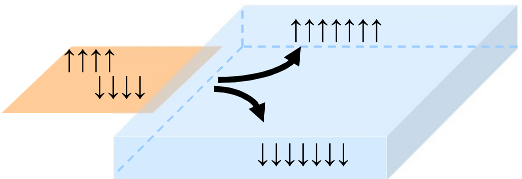


- Bi_2Te_3 doped with Cr etc
- $MnBi_2Te_4$
- …

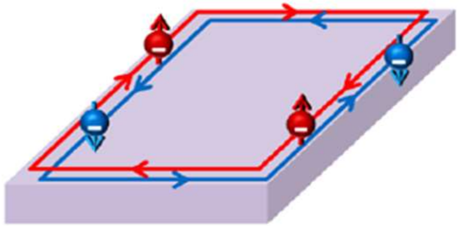
(2D only)

w/ TRS

- SHE (2004, intrinsic)



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



- HgTe QW
- WTe_2
- …

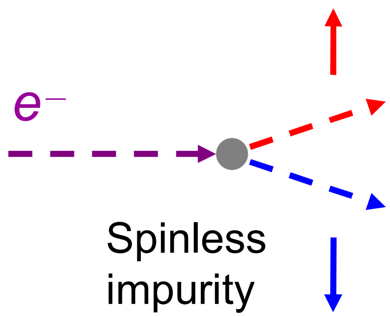
Chang and Li, J Phys 2016

Spin Hall effect: <u>extrinsic mechanism</u>

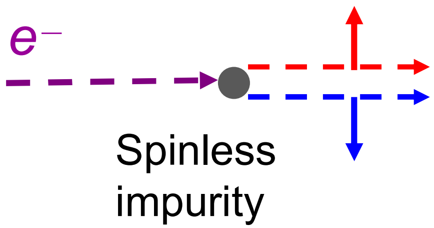
(Dyakonov and Perel, JETP 1971; J.E. Hirsch, PRL 1999.)

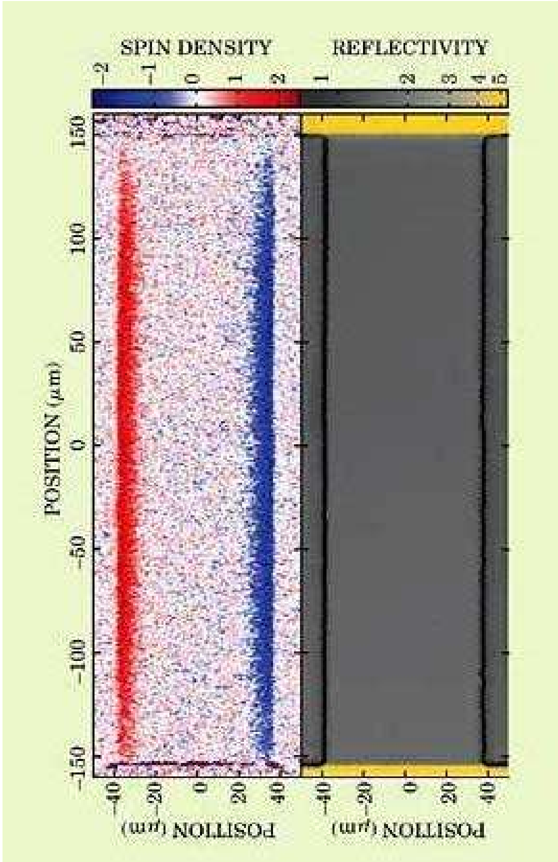
Due to SO interaction between electron and impurity

- Skew scattering (Smit, Physica 1955)



- Side jump (Berger, PRB 1970)





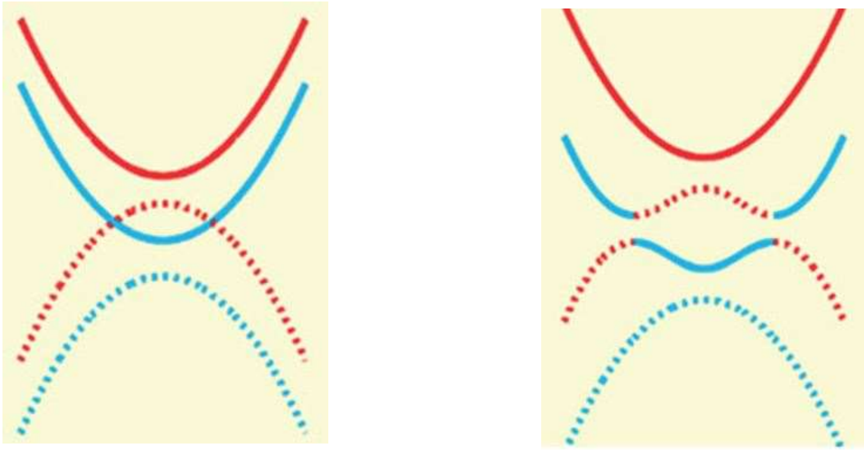
Local Kerr effect in strained n-type bulk InGaAs, 0.03% polarization

Kato et al, Science 2004

Band inversion and topology

QAH

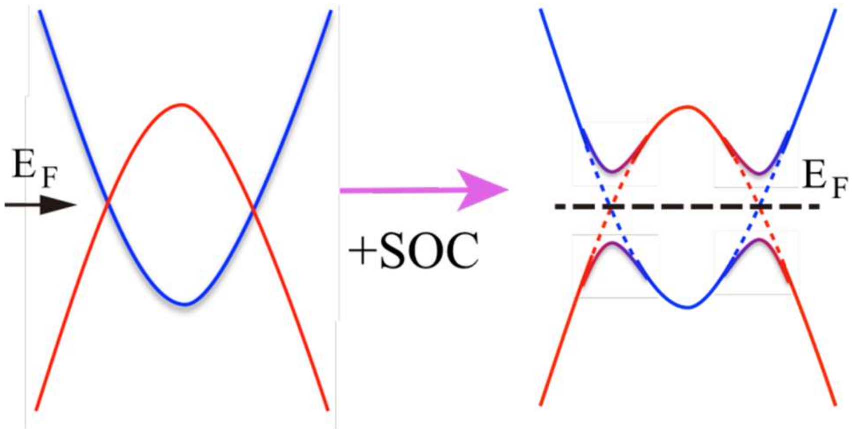
Band inversion



Turn on magnetization　　Turn on SOC

QSH

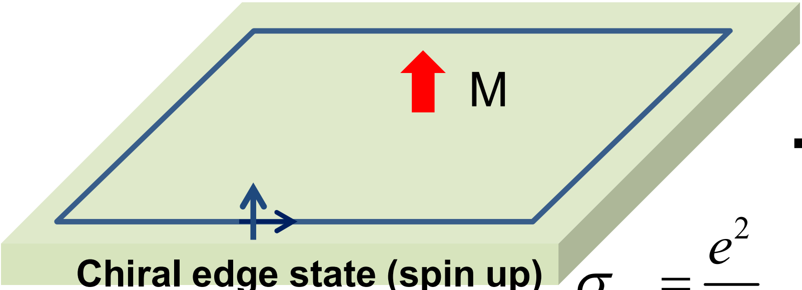
Band inversion



Degenerate spin levels with opposite Berry curvatures

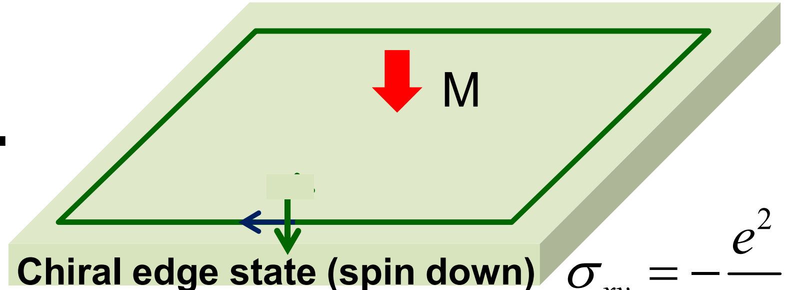
Inversion by nature (Time-Reversal Symm preserved)

Quantum spin Hall effect as two copies of QAHE



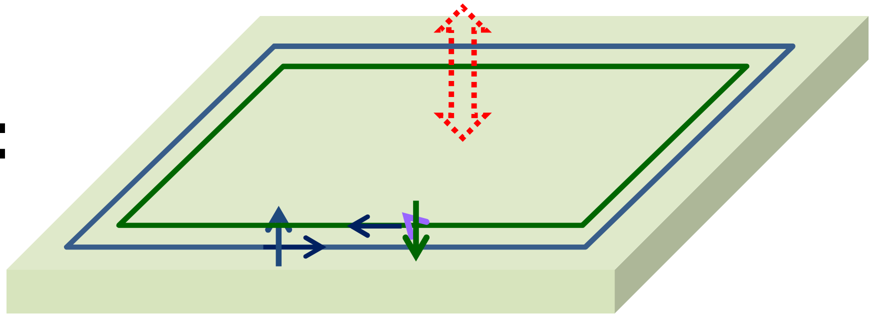
$$\sigma_{xy} = \frac{e^2}{h}$$

+



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

=



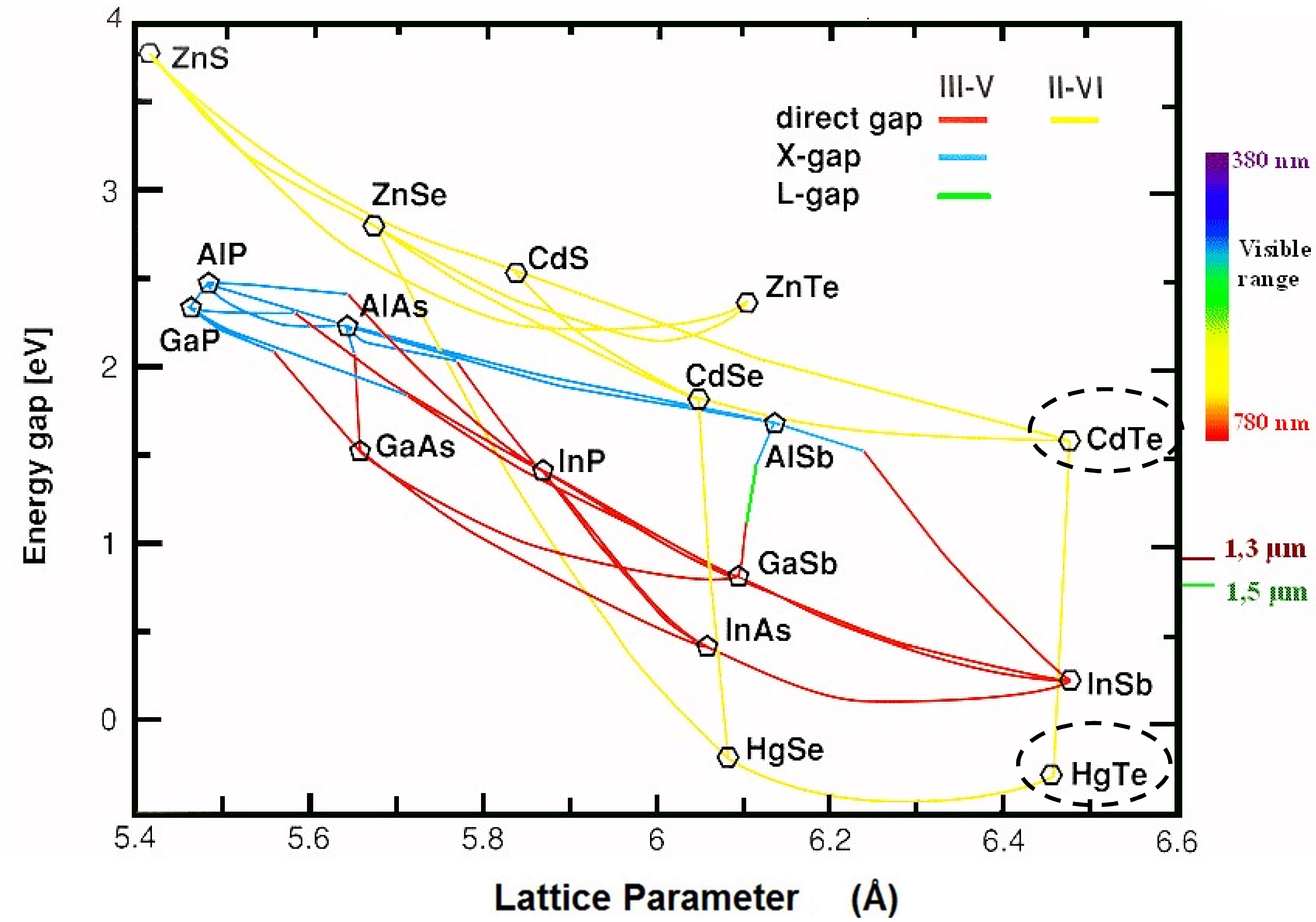
Helical edge state

$$\sigma_{xy} = 0$$

$$\text{but} \quad \sigma^{s}_{xy} = \frac{e}{2\pi}$$

- Spin current is no longer quantized when we turn on the spin-orbit coupling. But the edge states remain robust.

Band inversion

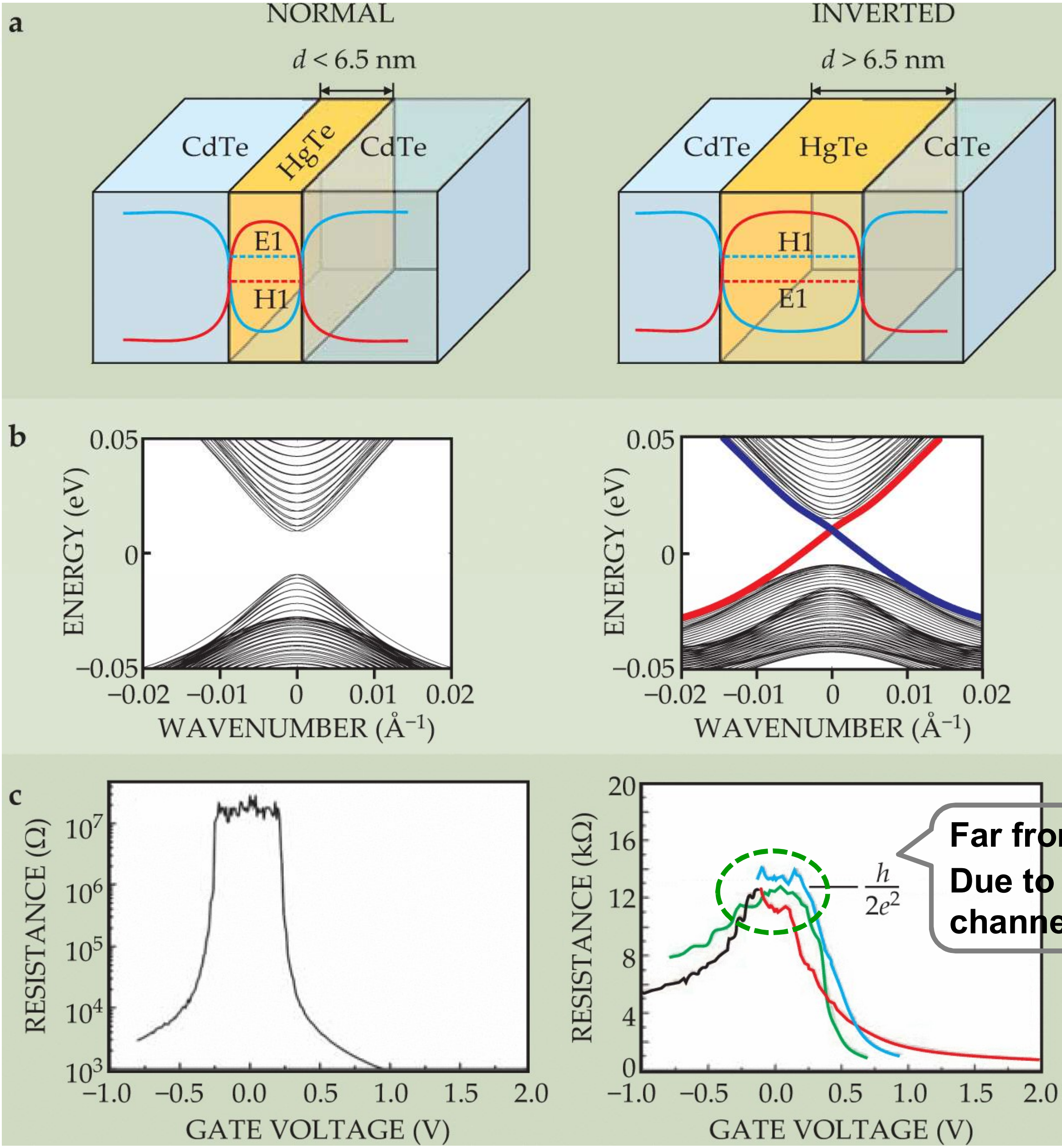


(Konig et al, Science 2007)

Quantum Spin Hall Insulator State in HgTe Quantum Wells

E1 ~ s orbital
H1 ~ p orbital

Band inversion, SO coupling

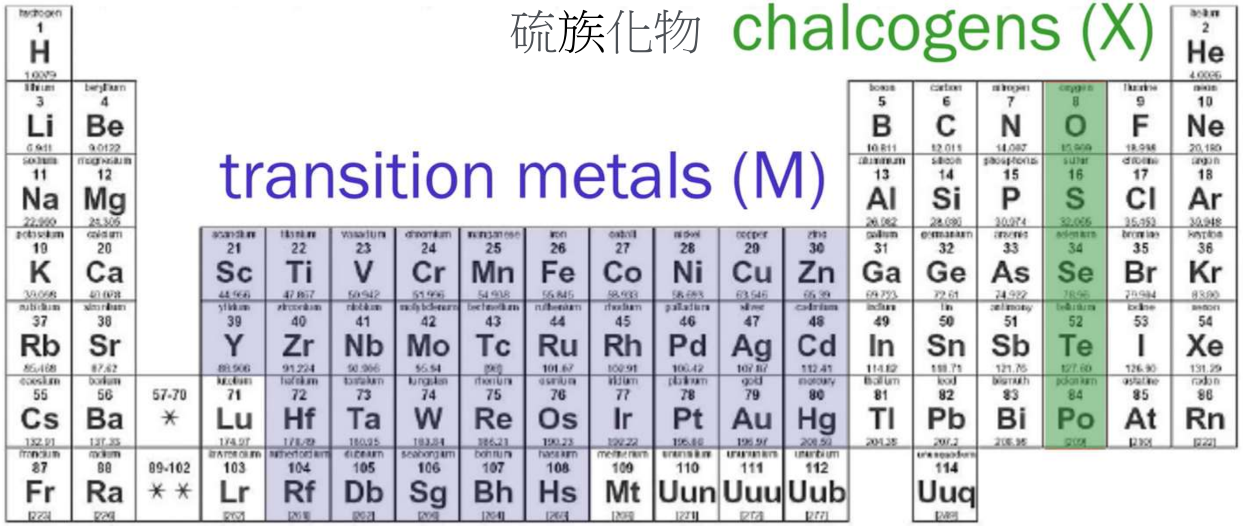


Far from ideal. Due to 2 edge channels

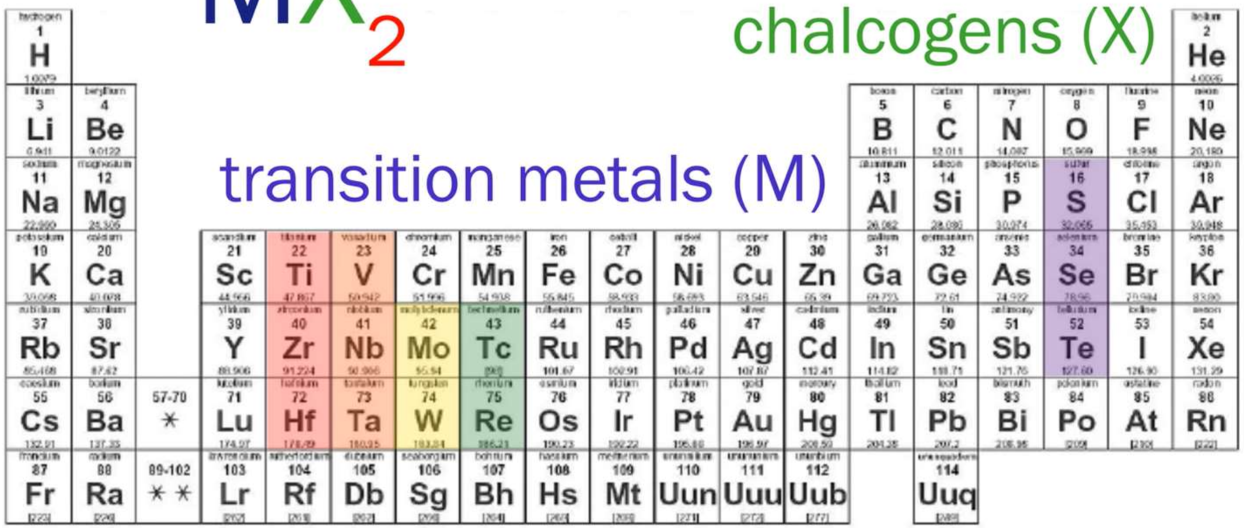
Qi and Zhang, Phys Today 2010

Science 2014

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



MX_2 Stable as a monolayer



3 possible forms:

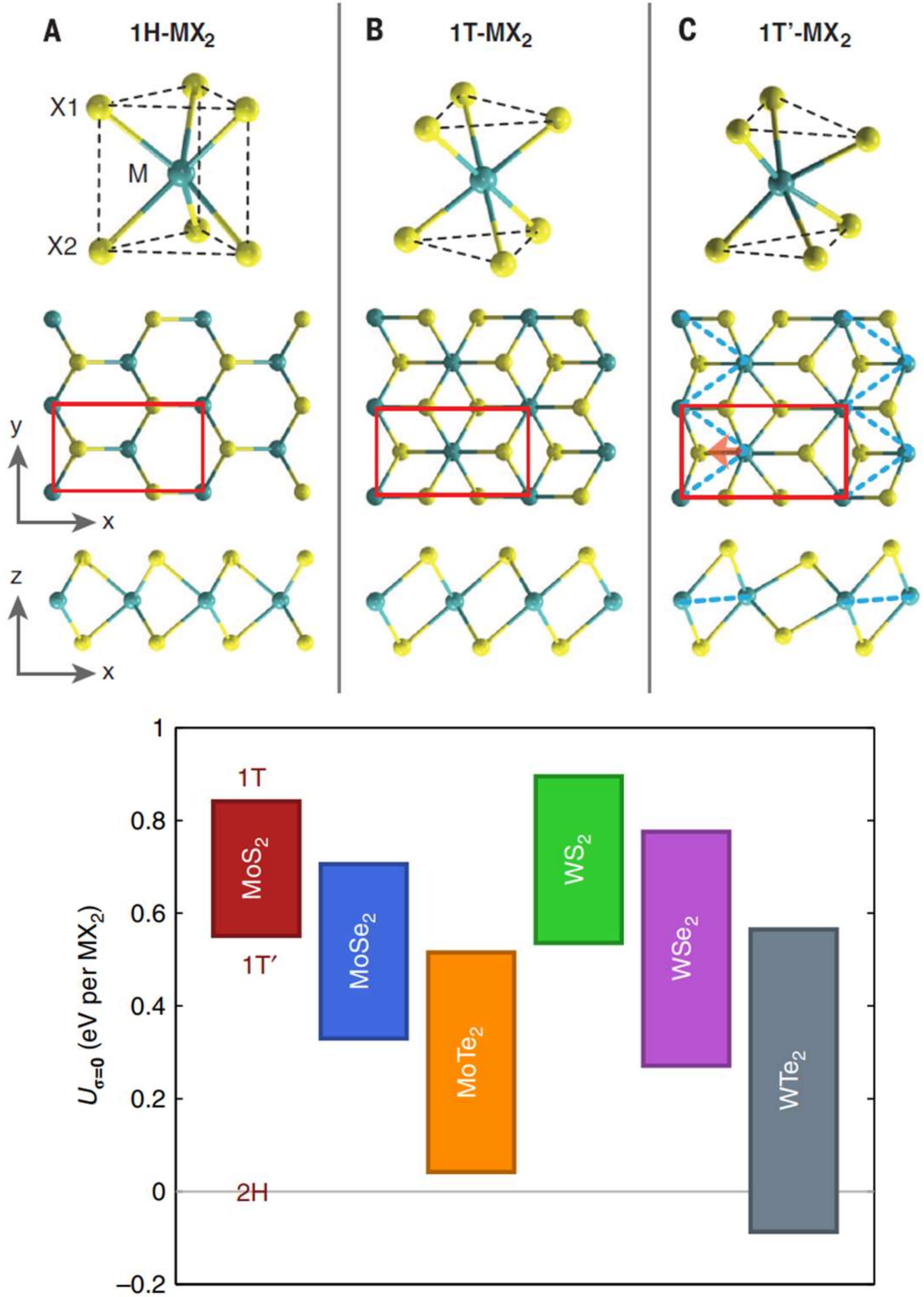
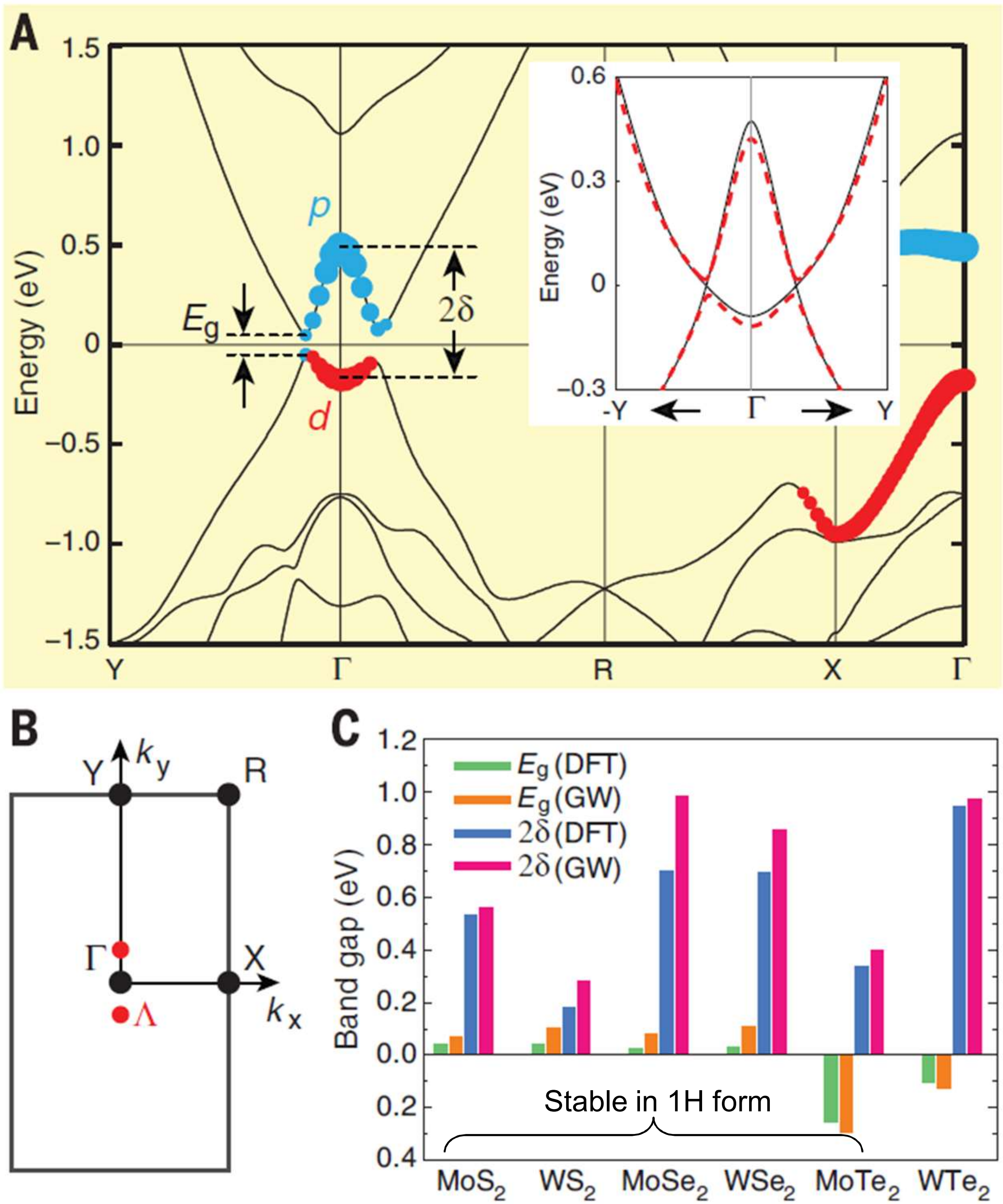


Figure 2 | Ground-state energy differences between monolayer phases of the six studied materials. The energy U is given per formula unit MX_2 for

Duerloo et al, Nat Comm 2014

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



w/o and w/ SOC

All are predicted to be QSHI in 1-T' form

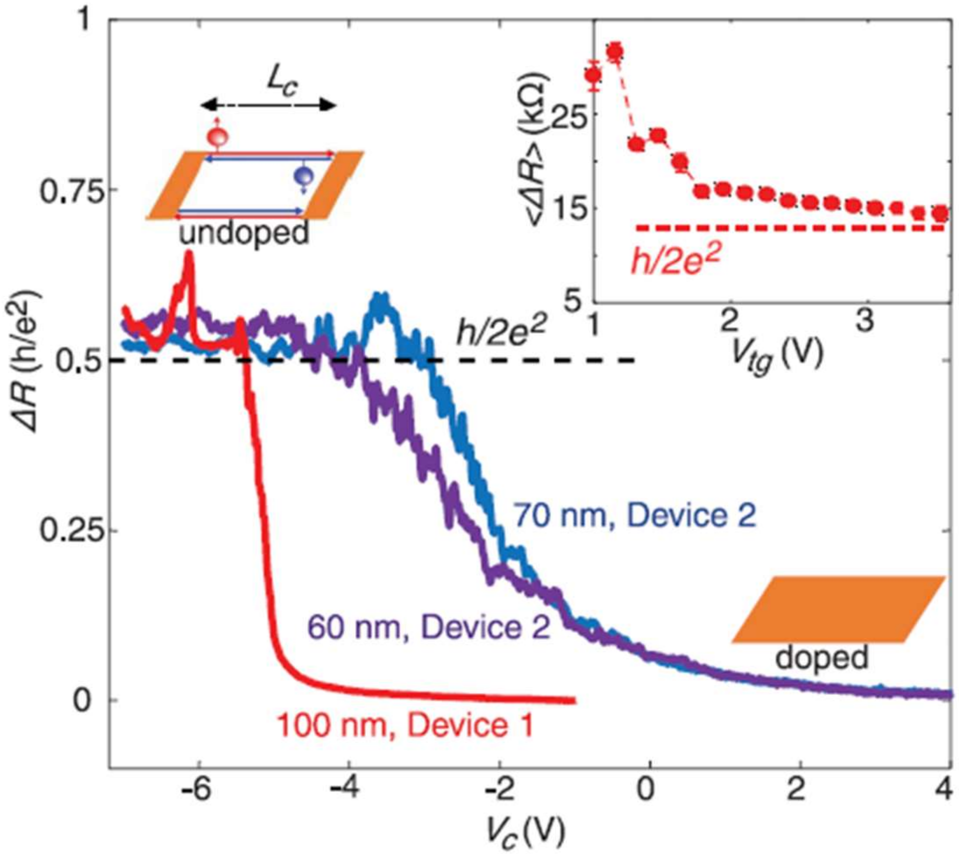
Qian, Science 2014

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]†

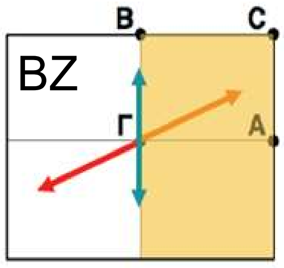
Science 2018



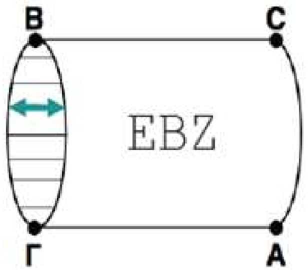
- “Plateau” exists only for ballistic transport
- Nothing is really quantized, except that there are “2” edge channels

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

Consider lattice fermion with time reversal symmetry (TRS)



- Without B field, Chern number C_1= 0
- Bloch states at *k*, -*k* are not independent, independent states live in EBZ.

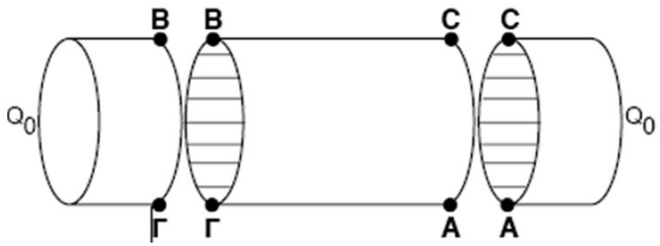


- EBZ is a cylinder, not a closed torus.

∴ 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"

Z_2 topological number

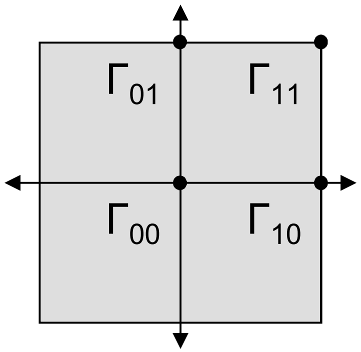
For a 2D insulator with SIS

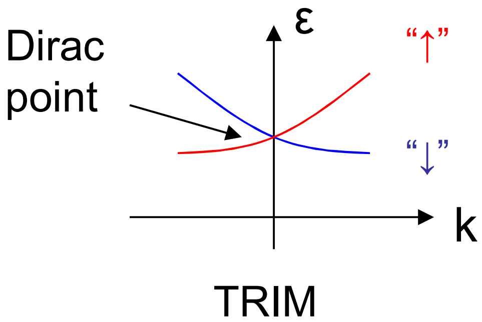
there is a simple way to determine the Z_2 integer
(unfortunately, there is no simple explanation)

Time reversal operator

$\Theta^2 = -1$ for fermions

- Kramer's degeneracy
- Time Reversal Invariant Momentum (TRIM)





If there is inversion symm,

then Bloch state at TRIM Γ_i has a definite parity

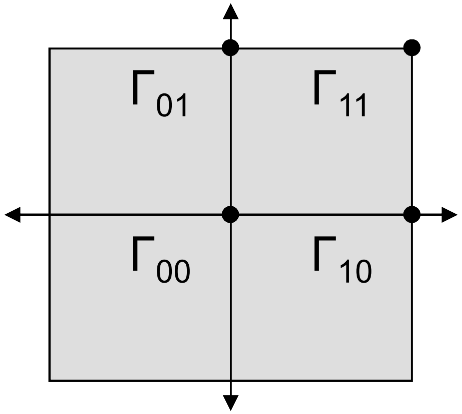
- Parity eigenvalue $\Pi\psi_{n\Lambda_i\alpha}(\mathbf{r}) = \zeta_{n\Lambda_i}\psi_{n\Lambda_i\alpha}(\mathbf{r})$ same for this pair

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

The Z_2 topological number (Fu and Kane 2006)

- Cumulative parity at Γ_i

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

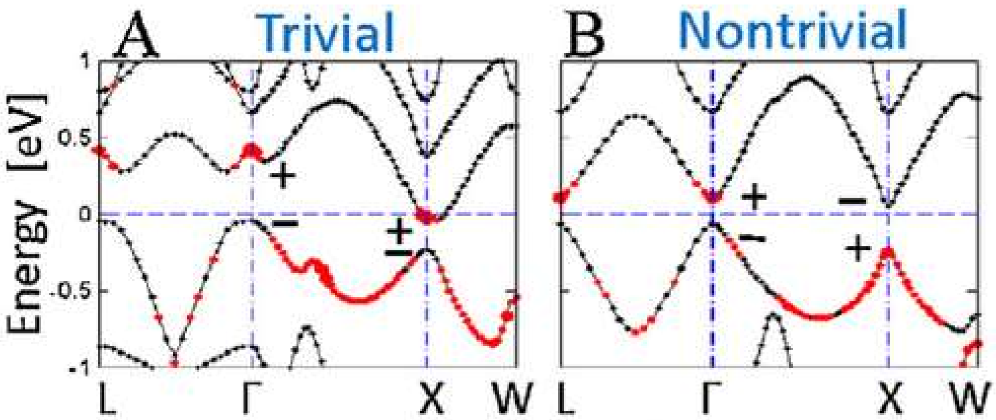


- Z_2 class

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

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

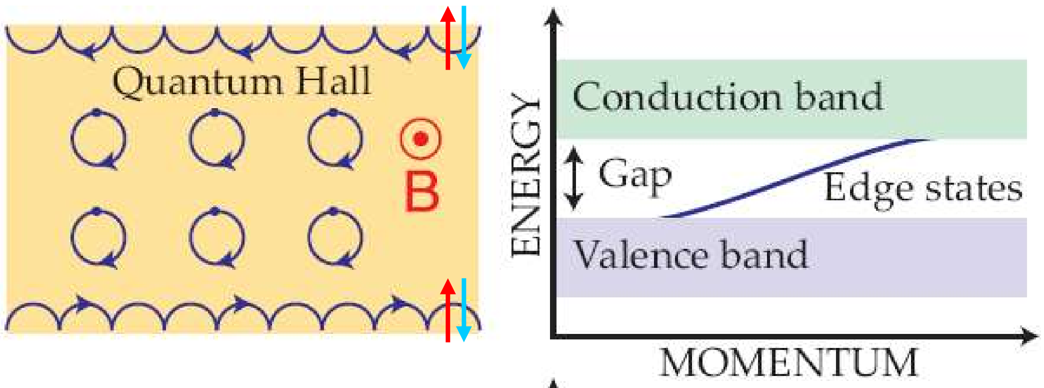
Band inversion and parity change



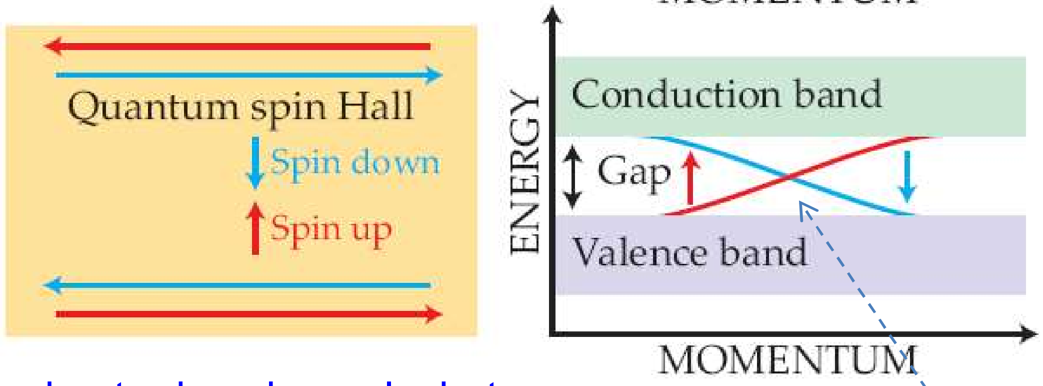
Edge state: *QH insulator* vs *QSH insulator* (aka 2D TI)

Real space | Energy spectrum

Robust
chiral edge state



Robust
helical edge state



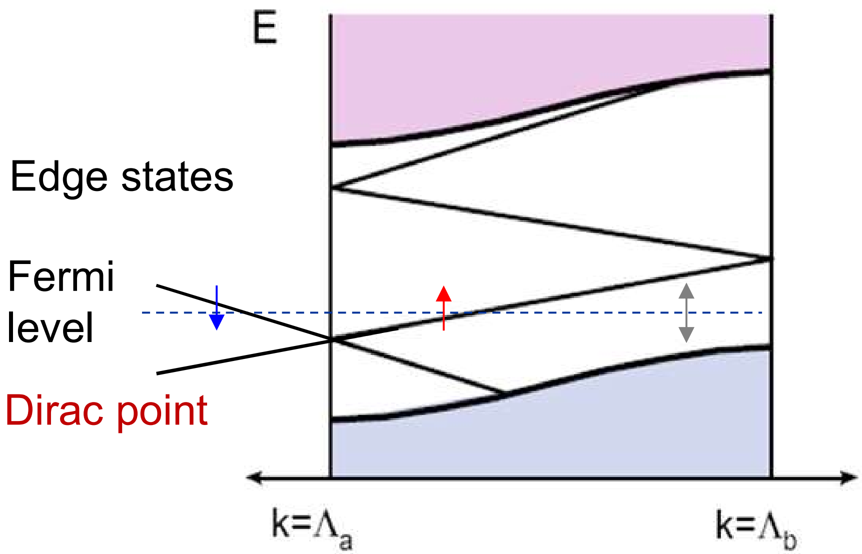
backscattering by non-magnetic impurity forbidden

2 robust edge channels, but
spin transport is not quantized.

- **Dirac point at TRIM**
- **Spin couples with momentum**

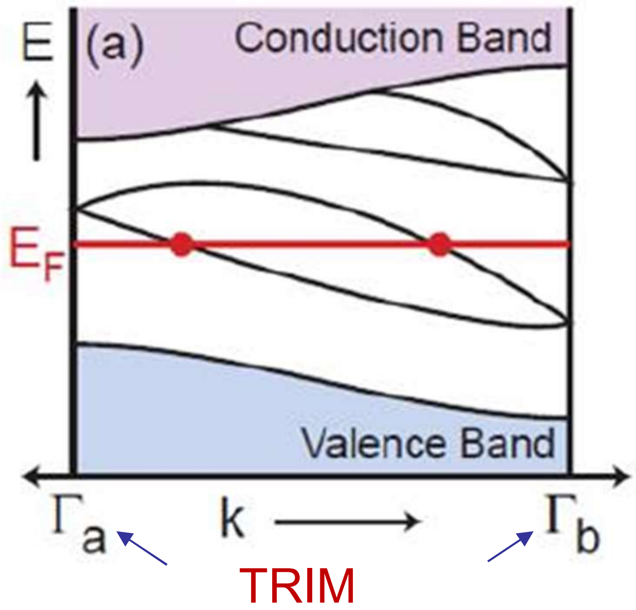
Edge states in 2D TI (Fu and Kane)

Non-trivial



- odd # of Dirac points
- odd # of crossings
- robust surface state

Trivial



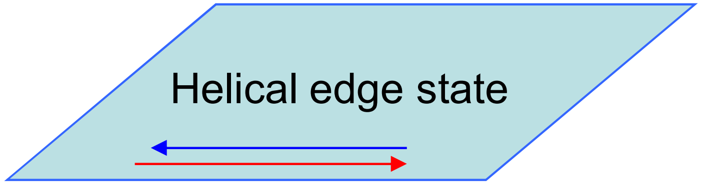
- even # of Dirac points
- even # of crossings
- fragile surface state

I. 3D Topological insulator

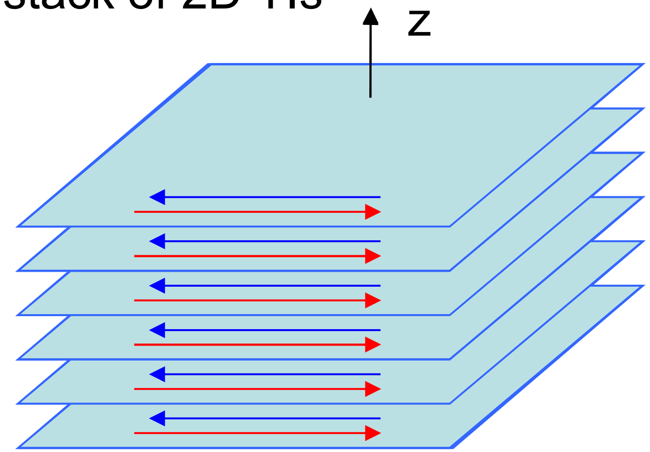
A. Fermi circle of the surface state
B. Weak topological indices
C. Topological crystalline insulator and beyond

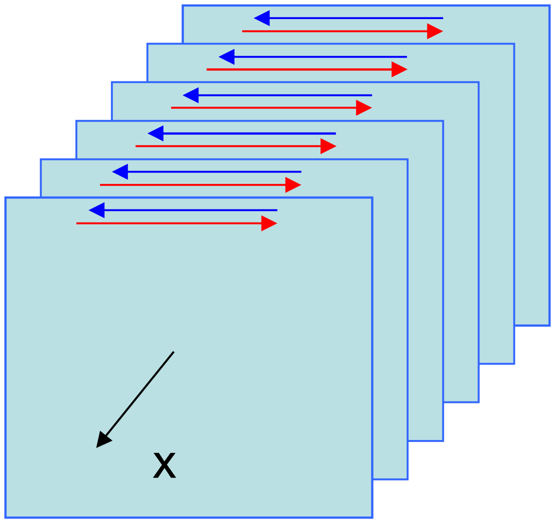
From 2D TI to 3D TI

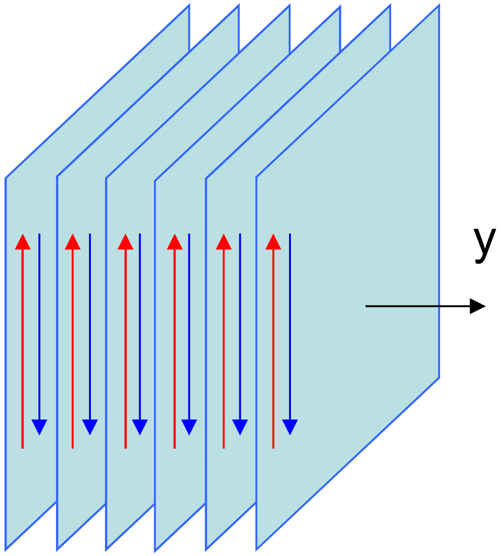
Real space



A stack of 2D TIs





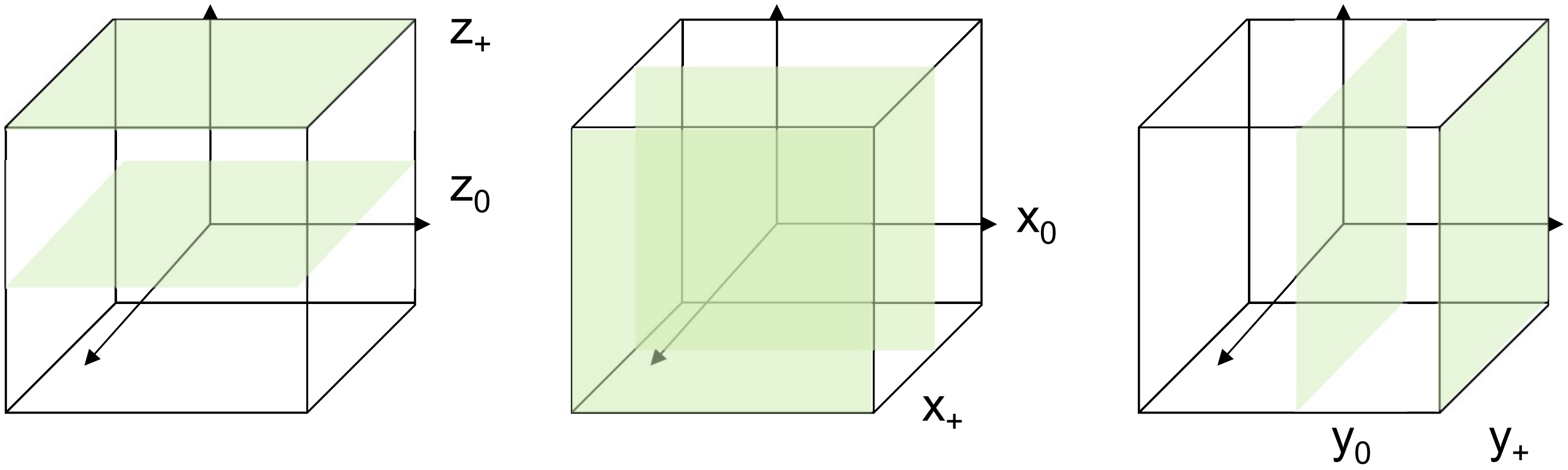


3 TI indices

Momentum space

Time-reversal invariant plane

Each 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,

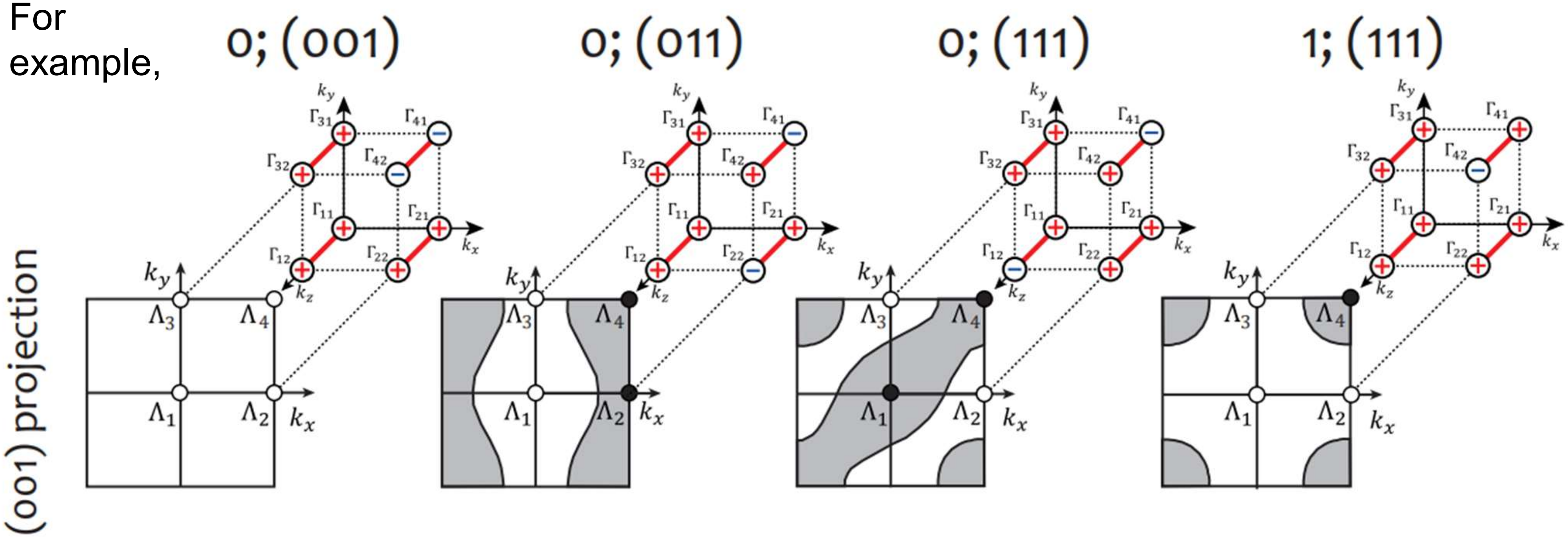
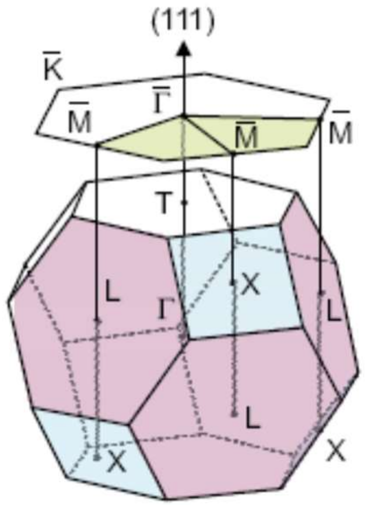


Fig. from Eschbach, 2016

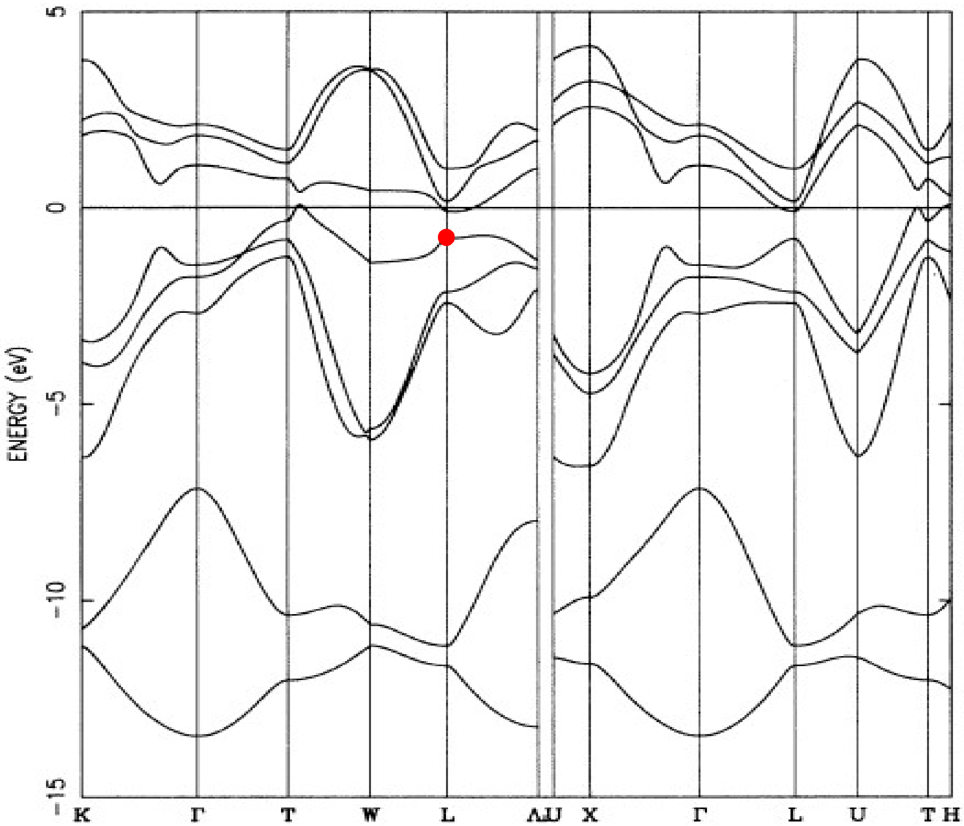
~ 2D TIs stacked along $\vec{M}_\nu = \left(\nu_1\vec{b}_1 + \nu_2\vec{b}_2 + \nu_3\vec{b}_3\right)/2$

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

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

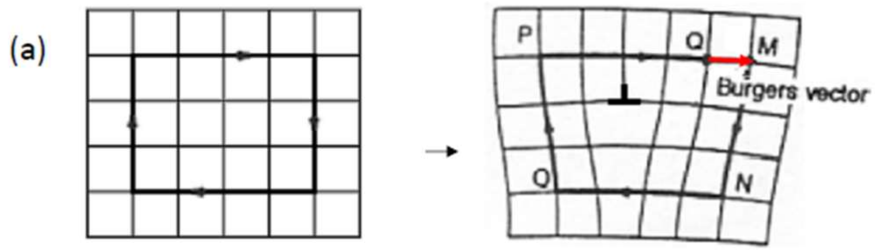


Band structure of Sb (Liu and Allen PRB95)



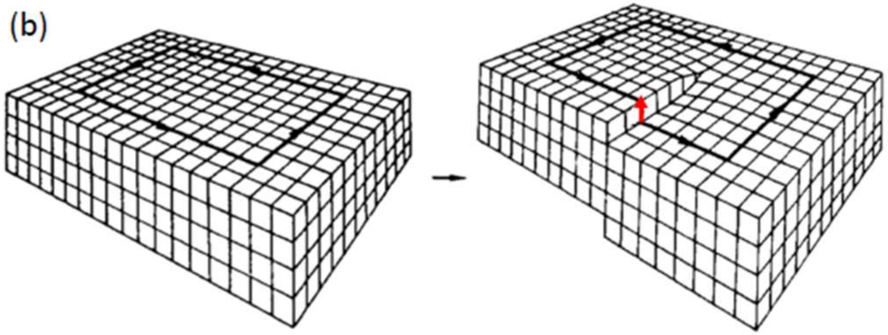
Bismuth	
$\Gamma_6^+ \Gamma_6^- \Gamma_6^+ \Gamma_6^+ \Gamma_{45}^+$	$-$
$L_s L_a L_s L_a L_a$	$-$
$X_a X_s X_s X_a X_a$	$-$
$T_6^- T_6^+ T_6^- T_6^+ T_{45}^-$	$-$
Z_2 class	(0;000)
Antimony	
$\Gamma_6^+ \Gamma_6^- \Gamma_6^+ \Gamma_6^+ \Gamma_{45}^+$	$-$
$L_s L_a L_s L_a L_s$	$+$
$X_a X_s X_s X_a X_a$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

Weak TI index and defect

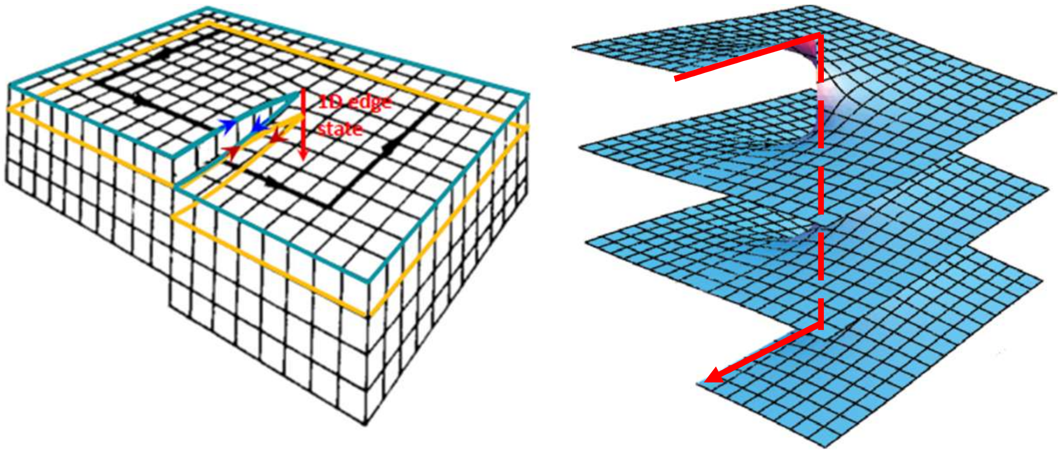


Two types of dislocation:

- Edge dislocation



- Screw dislocation



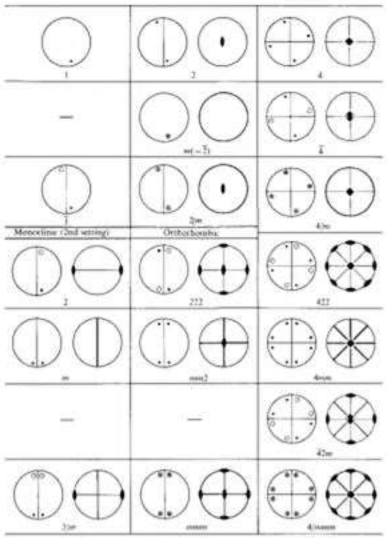
Electronic state along 1D defect

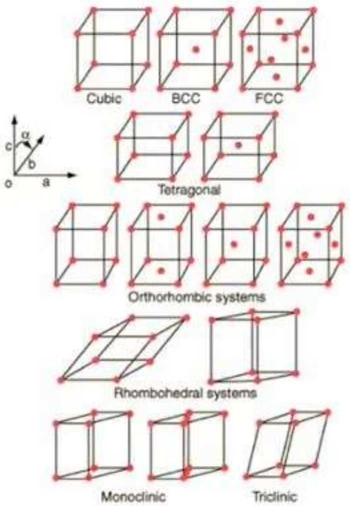
- robust against disorder
- chiral quantum wire

Ran Y et al, Nature Phys 2009

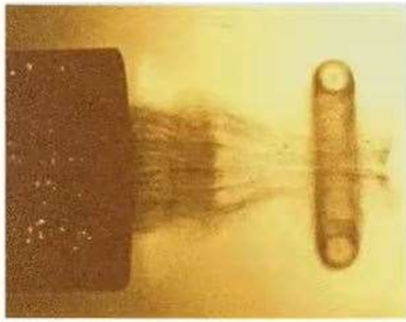
Symmetry and Topology in Insulators

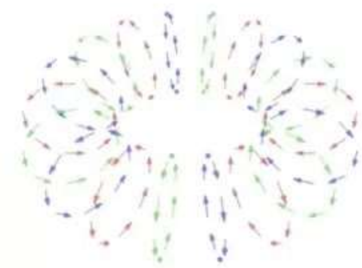
- Symmetry

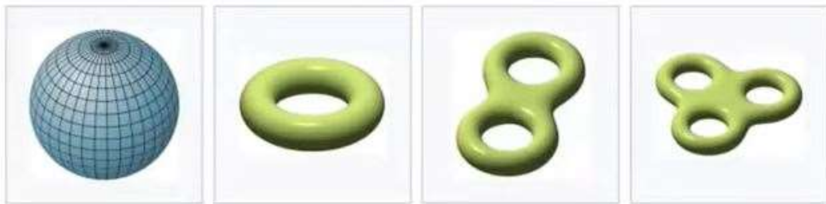




- Topology







genus 0 genus 1 genus 2 genus 3

TI protected by crystalline symmetry, instead of TRS << SPT phase

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)

The recent discovery of topological insulators has revived interest in the band topology of insulators. In this Letter, we extend the topological classification of band structures to include certain crystal point group symmetry. We find a class of three-dimensional "topological crystalline insulators" which have metallic surface states with quadratic band degeneracy on high symmetry crystal surfaces. These topological crystalline insulators are the counterpart of topological insulators in materials without spin-orbit coupling. Their band structures are characterized by new topological invariants. We hope this work will enlarge the family of topological phases in band insulators and stimulate the search for them in real materials.

DOI: 10.1103/PhysRevLett.106.106802 PACS numbers: 73.20.−r, 73.43.−f

- 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

ARTICLE

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

Check

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)

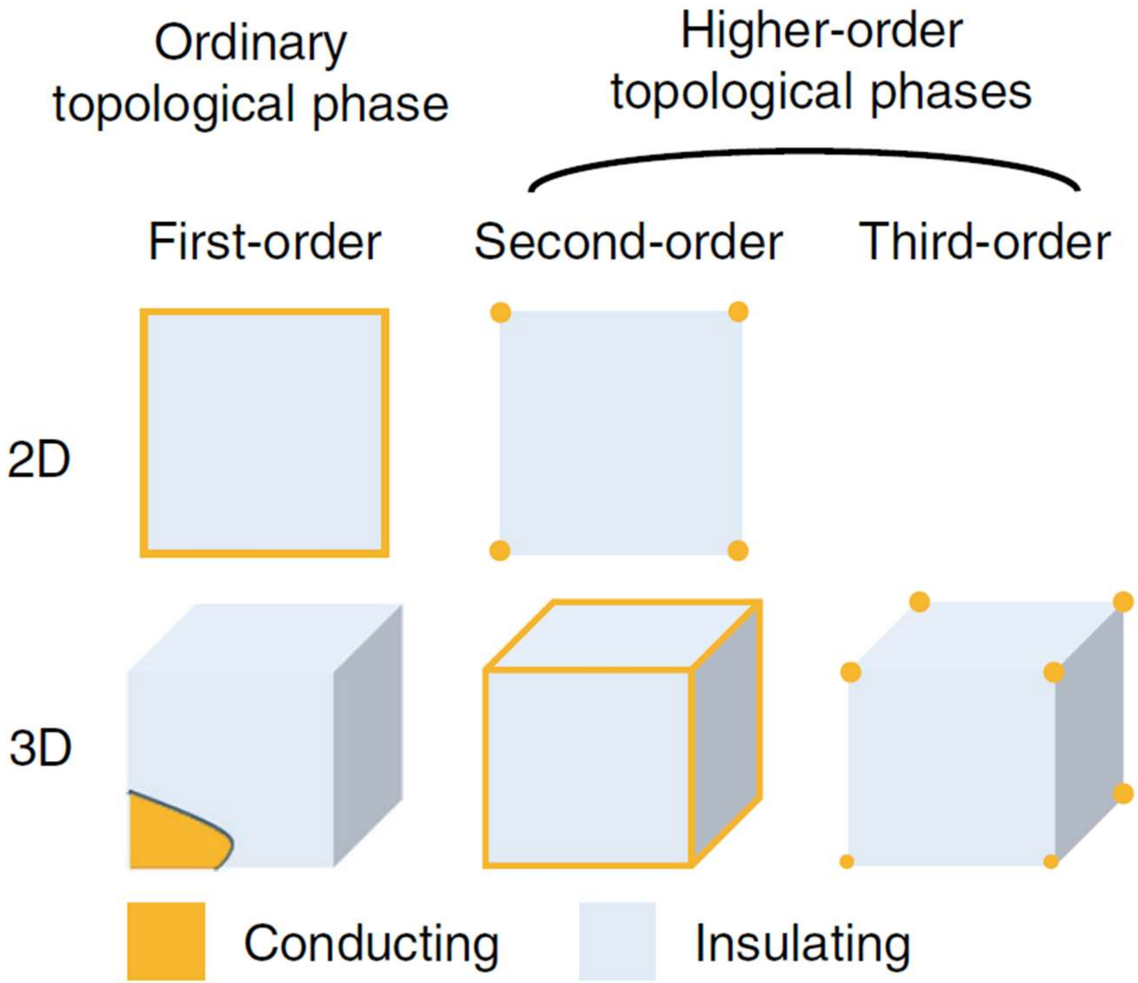


Fig from Kim et al, in Light: Science & Applications (2020)