Crystal symmetry meets band topology

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Classification of topological insulators with internal symmetry

Ryu, Schnyder, Furusaki, Ludwig, New J. Phys. (2010)

Classified by time-reversal and charge-conjugation symmetries

complex case:

no symmetry →

Cartan\d	0	1	2	3	4	5	6	7	8	9	10	11	⋯
A	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	⋯
AIII	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	⋯

Integer quantum Hall

real case:

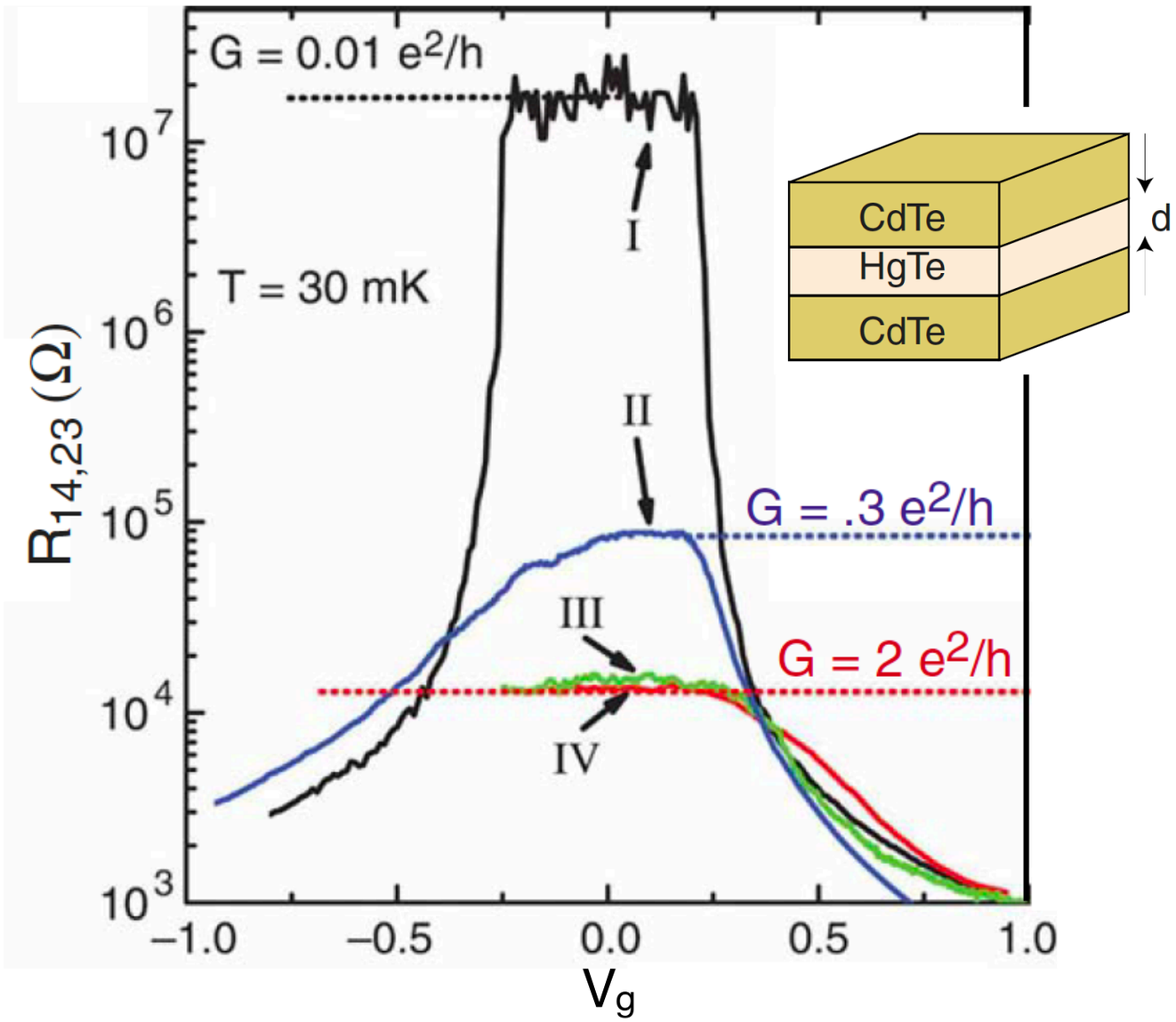
fermions w/ time-reversal →

Cartan\d	0	1	2	3	4	5	6	7	8	9	10	11	⋯
AI	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	⋯
BDI	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	⋯
D	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	⋯
DIII	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	⋯
AII	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	⋯
CII	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	⋯
C	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	⋯
CI	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	⋯

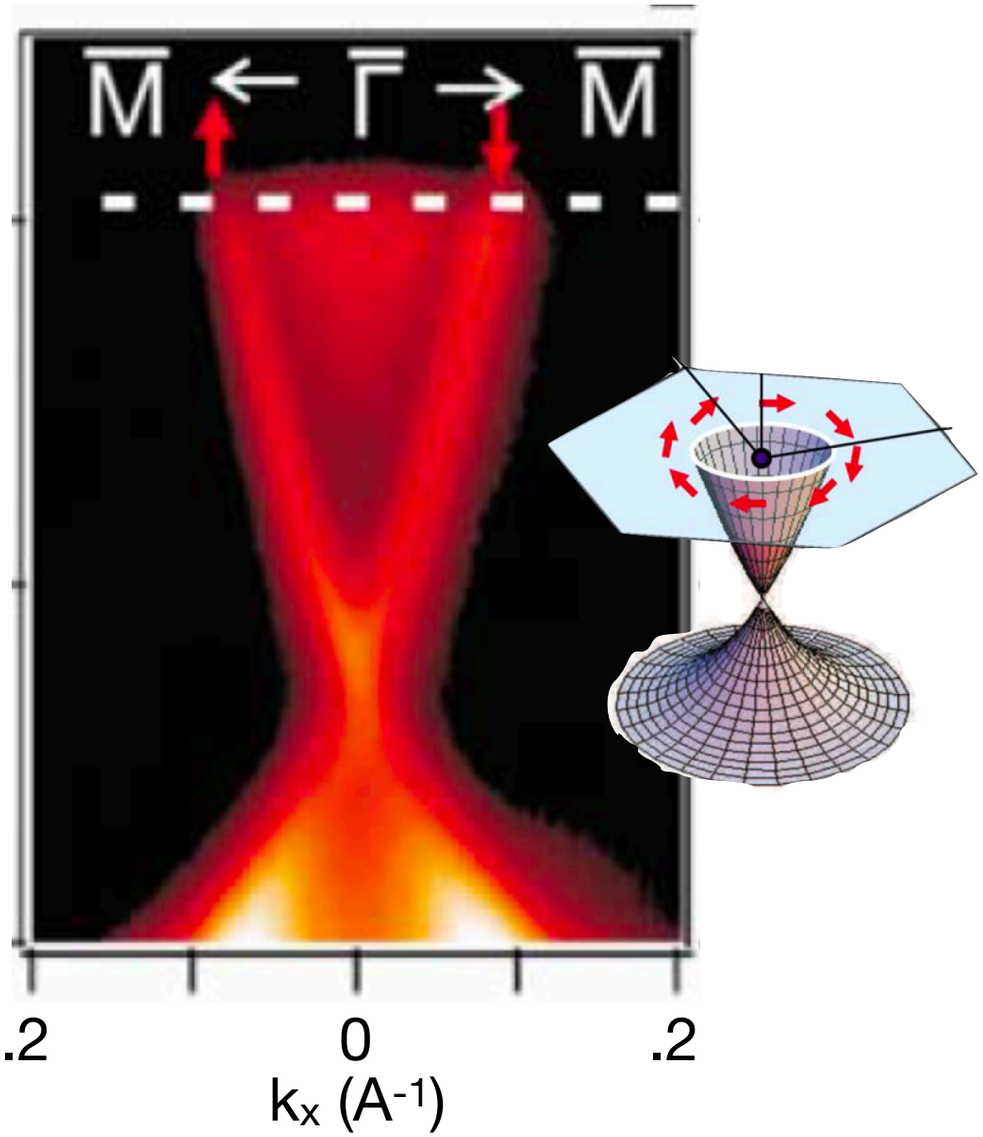
2d and 3d topological insulators

Topological insulators have gapless surface states that are robust to small perturbations

2D: HgTe/CdTe quantum well (BHZ)
Molenkamp group (Würzburg)

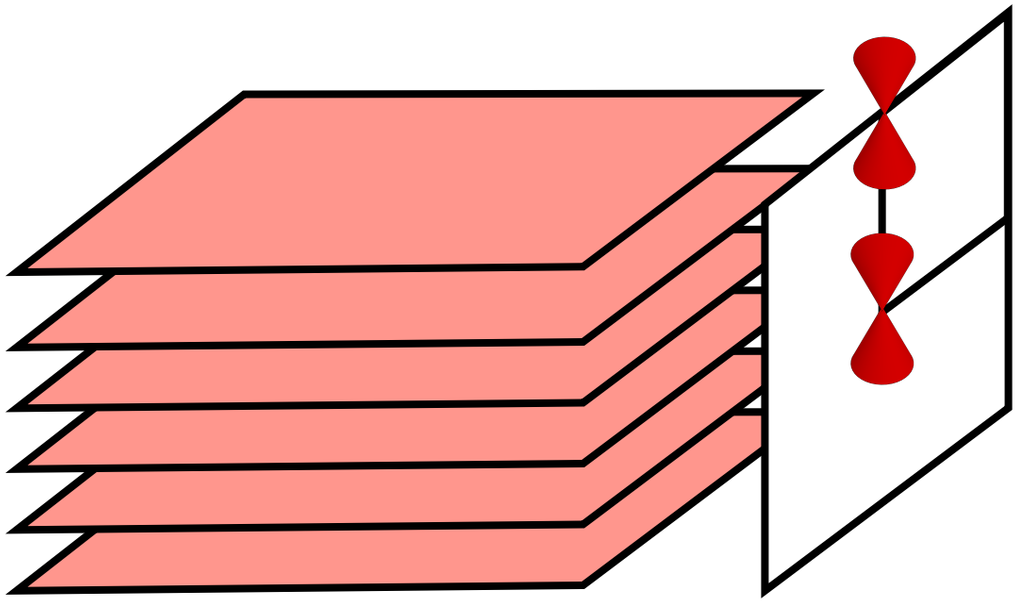


3D: Bi_2Se_3
Hasan group (Princeton)



Figures from Hasan + Kane RMP

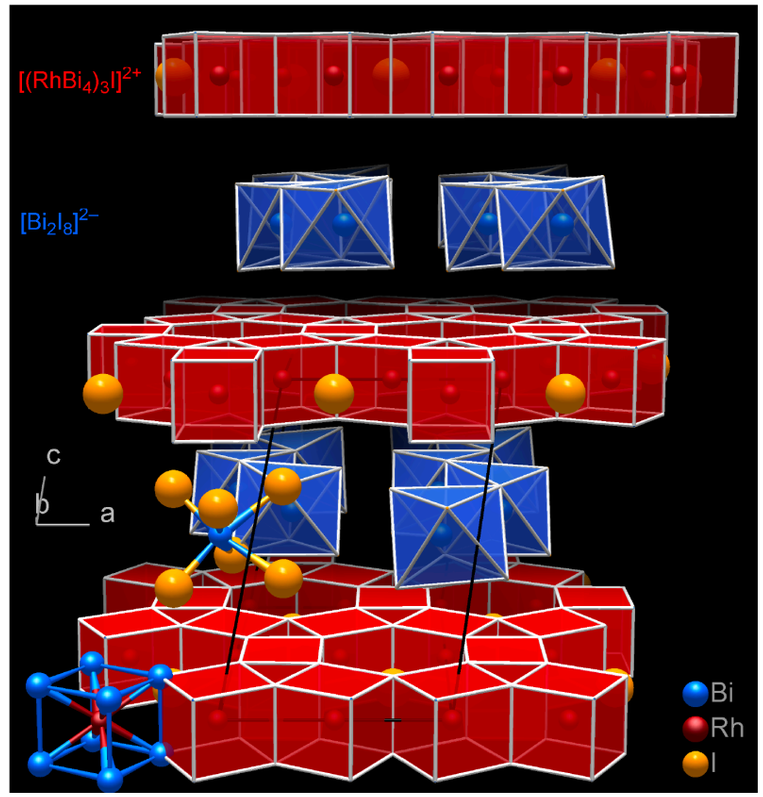
Refined classification of topological insulators with translation symmetry



Stacked 2D TIs

Two surface Dirac cones

$Bi_{14}Rh_3I_9$



Rasche, et al, Nat. Mat. (2013)

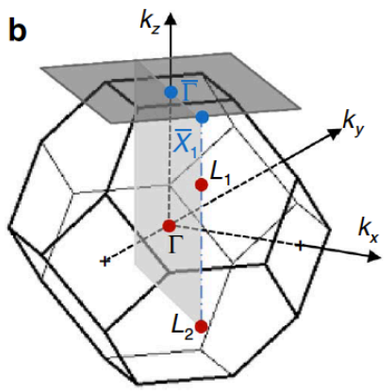
One “strong” and three “weak” indices $(\nu_0; \nu_1, \nu_2, \nu_3)$

Fu, Kane, Mele PRL 2007; Moore, Balents PRB 2007; Roy PRB 2009

Point group symmetry can also protect a topological insulator

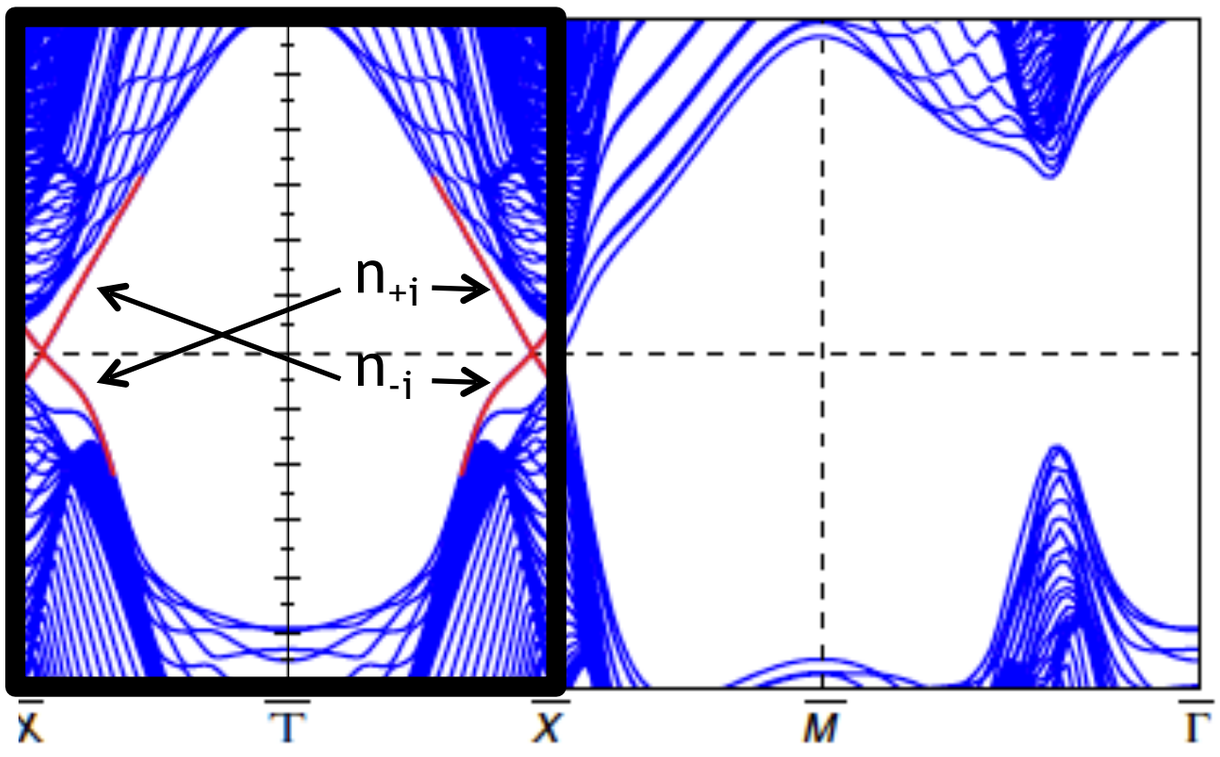
Fu PRL 2011

Teo, Fu, Kane PRB 2008



Ex: Mirror Chern insulator in SnTe

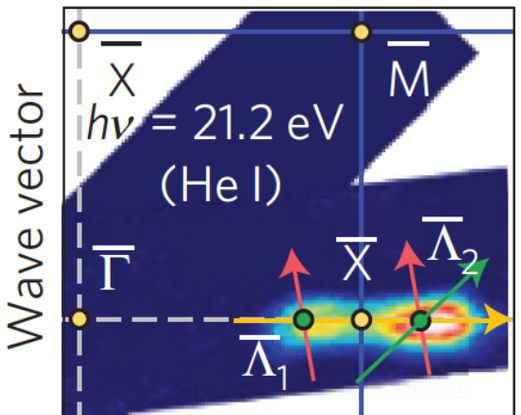
Hsieh, *Nat. Comm.* **3** 982 (2012)

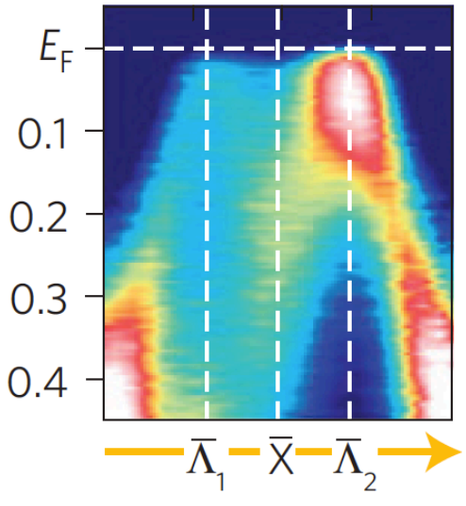


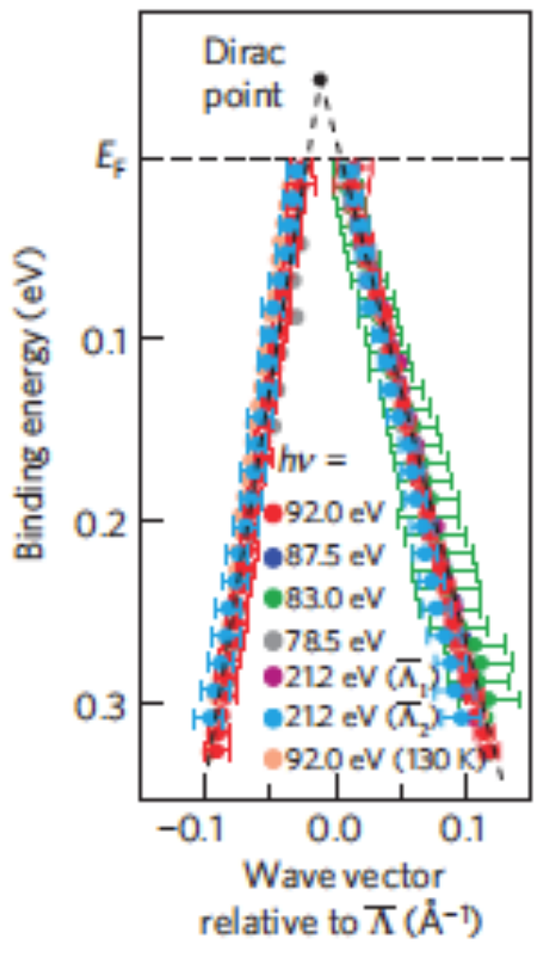
Dirac cones protected by mirror symmetry!

Observation by Ando group

Tanaka, et al, *Nat. Phys.* **8** 800 (2012)

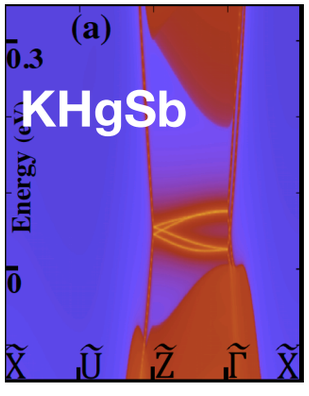






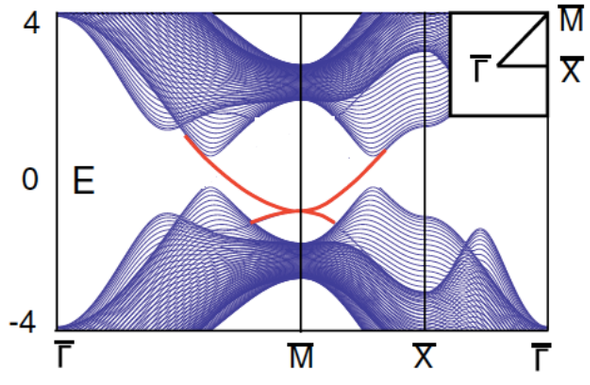
More topological phases with crystal symmetry

Hourglass fermion: Z_4



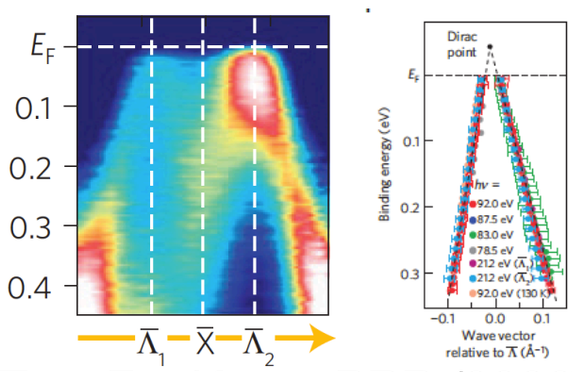
Wang, et al Nature (2016)
Shiozaki, Sato, Gomi, PRB (2016))

C_4 rotation: Z_2



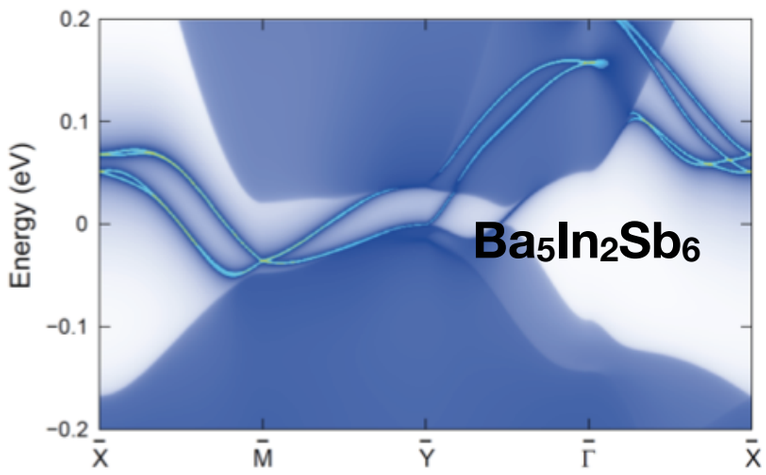
Fu, PRL (2011)

Mirror Chern: Z



Teo, Fu, Kane, PRB (2008)
Hsieh, et al, Nat. Comm. (2012)
Tanaka, et al, Nat. Phys. (2012)

Dirac insulator: Z_2 x Z_4



Wieder, **JC** et al, Science 2018

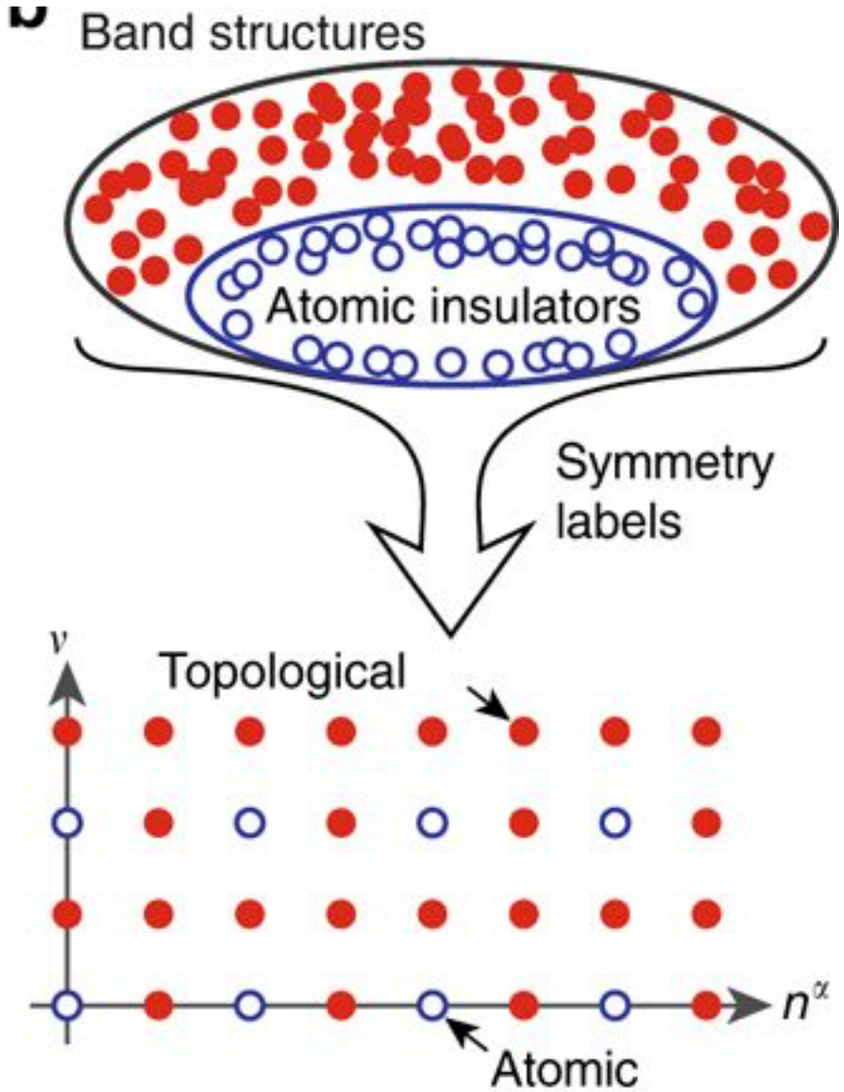
2017: Classification of topological crystalline insulators in any space group

Topological quantum chemistry

Bradlyn, JC, et al Nature 2017

Symmetry indicators

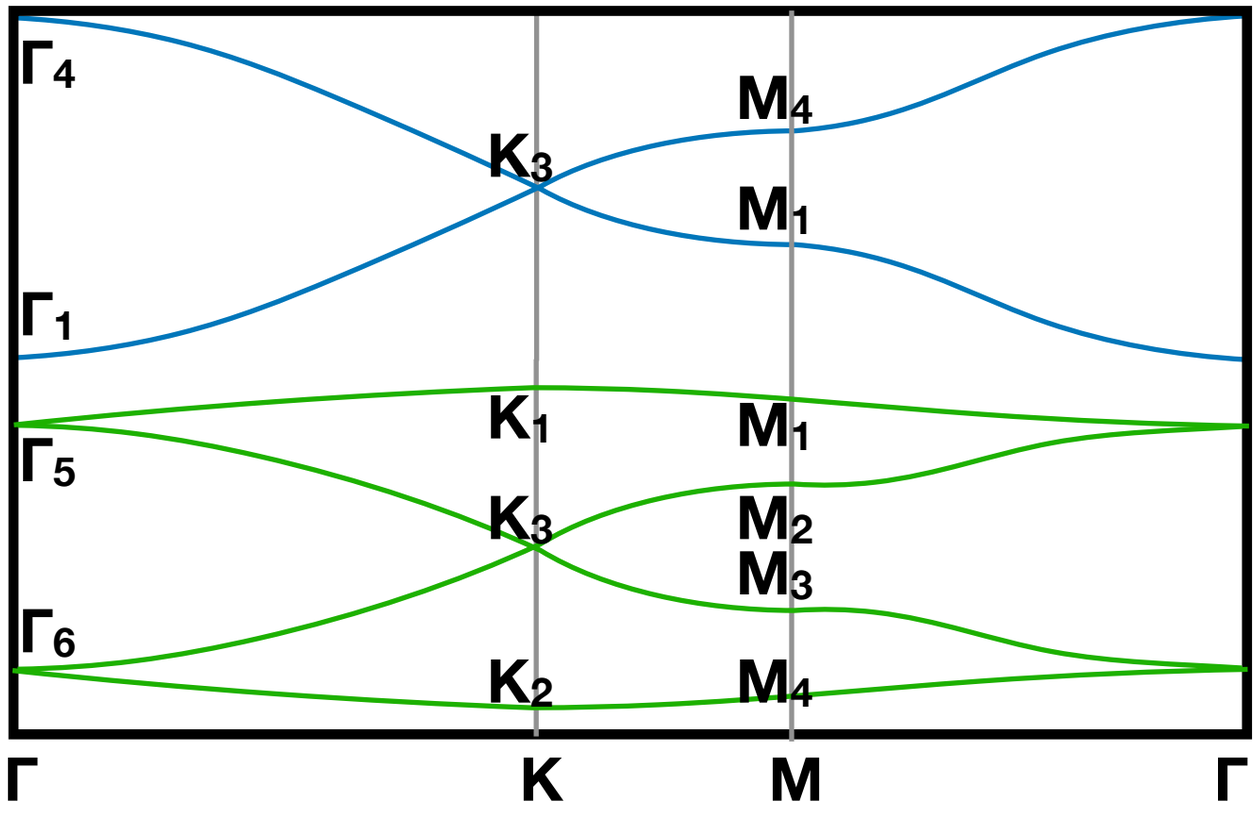
Po, Vishwanath, Watanabe, Nat. Comm. 2017



How to identify topological phases by symmetry eigenvalues

1. Identify symmetry eigenvalues of *all* atomic limit phases

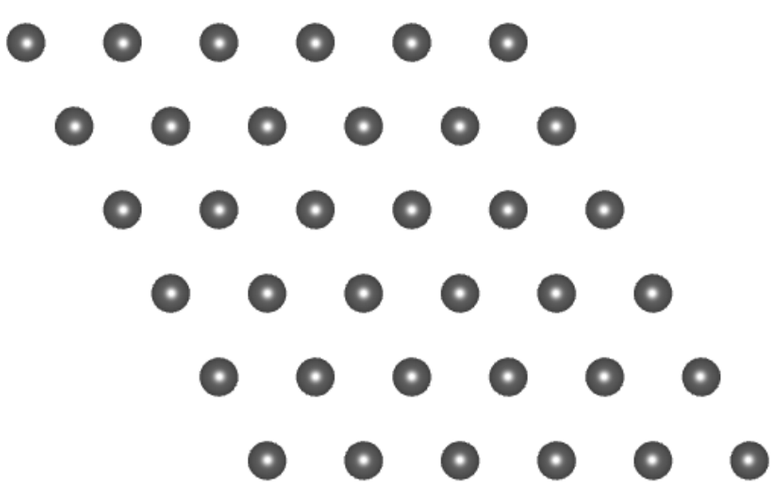
2. Groups of bands whose symmetry eigenvalues do not match those of an atomic limit must be topological



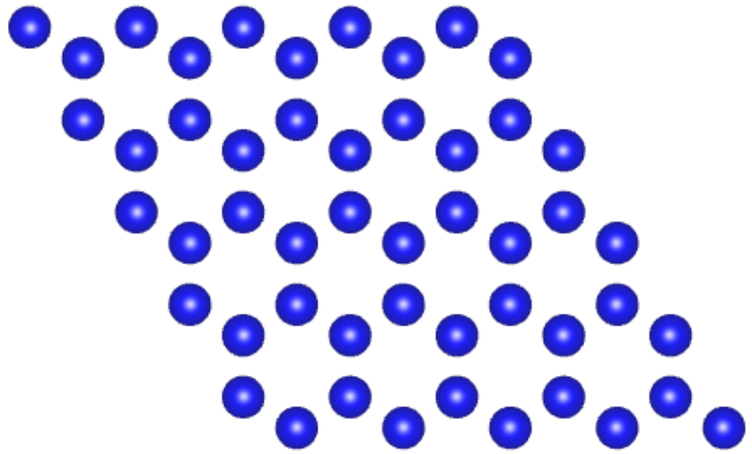
How to identify all atomic limits?

Within one space group, many ways to arrange atoms

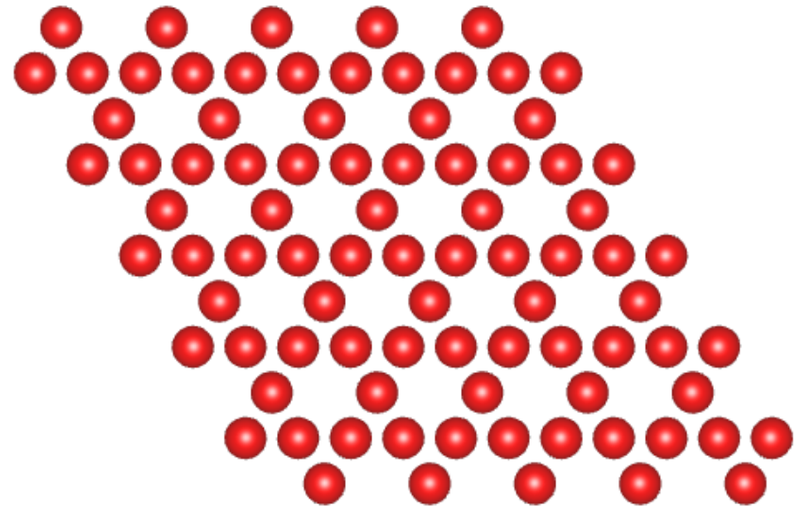
“Wyckoff positions”



1 atom/unit cell
(triangular)



2 atoms/unit cell
(honeycomb)

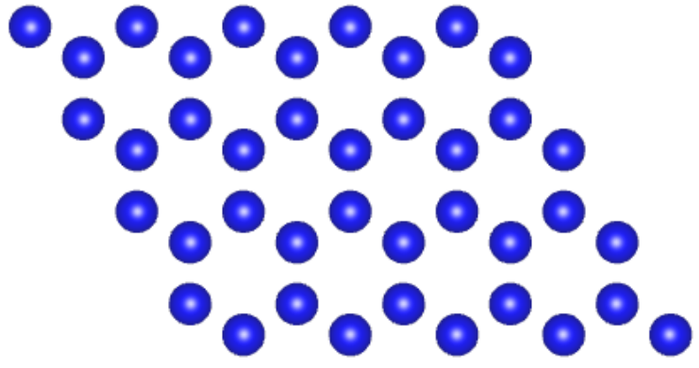


3 atoms/unit cell
(kagome)

All atoms are related by symmetry

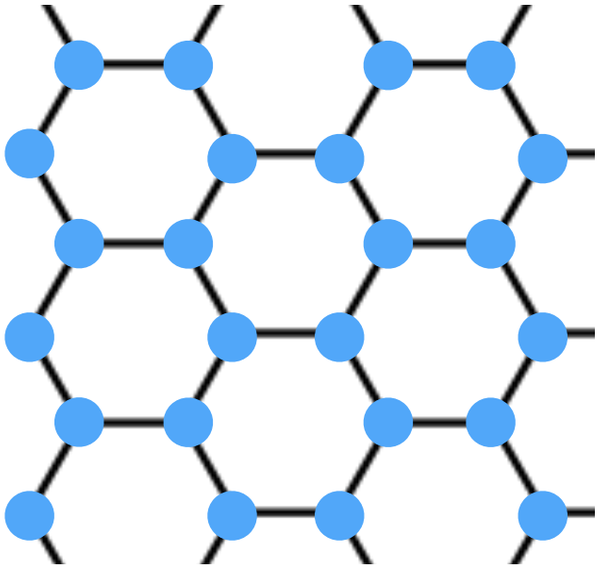
How to identify all atomic limits?

Within one arrangement, many choices of orbitals

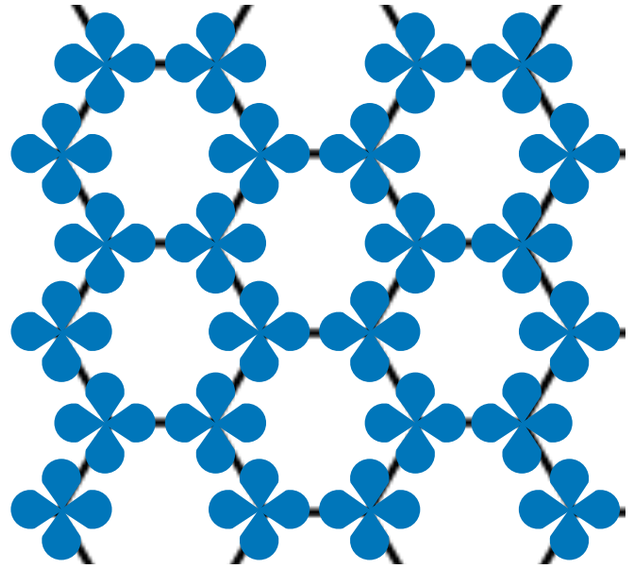


2 atoms/unit cell

s (or p_z) orbitals



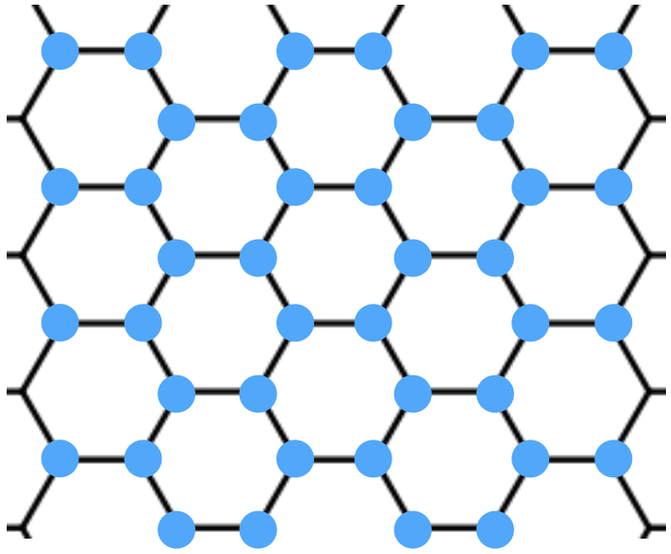
p_x and p_y orbitals



A space group, Wyckoff position, and orbital define an atomic limit

Mathematically: a Wyckoff position, and orbital determine a “band representation” of the space group

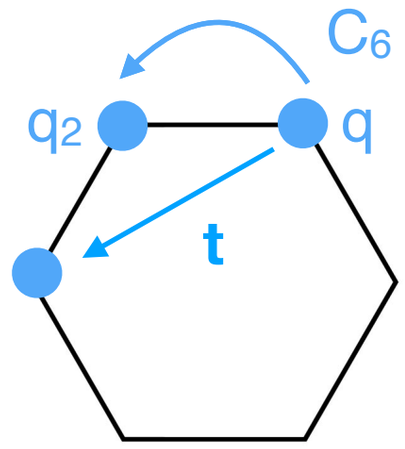
Zak PRL 1980, PRB 1981, 1982



How to construct such a representation?

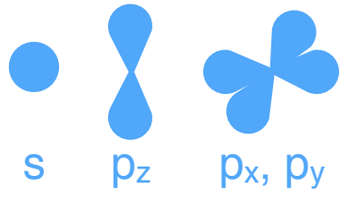
1. Identify “site-symmetry group”:

G_q = symmetries that leave q invariant



C_3, m_y

2. Orbitals at q transform under a rep, $\rho(g)$, of G_q



3. Elements that do not leave q invariant tile lattice

C_6, t, …

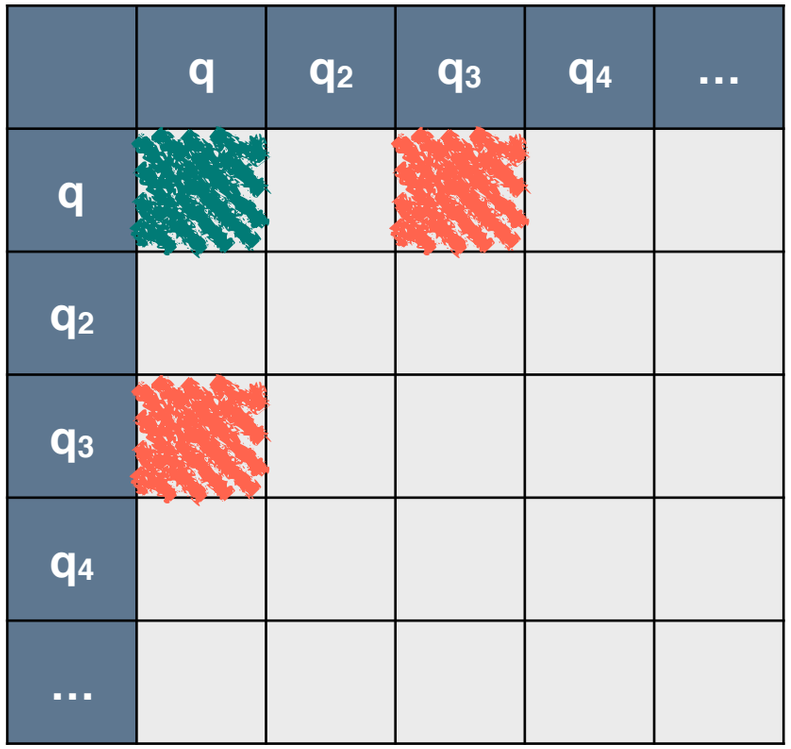
Mathematically: a space group, Wyckoff position, and orbital determine a representation of the space group

Zak PRL 1980, PRB 1981, 1982

Each symmetry operation represented by BIG matrix

Diagonal block
if $g \in G_q$, i.e, $gq = q$

Off-diagonal block if g interchanges sites



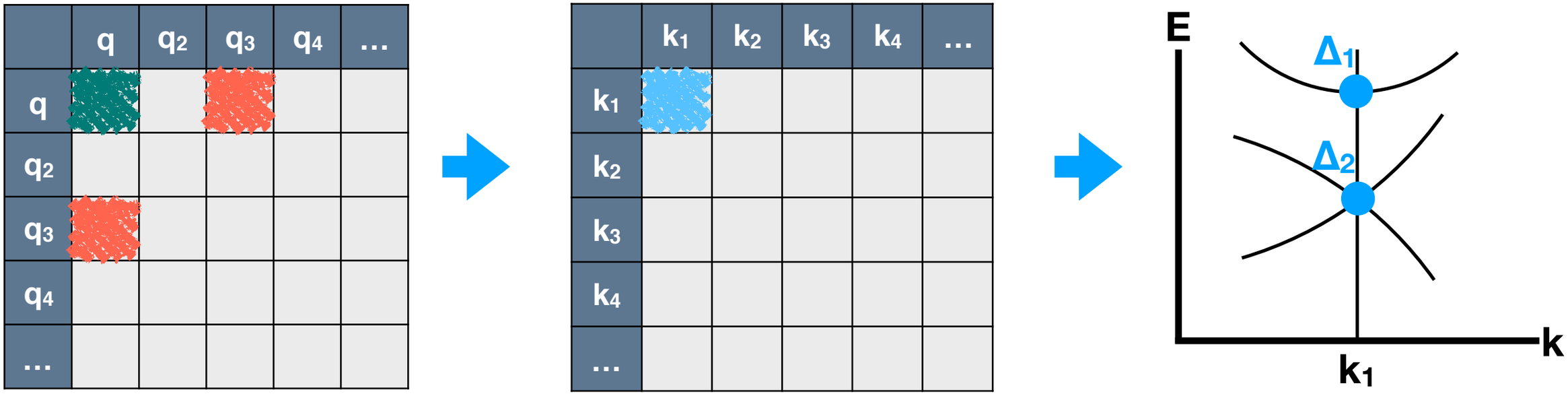
Group theory: induced representation of subgroup uniquely determines representation of group

$$\mathrm{Ind}_{G_{\mathbf{q}}}^{G} \rho$$

Fourier transform yields the symmetry irreps at each point in the Brillouin zone

“Band representation”

Zak PRL 1980, PRB 1981, 1982



Diagonal blocks form representation of symmetry group that leaves k invariant
(“the little group at k”)

The set of these representations serves as an identifier for the band representation

We want to identify <u>all</u> atomic limit phases for <u>all</u> space groups, but how to enumerate an infinite list?

Band representations decompose into (finite number of) elementary band representations Zak 1980

1. Elementary band reps are induced from irreducible representations of G_q

$$(\rho_1 \oplus \rho_2) \uparrow G = (\rho_1 \uparrow G) \oplus (\rho_2 \uparrow G)$$

2. All EBRs can be induced from representations of <u>maximal</u> site-symmetry groups

$$(\rho \uparrow H) \uparrow G = \rho \uparrow G$$

⇒ Finitely many EBRs

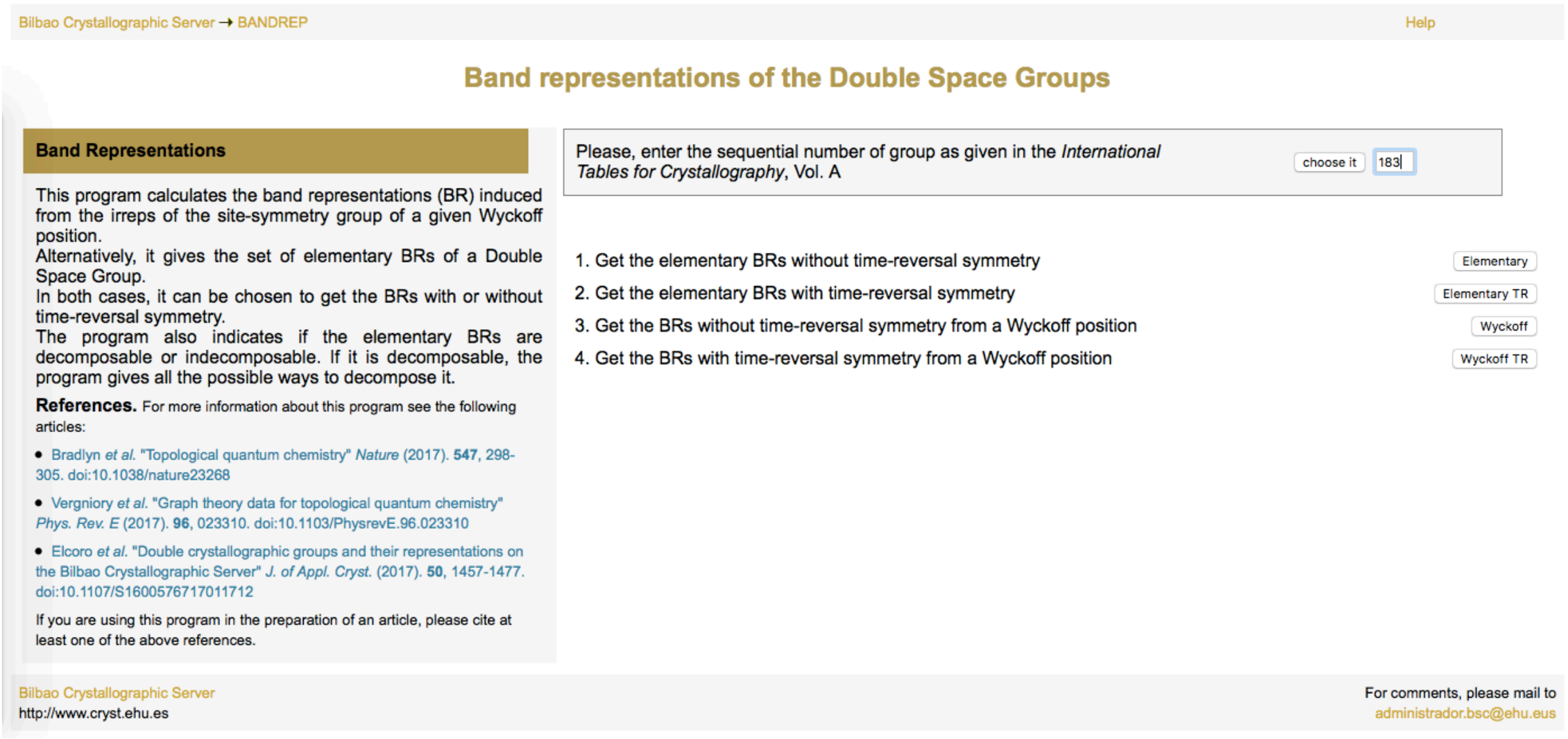
Symmetry labels for all EBRs are enumerated on the Bilbao Crystallographic Server

bilbao crystallographic server

http://www.cryst.ehu.es/

Elcoro, JC, et al J. Appl. Cryst. 50, 1457 (2017)

Bradlyn, Elcoro, JC, Vergniory, Wang, Felser, Aroyo, Bernevig Nature 547, 298–305 (2017)



Each column is elementary band representation

Bilbao Crystallographic Server → BANDREP Help

Elementary band-representations without time-reversal symmetry of the Double Space Group *P6mm* (No. 183)

The first row shows the Wyckoff position from which the band representation is induced.
In parentheses, the symbol of the point group isomorphic to the site-symmetry group.

The second row gives the symbol ρ↑G, where ρ is the irrep of the site-symmetry group.
In parentheses, the dimension of the representation.

The output shows the decomposition of the band representations into irreps of the little groups of the given k-vectors in the first column.
In parentheses, the dimensions of the representations.

Minimal set of paths and compatibility relations to analyse the connectivity

Show all types of k-vectors

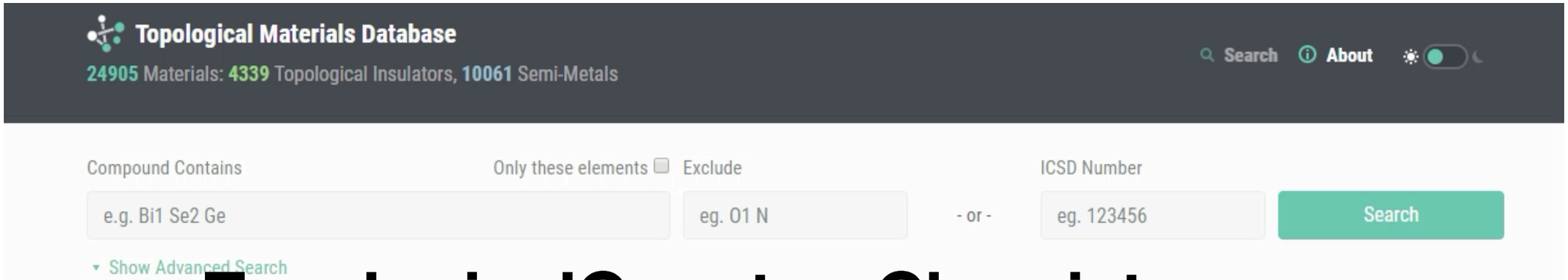
Wyckoff pos.	1a(6*mm*)	1a(6*mm*)	1a(6*mm*)	1a(6*mm*)	1a(6*mm*)	1a(6*mm*)	2b(3*m*)	
Band-Rep.	$A_1\uparrow G(1)$	$A_2\uparrow G(1)$	$B_1\uparrow G(1)$	$B_2\uparrow G(1)$	$E_1\uparrow G(2)$	$E_2\uparrow G(2)$	$A_1\uparrow G(2)$	
Decomposable\ Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Ir
Γ:(0,0,0)	$\Gamma_1(1)$	$\Gamma_2(1)$	$\Gamma_4(1)$	$\Gamma_3(1)$	$\Gamma_6(2)$	$\Gamma_5(2)$	$\Gamma_1(1) \oplus \Gamma_4(1)$	
A:(0,0,1/2)	$A_1(1)$	$A_2(1)$	$A_4(1)$	$A_3(1)$	$A_6(2)$	$A_5(2)$	$A_1(1) \oplus A_4(1)$	
K:(1/3,1/3,0)	$K_1(1)$	$K_2(1)$	$K_2(1)$	$K_1(1)$	$K_3(2)$	$K_3(2)$	$K_3(2)$	
H:(1/3,1/3,1/2)	$H_1(1)$	$H_2(1)$	$H_2(1)$	$H_1(1)$	$H_3(2)$	$H_3(2)$	$H_3(2)$	
M:(1/2,0,0)	$M_1(1)$	$M_2(1)$	$M_4(1)$	$M_3(1)$	$M_3(1) \oplus M_4(1)$	$M_1(1) \oplus M_2(1)$	$M_1(1) \oplus M_4(1)$	
L:(1/2,0,1/2)	$L_1(1)$	$L_2(1)$	$L_4(1)$	$L_3(1)$	$L_3(1) \oplus L_4(1)$	$L_1(1) \oplus L_2(1)$	$L_1(1) \oplus L_4(1)$	

Atom arrangement
Orbital
High-symmetry points

Materials search:

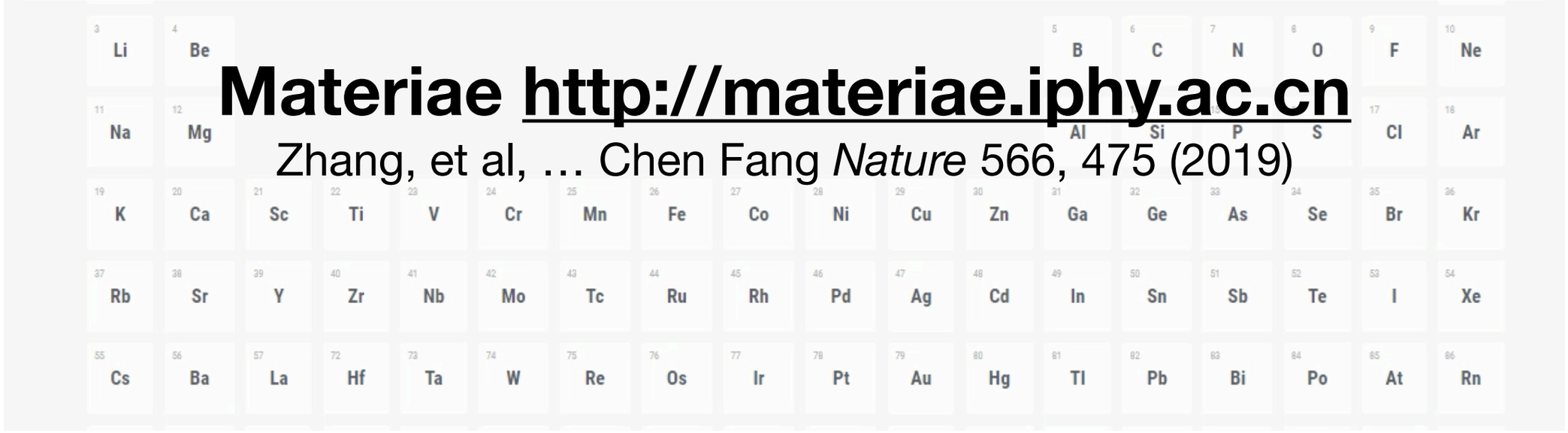
For every known chemical compound:

1. compute band structure
2. compute symmetry irreps
3. compare to irreps on server



TopologicalQuantumChemistry.com

Vergniory, Elcoro, Felser, Regnault, Bernevig, Wang *Nature* 566, 480 (2019)



Materiae http://materiae.iphy.ac.cn

Zhang, et al, … Chen Fang *Nature* 566, 475 (2019)

What have we learned from this enterprise?

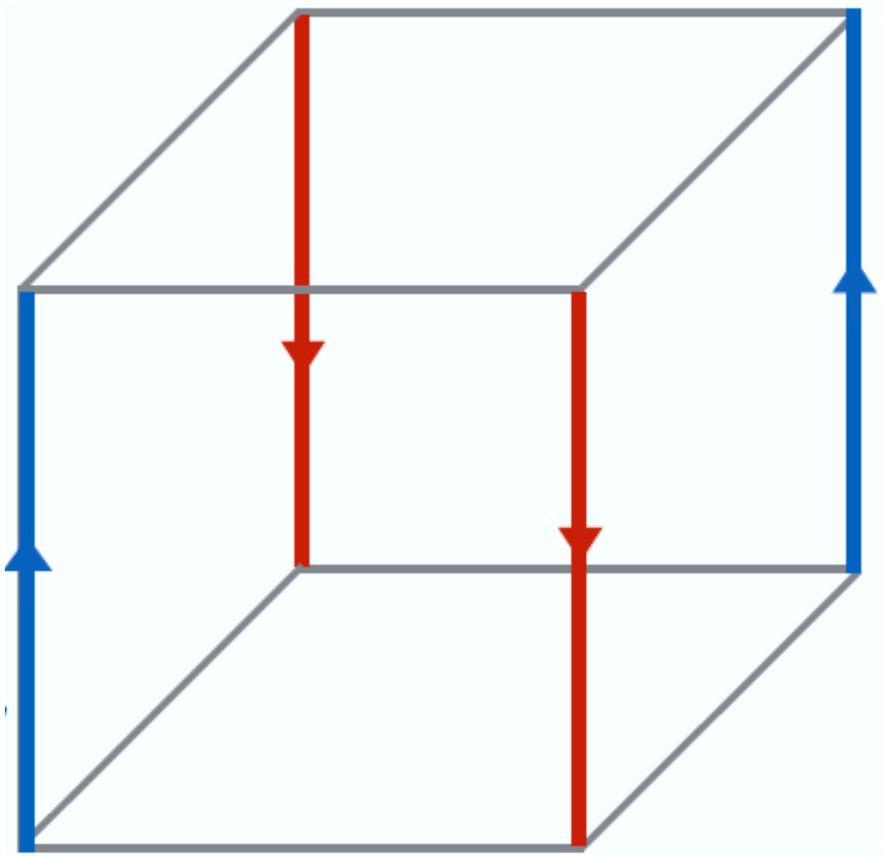
New, freely available topological materials databases and tools

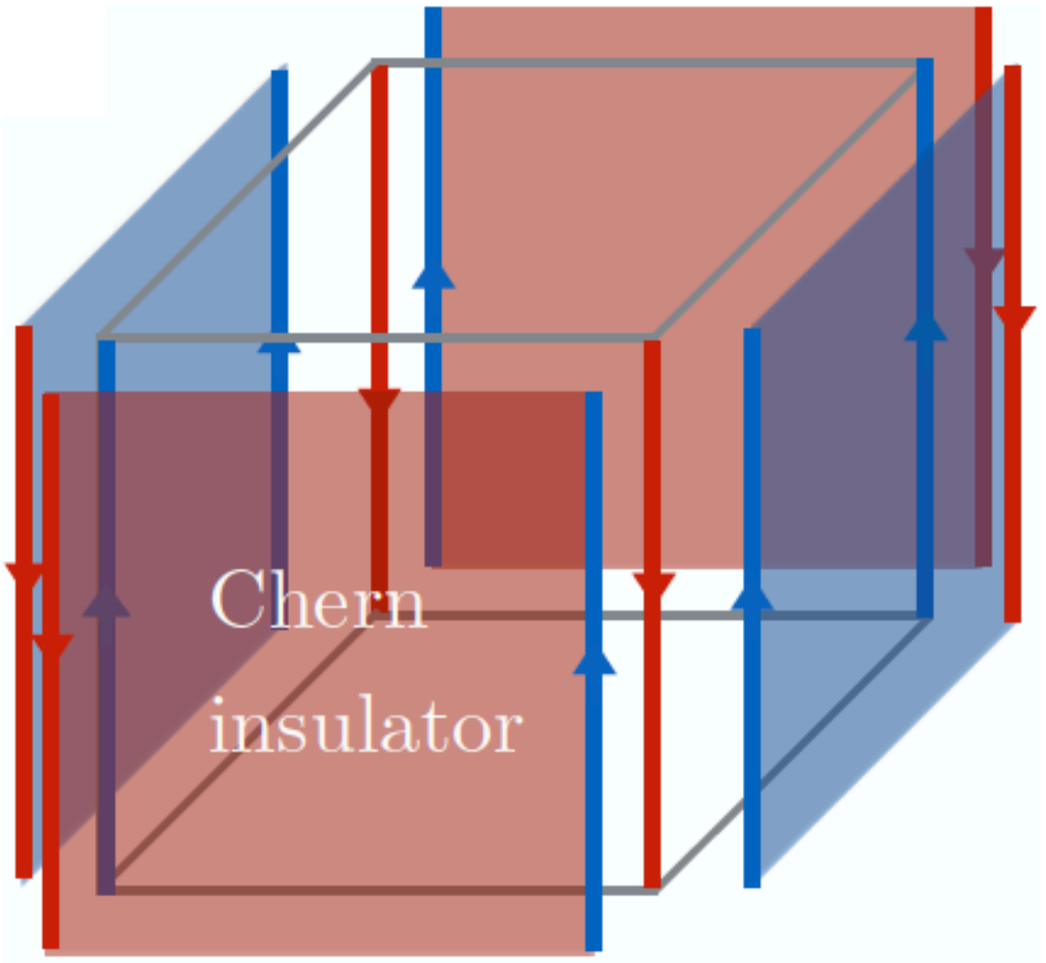
- Bilbao Crystallographic Server
- TopologicalQuantumChemistry.com
- Materiae: http://materiae.iphy.ac.cn

Refined bulk-edge correspondence: “higher order topological insulators”

Distinction between stable and “fragile” topological insulators

Higher-order topological insulators (HOTIs) have gapless modes where two edges meet



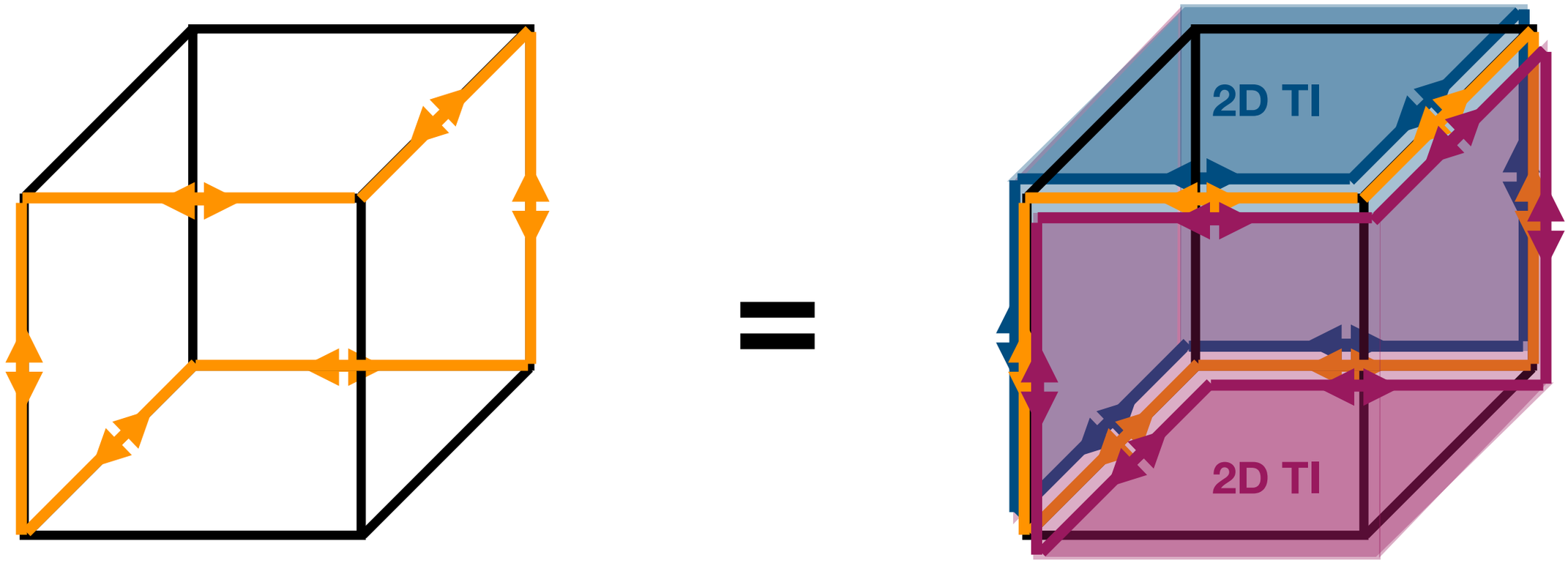


Ex: Product of C_{4z}*TR protects gapless chiral modes

Figure: Schindler, et al, Sci. Advances eaat0346 2018
Refs: Benalcazar, Bernevig, Hughes, Science 2017;
Khalaf, Po, Vishwanath, PRX 2018; Fang and Fu ArXiv: 1709.01929

Today: HOTIs with **inversion** and **time-reversal**

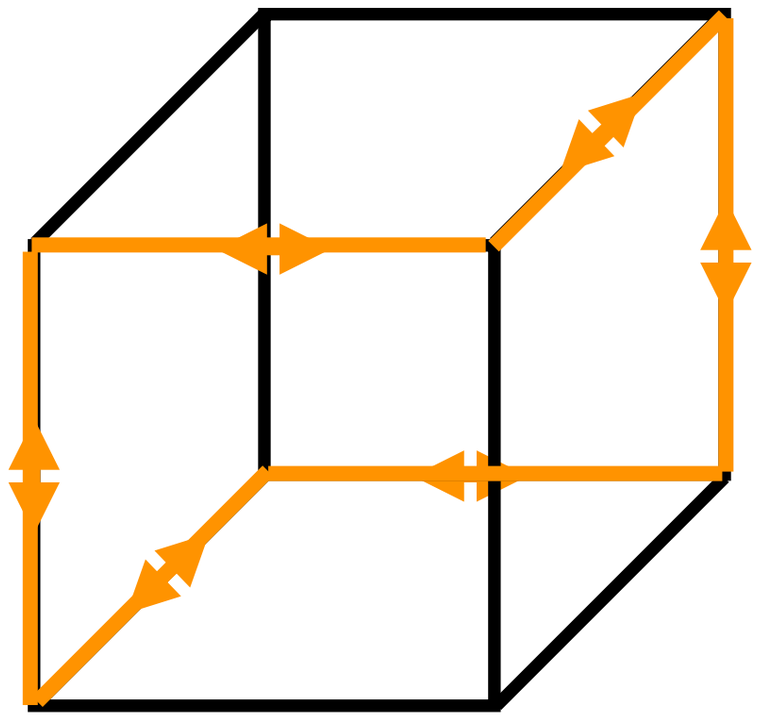
Khalaf, Po, Vishwanath, PRX 2018



Symmetries ensure HOTI is bulk state

Inversion and TR yield Z_4 classification

Khalaf, Po, Vishwanath, PRX 2018



Z_4 index determined by inversion eigenvalues:

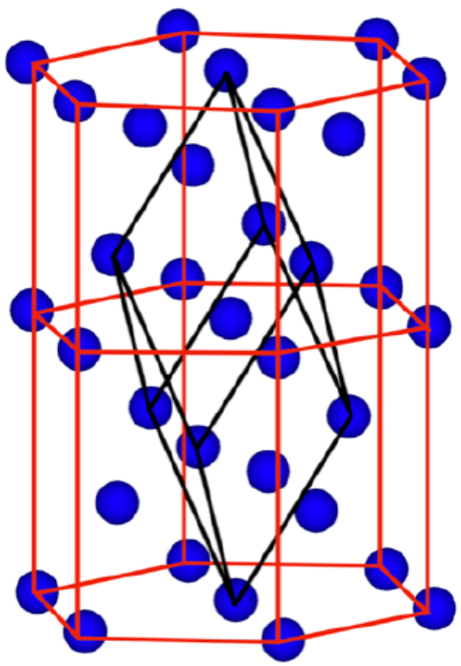
$$\kappa_1 = \frac{1}{4} \sum_{K \in \mathrm{TRIMs}} \left(n_K^+ - n_K^- \right) \mod 4$$

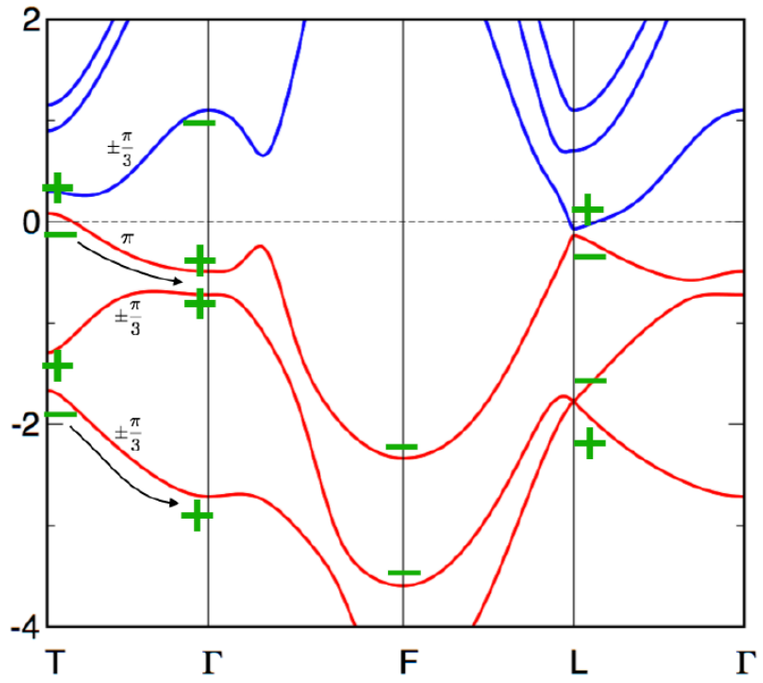
Parity of Z_4 index gives Z_2 index: $(-1)^{\nu_0} = (-1)^{\kappa_1}$

Hinge states are only possible when $\kappa_1 = 2$

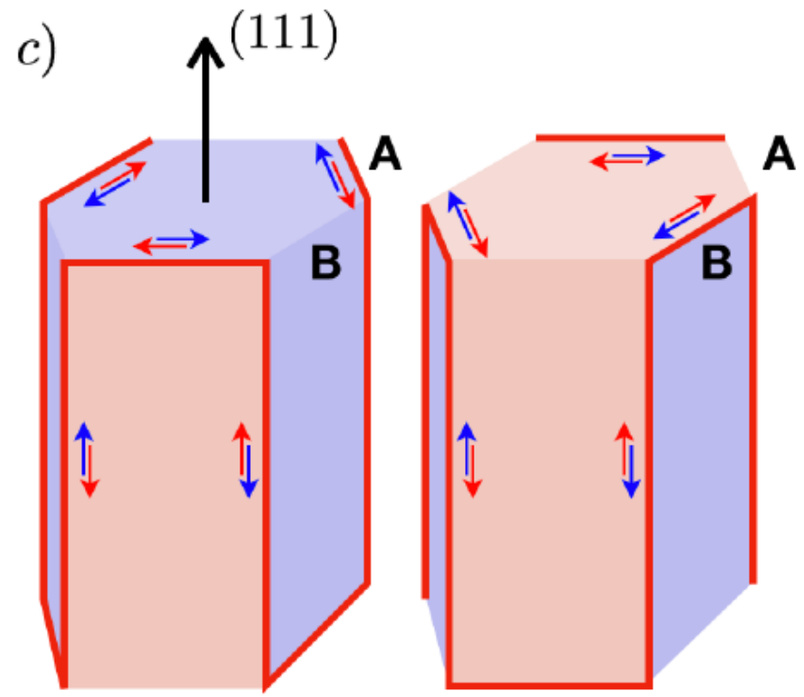
Bismuth: predicted HOTI

Schindler, et al, Sci. Adv. 2018

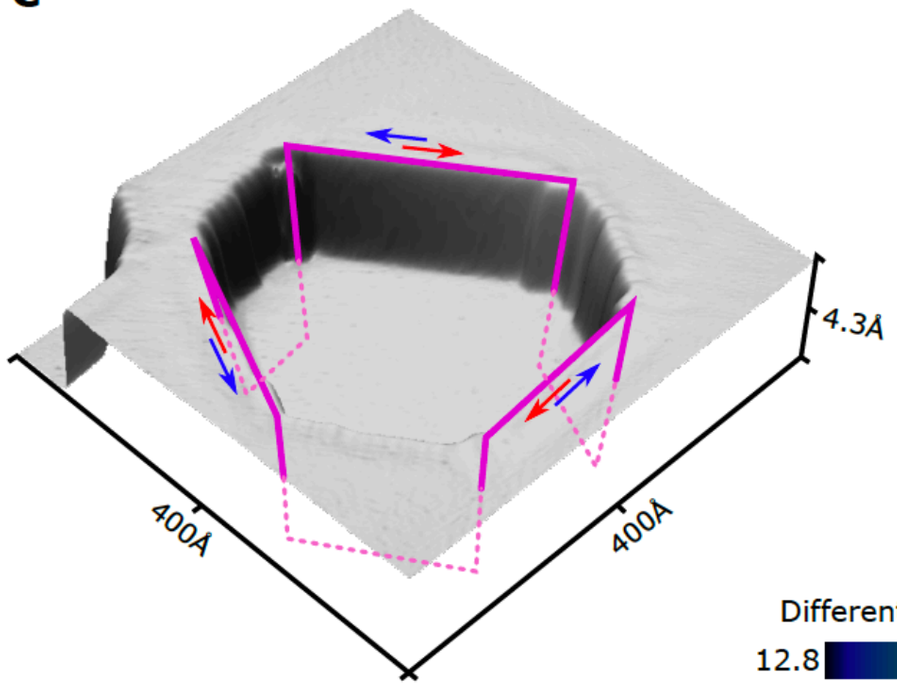


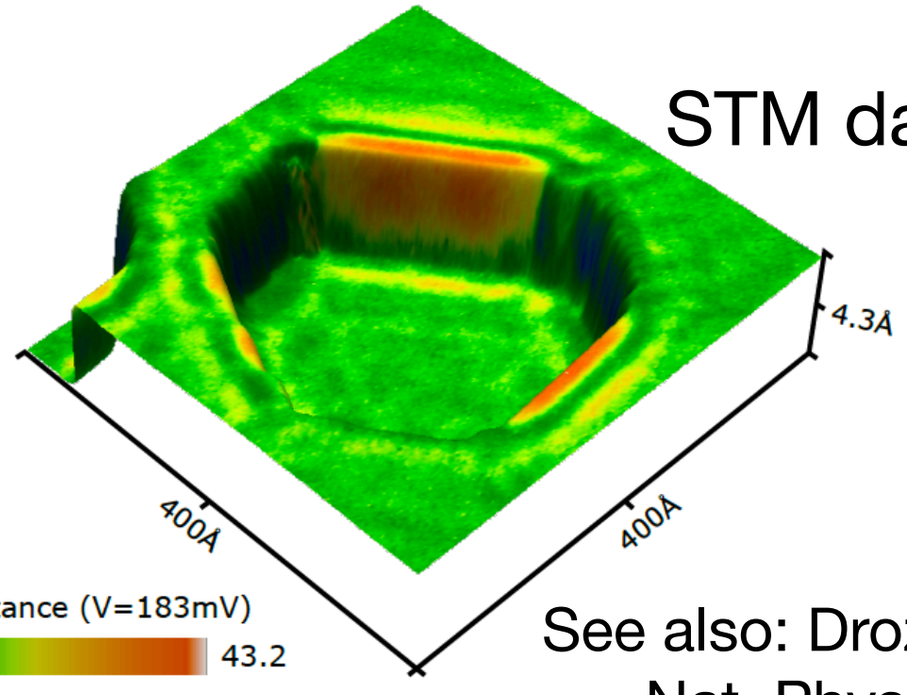


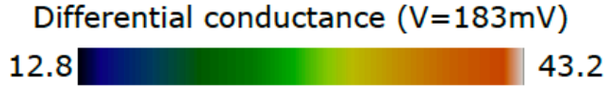
Topography



Differential conductance map

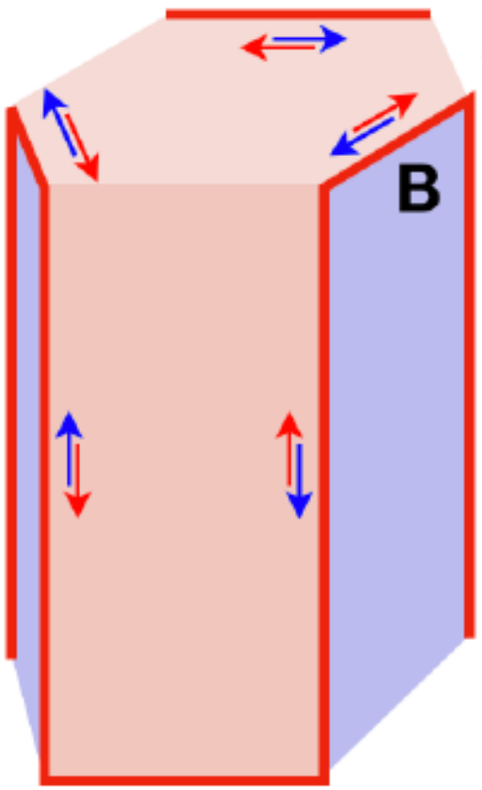




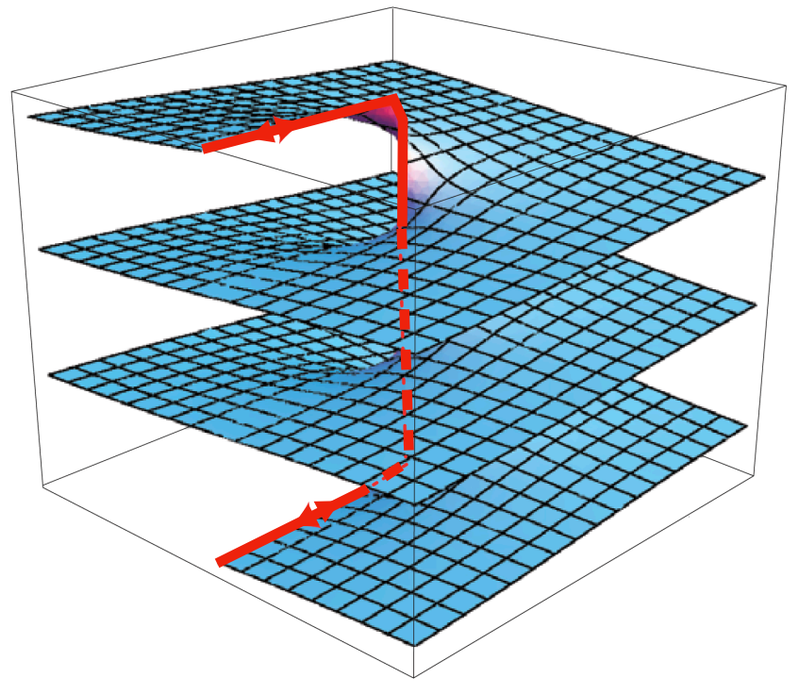


STM data

See also: Drozdov et al, Nat. Phys. 2014



Problem: challenging to precisely cleave crystal to observe hinge states



We propose gapless modes on dislocations to probe HOTIs

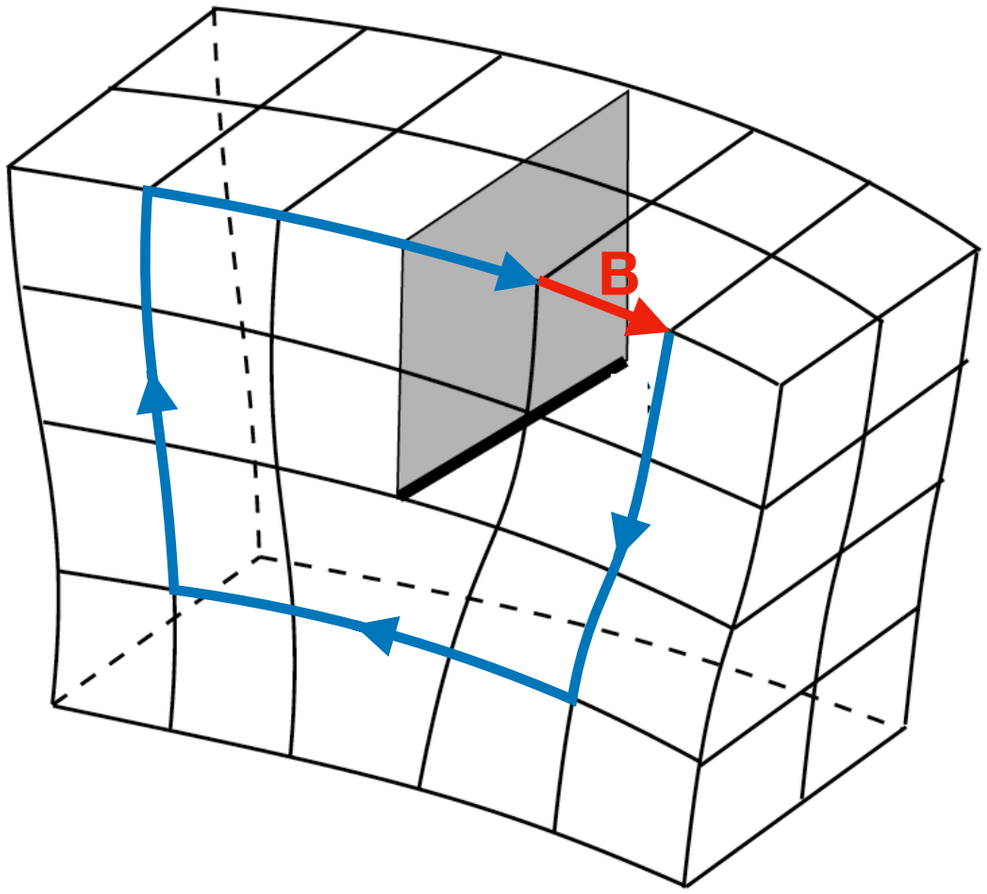
Raquel Queiroz
@KITP til Nov. 22

Collaboration with Raquel Queiroz, Cosma Fulga, Nurit Avraham and Haim Beidenkopf

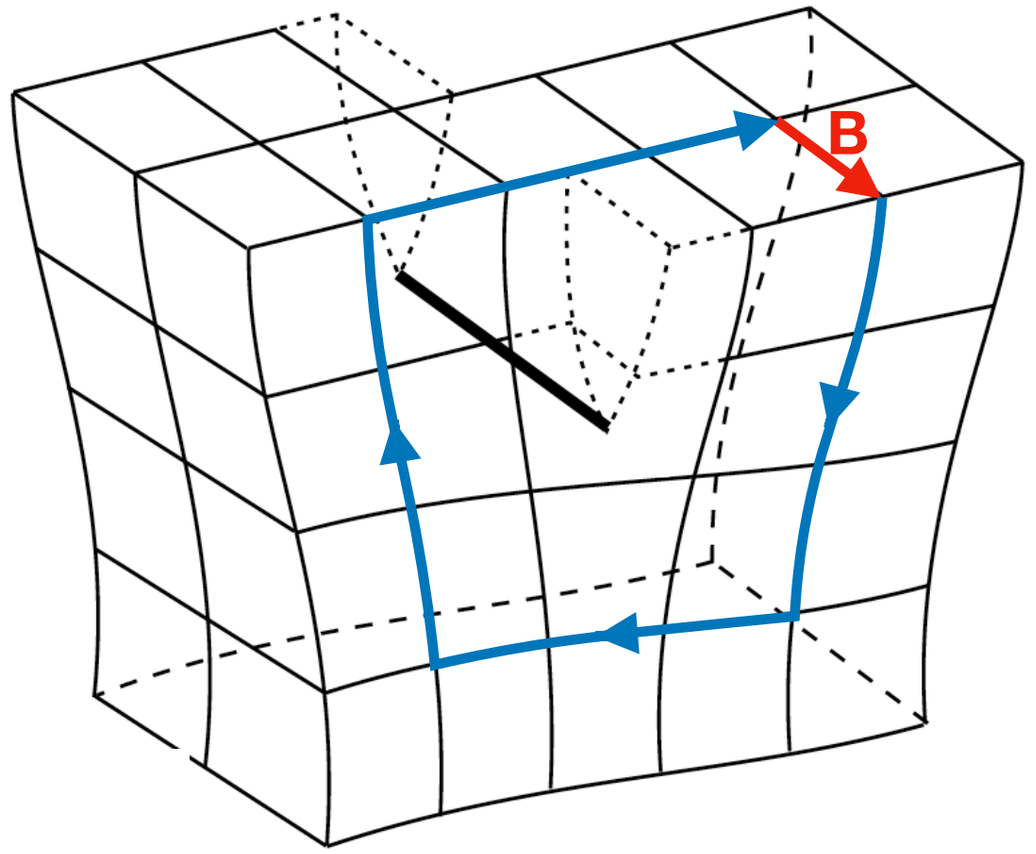
Reference: ArXiv 1809.03518

Dislocations introduce additional “hinge”

Edge dislocation



Screw dislocation

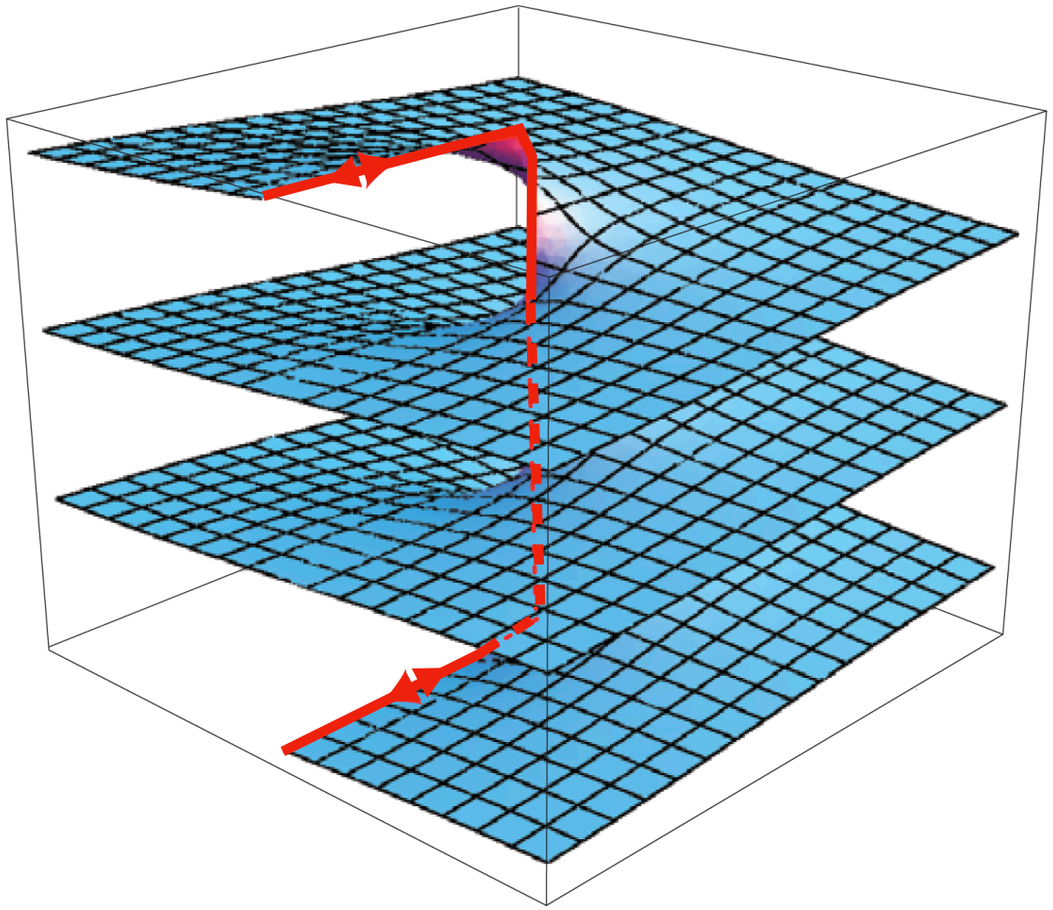


Burgers vector characterizes dislocation

Can dislocation bind gapless helical mode?

Dislocation in weak TI binds helical mode

Ran, Zhang, Vishwanath Nat. Phys. 2009

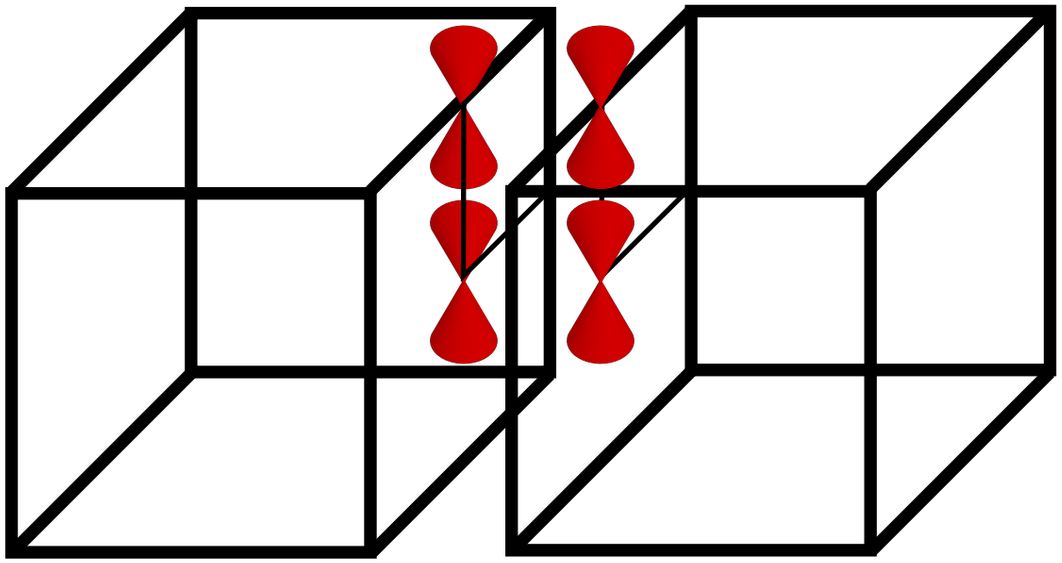


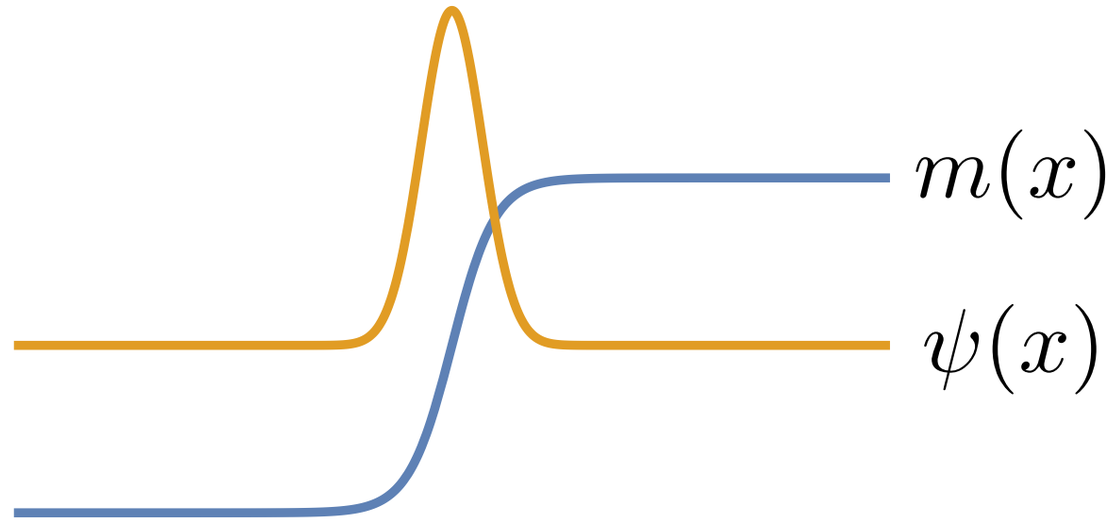
Heuristic:

step edge = gapless edge of TI

Dislocation in weak TI binds helical mode

Ran, Zhang, Vishwanath Nat. Phys. 2009





Domain wall in mass traps E=0 state
(Jackiw-Rebbi)

<u>Slice-and-glue argument:</u>

1. Slice: expose Dirac cones
2. Expand: $\Psi(\mathbf{x}) \sim e^{i\mathbf{k}_D \cdot \mathbf{x}} \psi(\mathbf{x})$
3. Glue: mass gap w/ dislocation has extra phase: $e^{i\mathbf{k}_D \cdot \mathbf{B}} = \pm 1$
4. Domain wall in mass iff: $e^{i\mathbf{k}_D \cdot \mathbf{B}} = -1$

Dislocation in weak TI binds helical mode

Ran, Zhang, Vishwanath Nat. Phys. 2009

General formula to bind helical mode along dislocation:

$$\mathbf{B}\cdot\mathbf{M}_\nu = \pi \,(\mathrm{mod}\, 2\pi)$$

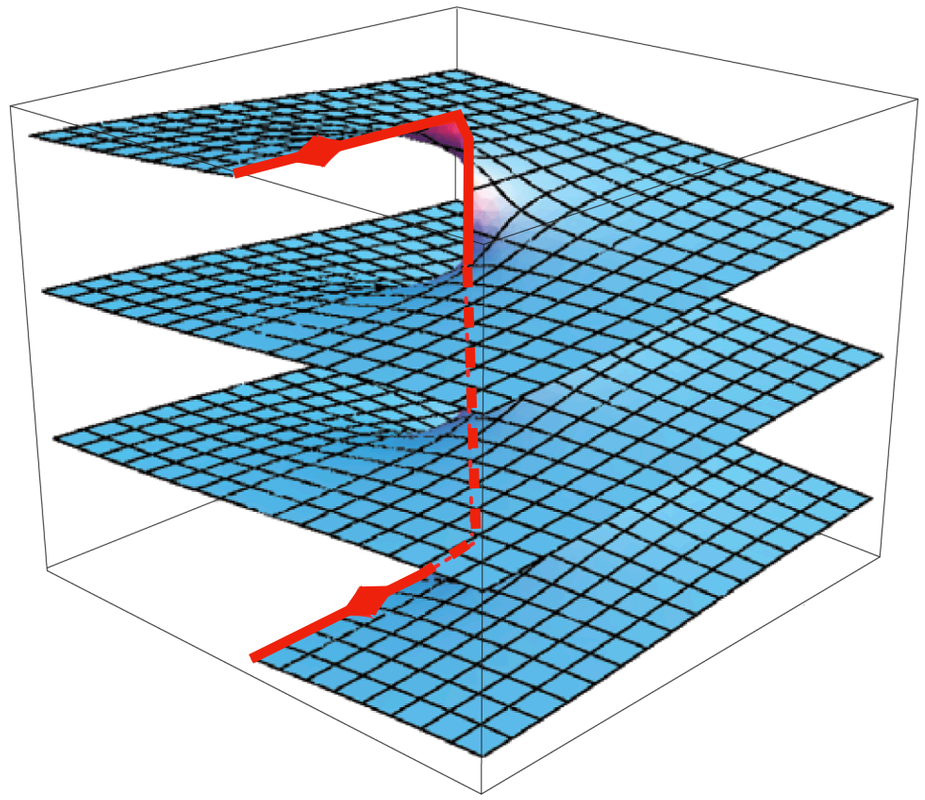
$$\mathbf{M}_\nu = (1/2)(\nu_1\mathbf{G}_1 + \nu_2\mathbf{G}_2 + \nu_3\mathbf{G}_3)$$

Example: stacked 2D TIs:

$$(\nu_0;\nu_1,\nu_2,\nu_3) = (0;0,0,1)$$

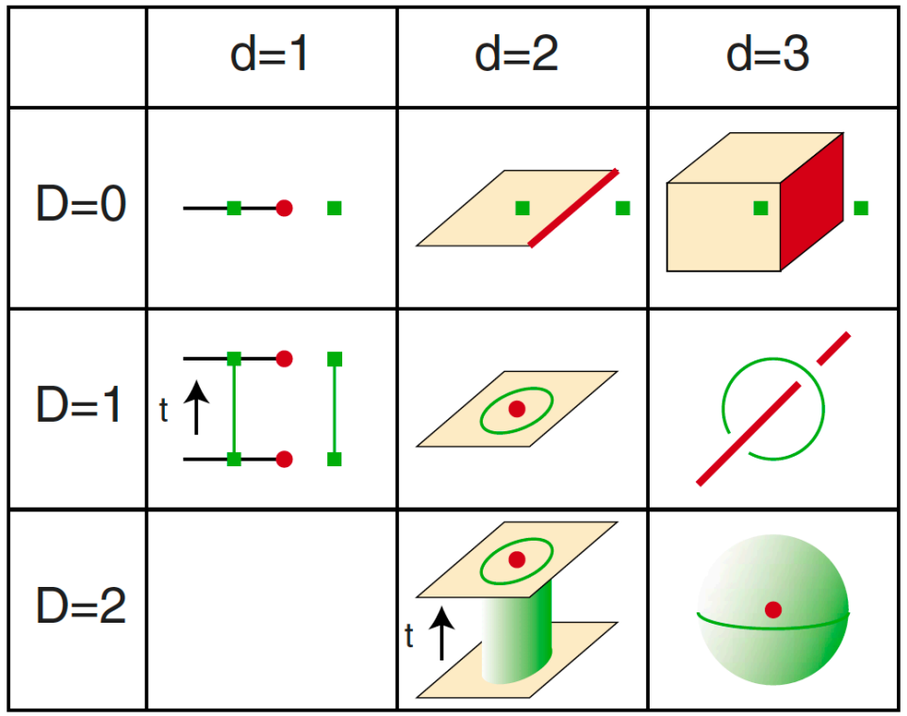
$$\mathbf{M}_\nu = \frac{1}{2}\mathbf{G}_z,\ \ \mathbf{B} = \hat{z}$$

$$\Rightarrow \mathbf{B}\cdot\mathbf{M}_\nu = \pi$$



Topological defect classification for all dimensions and symmetry classes

Teo and Kane PRB 2010



Class	$\delta = 0$	$\delta = 1$	$\delta = 2$	$\delta = 3$
AII	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$

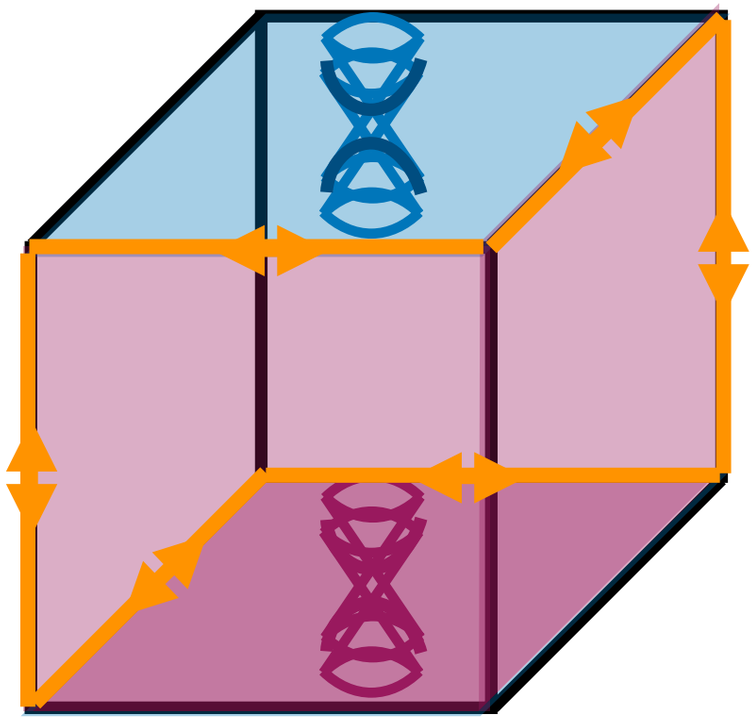
Teo, Hughes, Benalcazar: disclinations in topological superconductors

HOTI model: “Double strong topological insulator”

Po, Vishwanath, Watanabe (Nature Comm. 2017)
Fang and Fu (1709.01929); Khalaf, Po, Vishwanath (PRX 2018)

Two copies of a 3D topological insulator

Gapped by a mass term odd under inversion symmetry

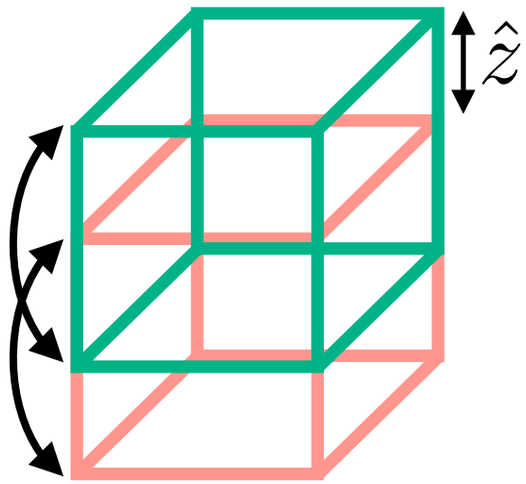


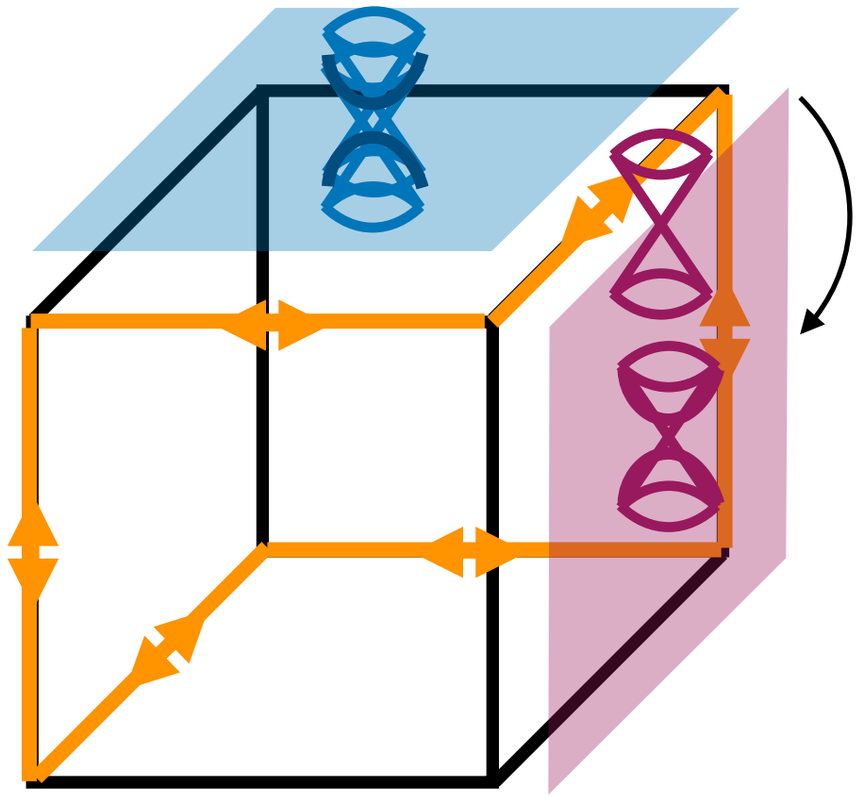
Mass domain walls bind helical mode

By construction: all weak/strong indices are zero; HOTI index is 2

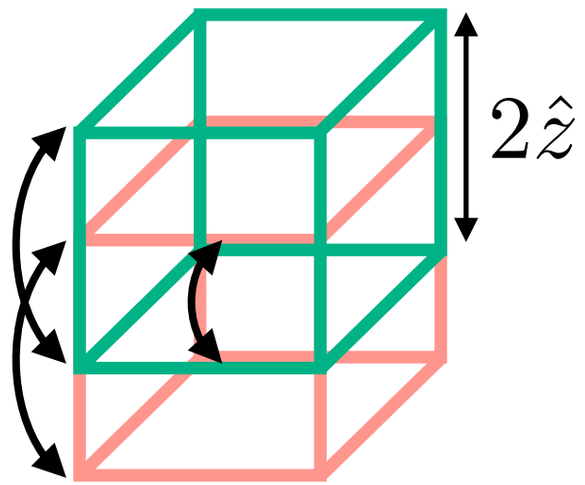
Our model: two 3D TIs offset by $\hat{z}$

Decoupled limit:
- weak TI
- z is lattice vec





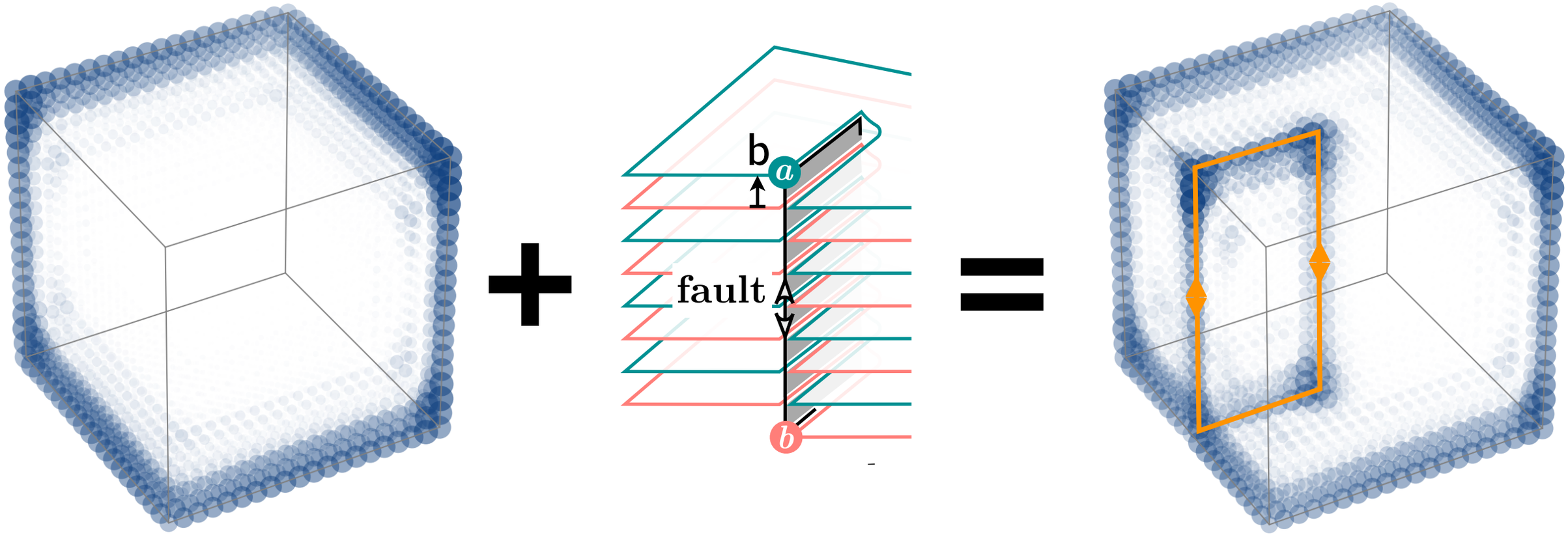
After coupling:
- no weak indices
- 2z is lattice vec
- HOTI index is 2



$$H_0(\mathsf{k}) = [M(\mathsf{k})\tau_z + A(\sin k_x \sigma_z \tau_x - \sin k_y \tau_y + \sin k_z \sigma_x \tau_x)]\mu_0$$

$$H_\delta(\mathsf{k}) = m \sin \frac{k_z}{2} \sigma_y \tau_x \mu_x + \delta \cos \frac{k_z}{2} (\sigma_x \tau_z + \sigma_y \tau_0)\mu_y$$

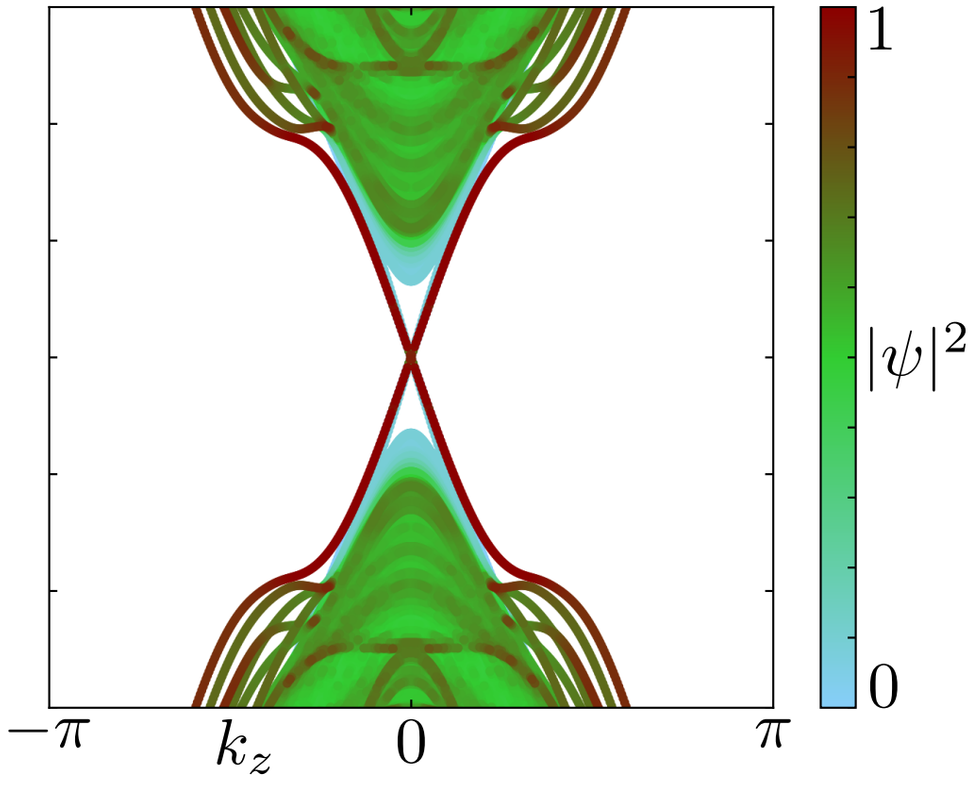
Consider a dislocation in a HOTI

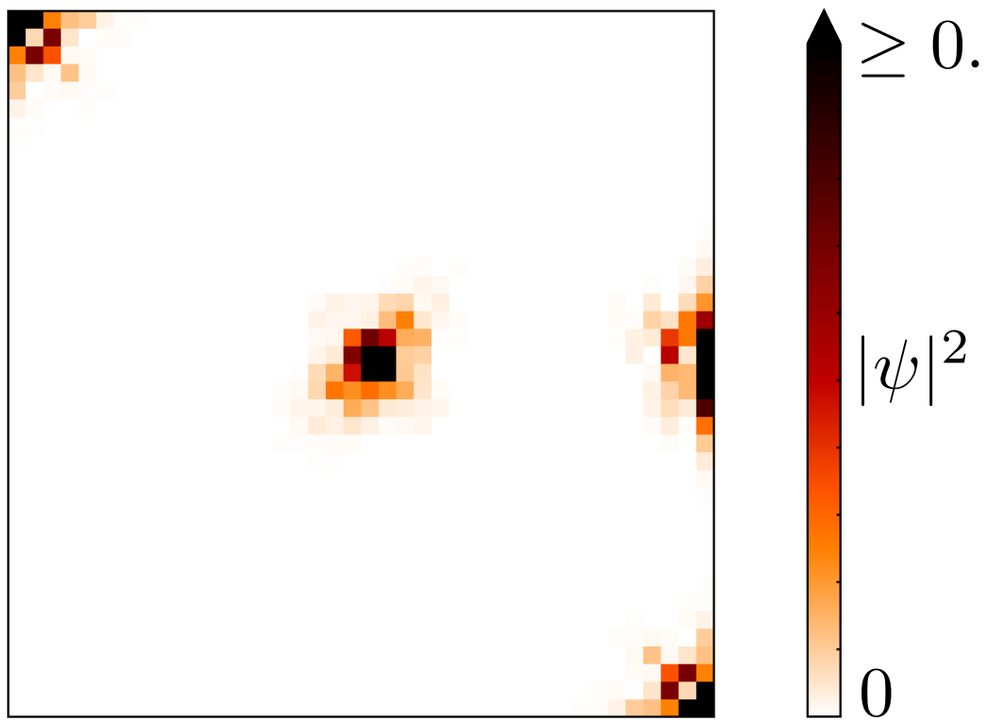


Double strong TI exhibits helical modes on hinges

Dislocation binds gapless mode

Band structure verifies gapless states are helical

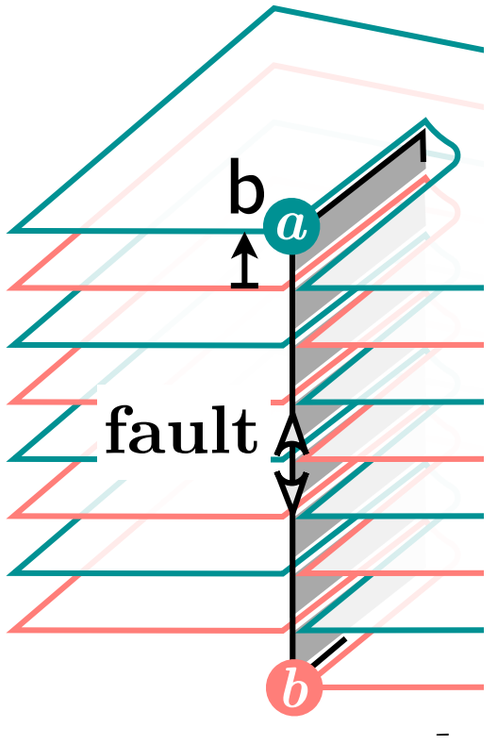




Contradiction: defect is not supposed to bind helical mode when weak indices are zero!

$$\mathbf{B} \cdot \mathbf{M}_\nu = 0$$

Understand helical mode from decoupled limit



Decoupled 3D TIs are weak TI:

$$(\nu_0; \nu_1, \nu_2, \nu_3) = (0; 0, 0, 1)$$

$$\mathbf{M}_\nu = \frac{1}{2}\mathbf{G}_z, \quad \mathbf{B} = \hat{z}$$

$$\Rightarrow \mathbf{B} \cdot \mathbf{M}_\nu = \pi$$

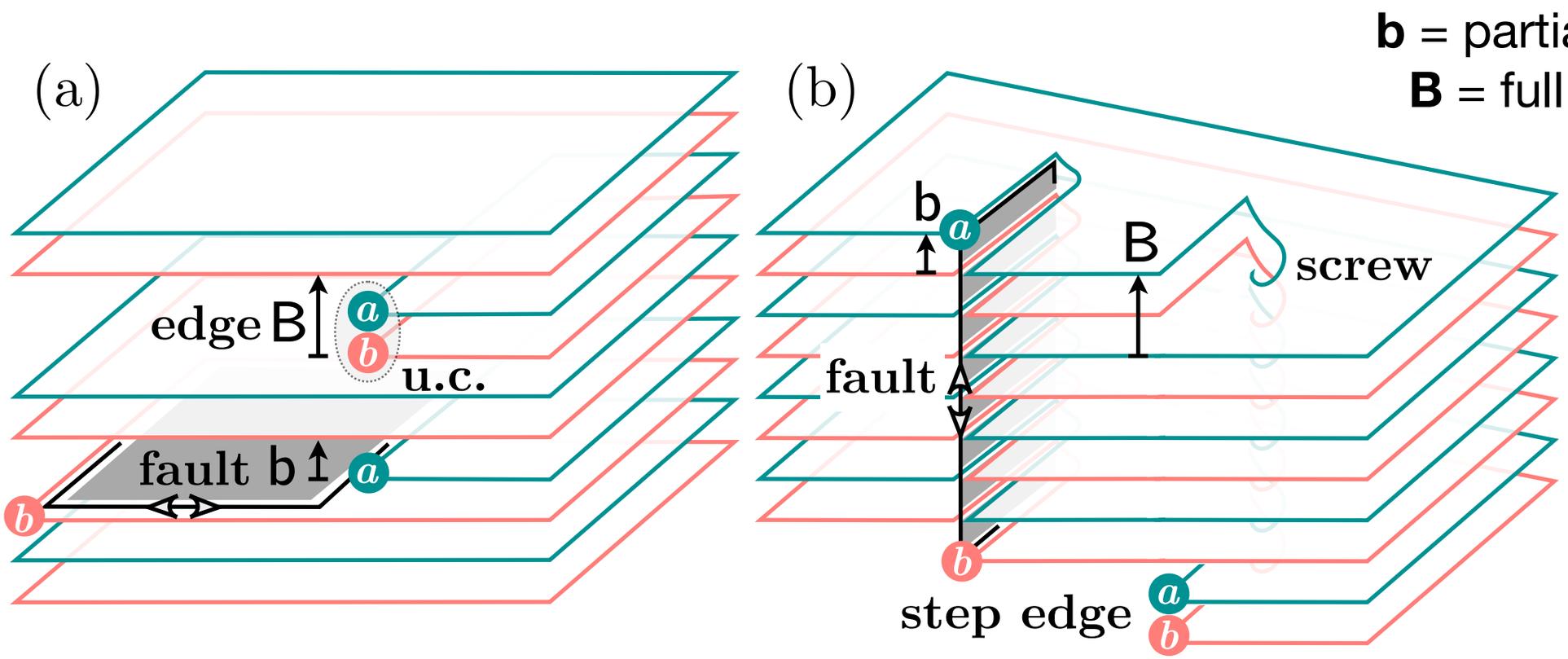
⇒ defect binds helical mode

Coupling 3D TIs reduces translation symmetry,
but helical mode is robust

So helical mode is correct…. how to reconcile with M=0 for HOTI?

Partial dislocations evade classification

Partial dislocation: Burgers vector is fraction of lattice vector



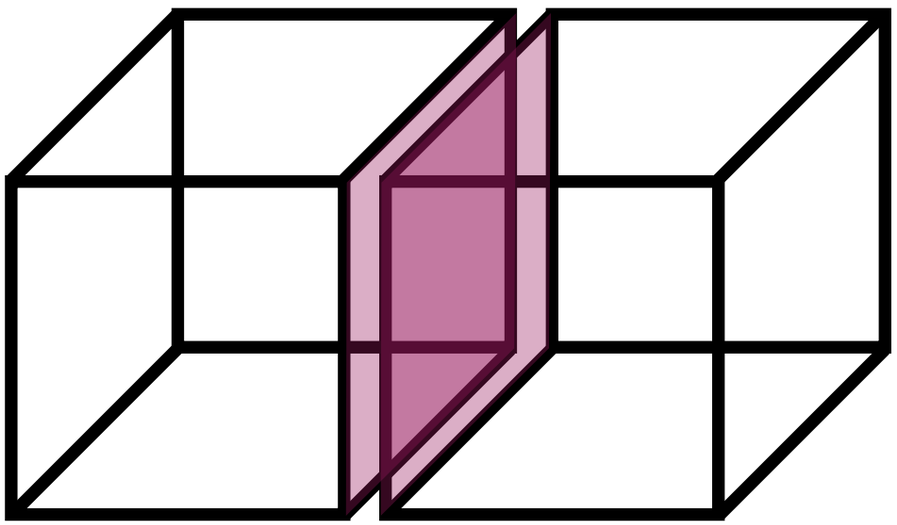
Partial lattice dislocations always introduce a stacking fault

Low-energy theory of stacking fault

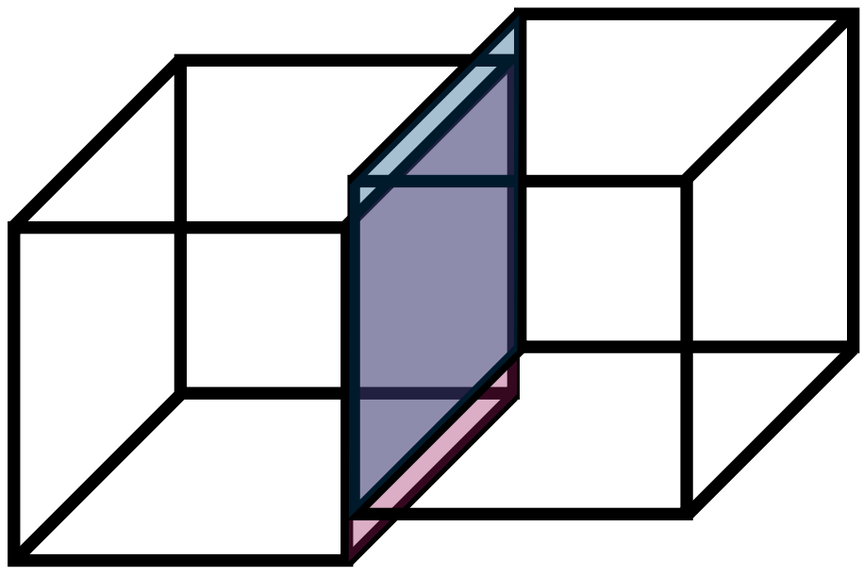
Slice-and-glue

1. Expand around band inversion point k ≈ 0
2. Bound state ansatz: $\psi = e^{-\int M(y)/A\, dy}\chi$
3. Bound state Hamiltonian: compare mass

Without stacking fault:



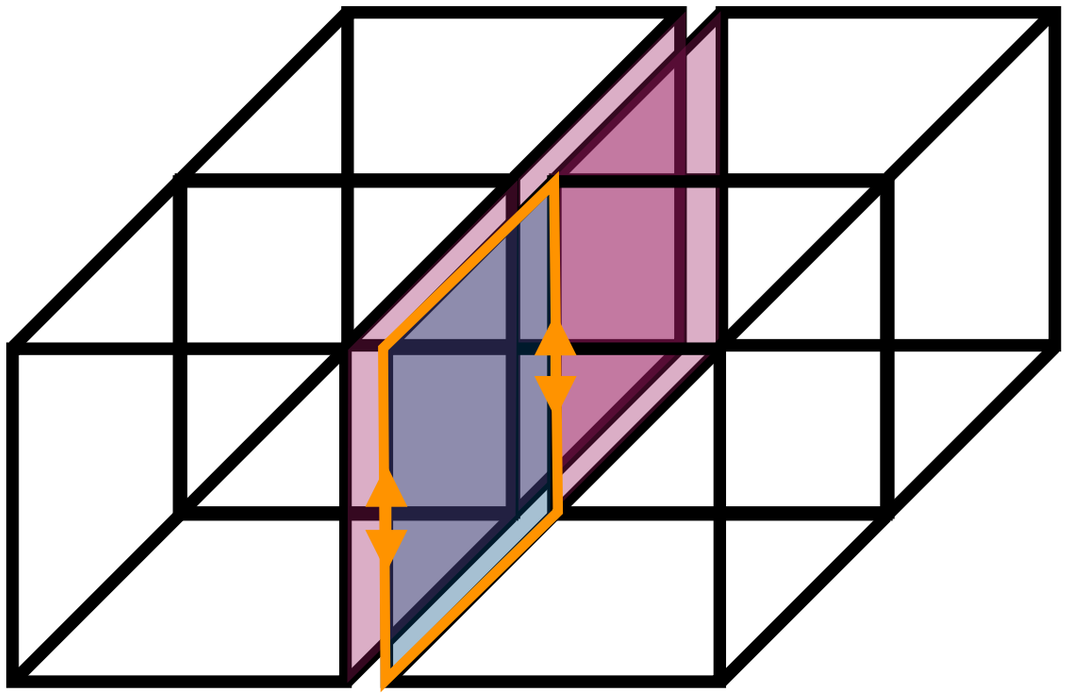
With stacking fault:

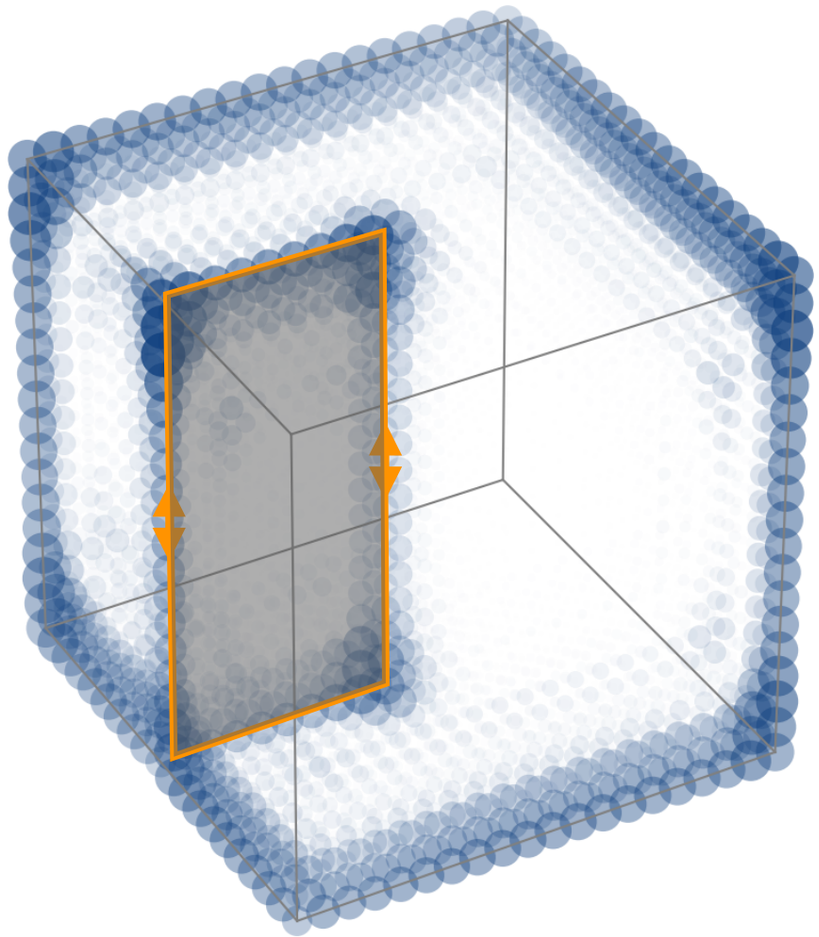


Result: Z_2 index changes with stacking fault!

Helical mode surrounds stacking fault
⇔ stacking fault is an “embedded 2D TI”

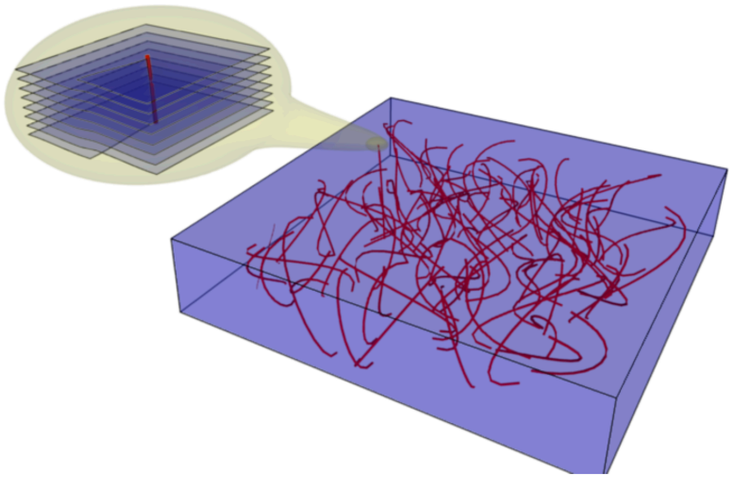
Embedded TI: Tuegel, Chua, Hughes 2018

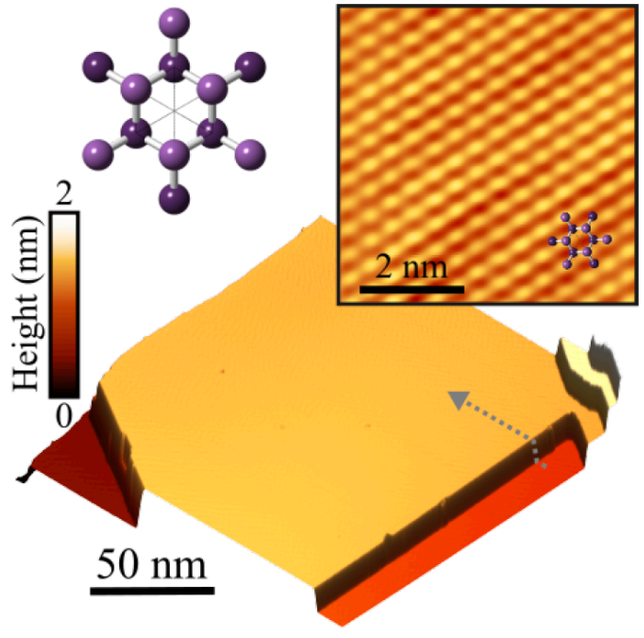




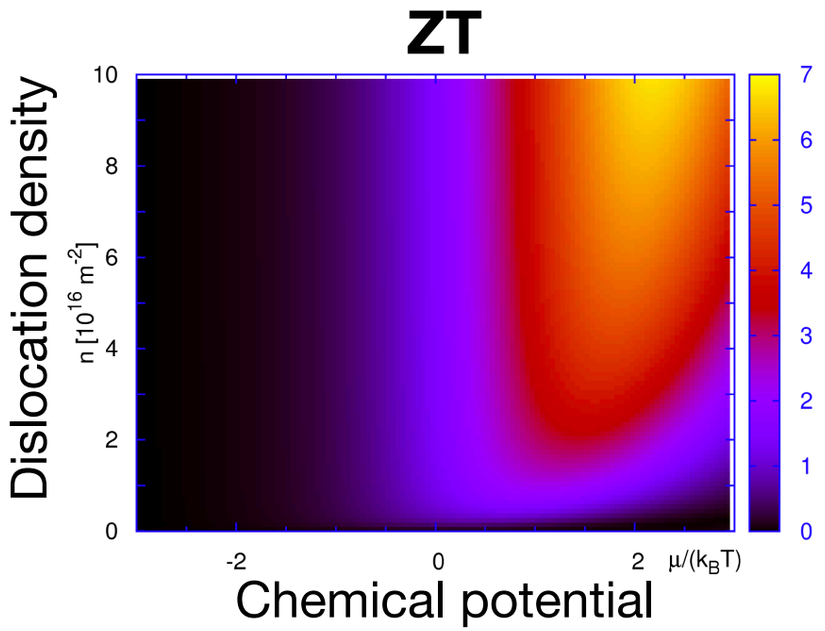
Experimental predictions

1. Helical modes along step edges detectable via STM





2. Enhanced bulk conductivity if many aligned dislocations



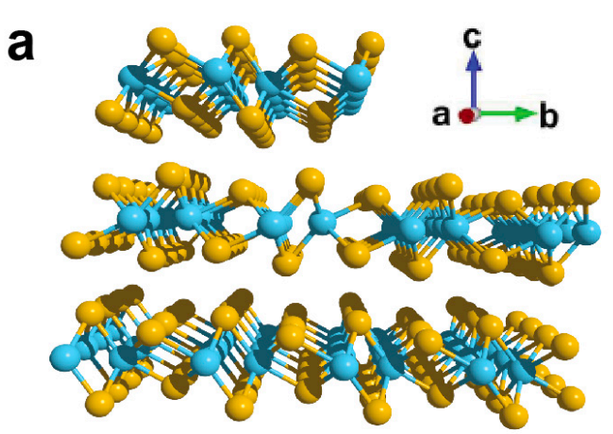
Est. max ZT ~6 in $(Bi_{1-x}Sb_x)_2Te_3$, $Bi_2(Te_{1-y}Se_y)_3$
Tretiakov, Abanov, Murakami, Sinova
(Appl. Phys. Lett. 97, 073108 (2010))

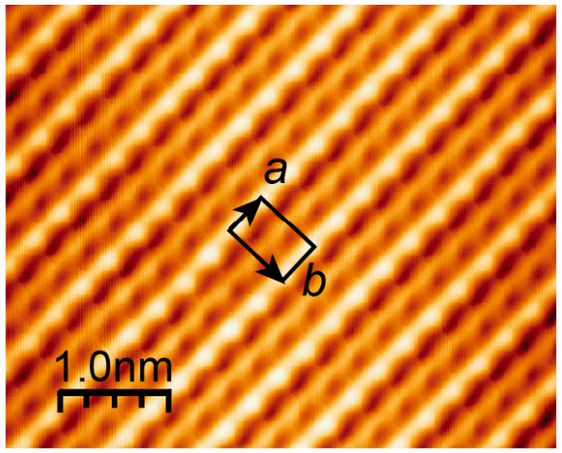
Prediction: helical mode on partial step edges in TMDs in 1T' structure

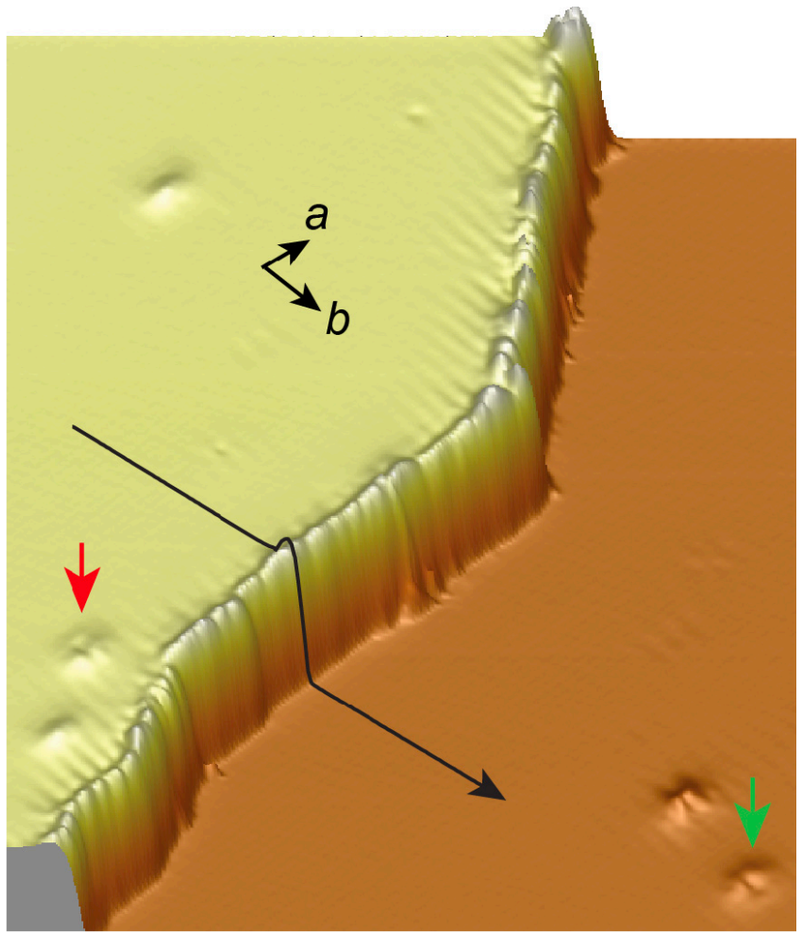
$MoTe_2$, WTe_2 predicted HOTI w/ two layers in unit cell
(Wang, et al ArXiv 1806.11116)

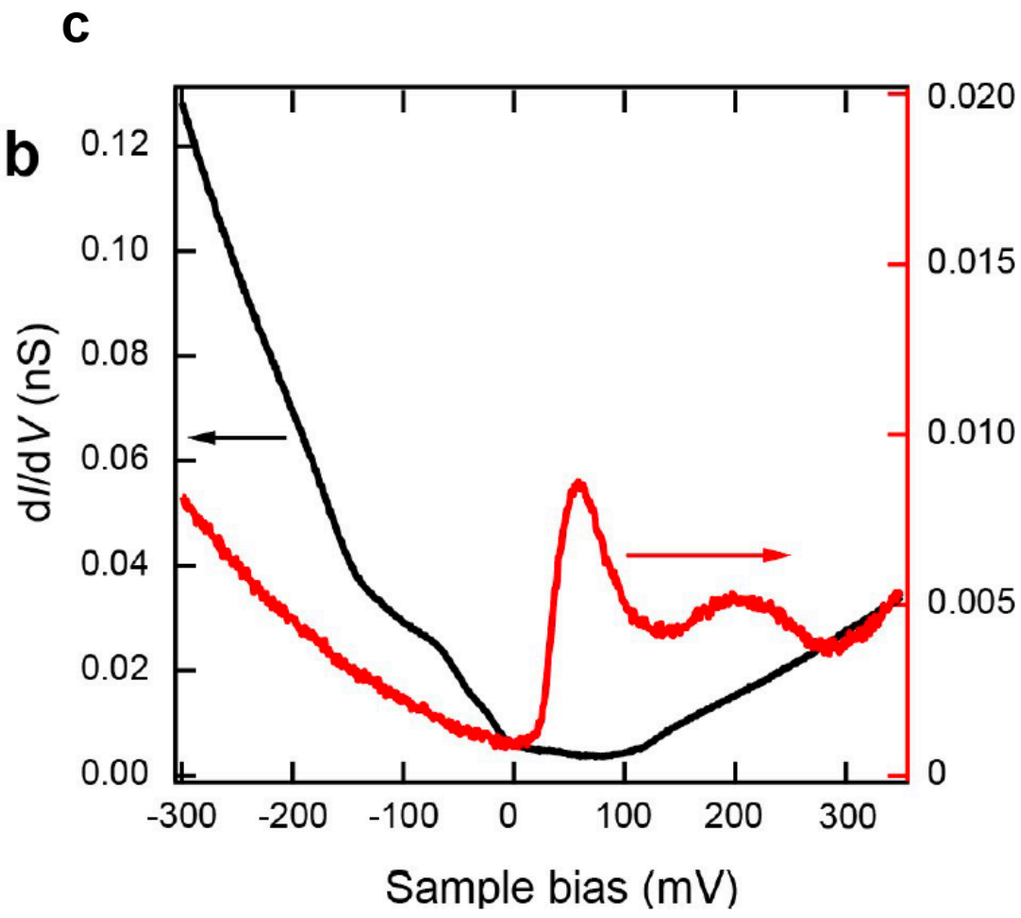
Promising: partial step edges in <u>monolayer</u> WTe_2 show d.o.s. peak
(Peng, et al, Nat. Comm. 8, 659 (2017); Jia, et al, PRB 96, 041108 (2017))

(2017)

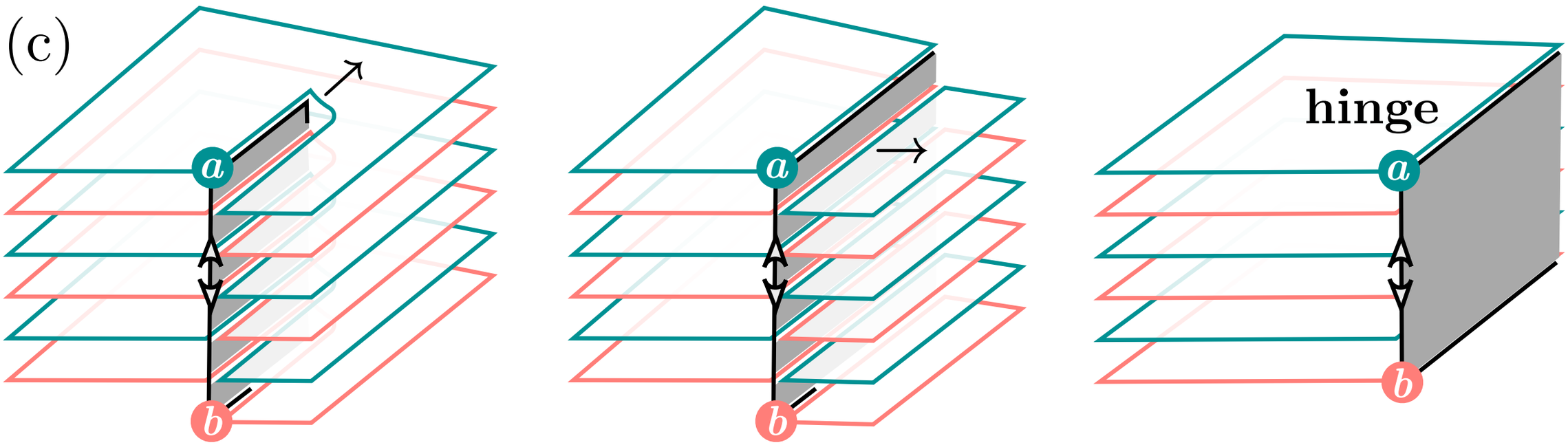






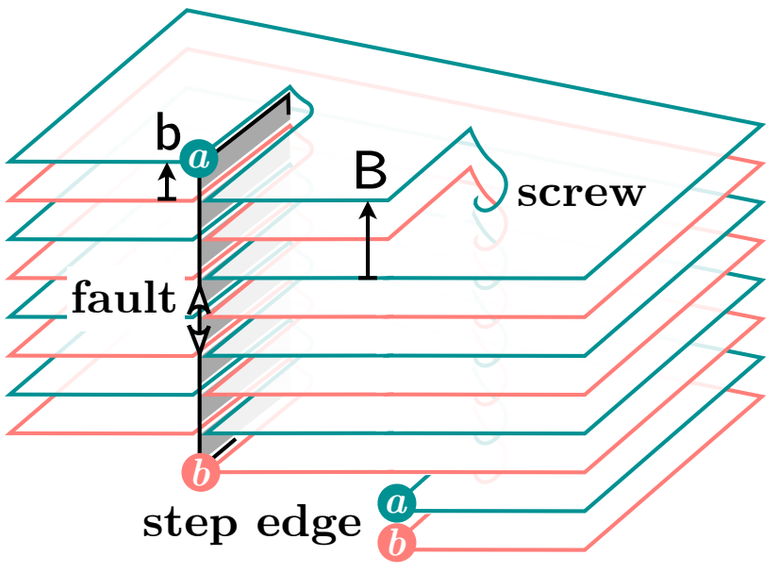


Expect general connection between helical mode on step edge and higher order topological insulator



Helical mode on step edge deforms to hinge mode

Whether a partial dislocation can bind a helical mode is constrained by M.B criterion



Consider a partial Burgers vector, **b**

Let *n* be smallest integer such that *n***b** is lattice vector

If dislocation **b** binds *h* helical modes, then:

$$n\mathrm{b} \cdot \mathrm{M}_\nu = nh\pi \mod 2\pi$$

	n even Double strong TI	*n* odd
$n\mathrm{b} \cdot \mathrm{M}_\nu = 0$	*h* = 0 or 1 (no constraint)	*h* = 0 (helical mode forbidden)
$n\mathrm{b} \cdot \mathrm{M}_\nu = \pi$	Gapped stacking fault does not exist!	*h* = 1 (helical mode required)

Conclusions

Crystal symmetry can be used to predict and identify topological materials
(Bradlyn, JC, et al Nature 2017;
JC et al PRB 97, 035139 (2018))

"Higher order topological insulators" (HOTIs) are a new type of topological phase that has come out of the symmetry classification

We propose partial lattice dislocations as surface/bulk signature of certain HOTIs
(ArXiv: 1809.03518)

General classification of defects remains an open question