

Topological Crystalline Insulators

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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/ Chern insulator

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	$2\mathbb{Z}$...

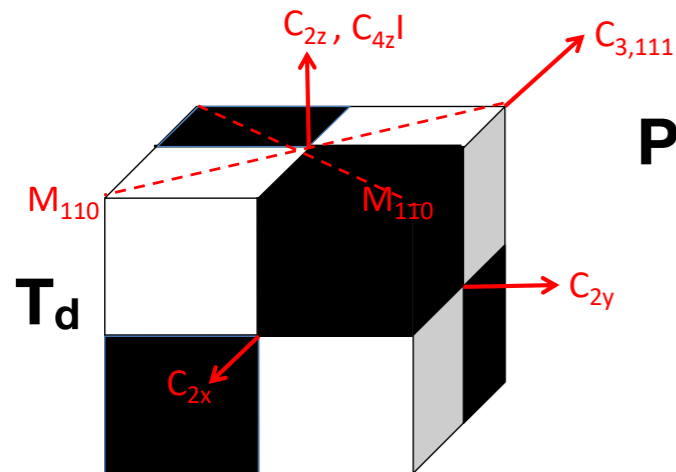
2d and 3d topological insulators
(weak index not captured)

Crystal symmetries can protect and identify topological phases

Outline:

- What are the possible crystal symmetries?
- Examples of topological phases with crystal symmetry
- Recent classification of band structures by symmetry irreps

What are crystal symmetries?



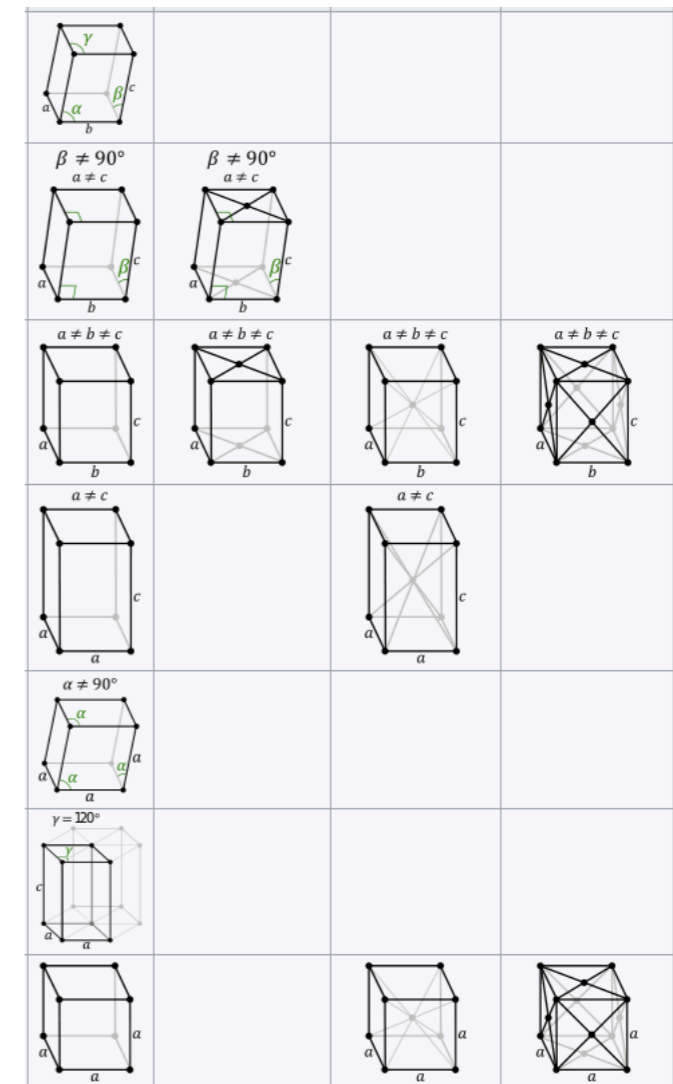
Point group symmetries: leave (at least) one point invariant

Consist of rotations, mirrors, inversion, and rotoinversion
32 crystallographic point groups

Translations: leave no point invariant

Generate one of the 14 Bravais lattices in 3D

Glide and screw symmetries: leave no point invariant, but also rotate/reflect



The 230 **space groups** enumerate all possible combinations of symmetries in 3D crystals

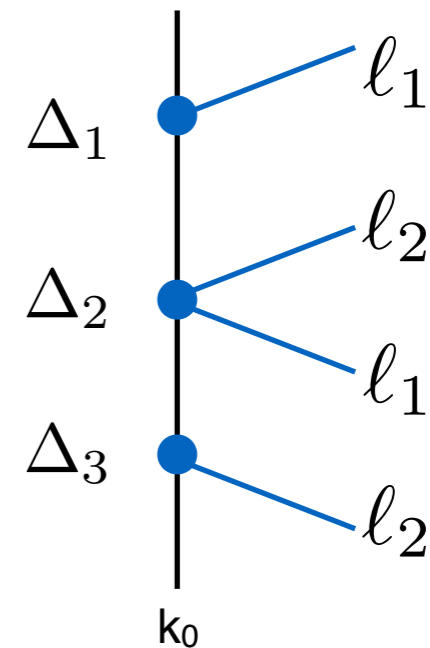
How do crystal symmetries act on a Hamiltonian?

Fourier-transformed Hamiltonian: $\Delta(\mathcal{G})H(\mathbf{k})\Delta(\mathcal{G})^{-1} = H(\mathcal{G}\mathbf{k})$
 matrix representative of symmetry operation

“Little group” of \mathbf{k}_0 : $\mathcal{G}\mathbf{k}_0 = \mathbf{k}_0$

Eigenstates transform under little group irreps

Irreps at \mathbf{k}_0 determine irreps along lines emanating from \mathbf{k}_0

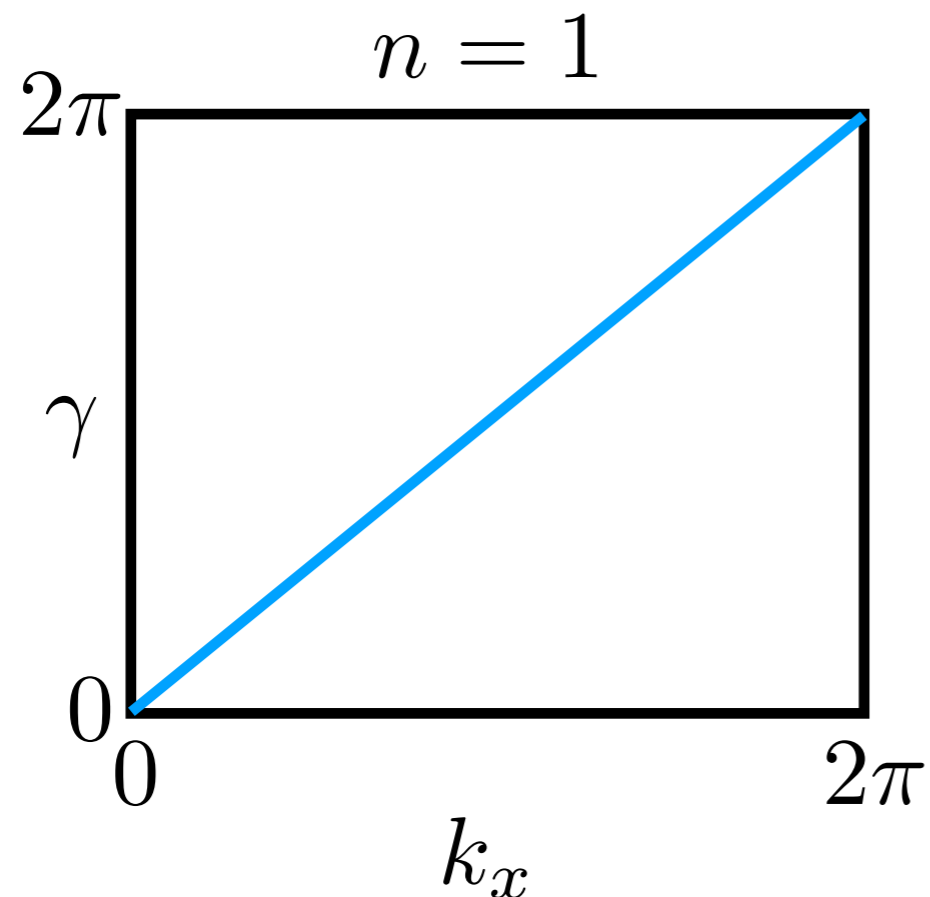


$$\left. \begin{array}{l} \Delta_1 \rightarrow l_1 \\ \Delta_2 \rightarrow l_1 \oplus l_2 \\ \Delta_3 \rightarrow l_2 \end{array} \right\} \text{Compatibility relations} \\ \text{between points and lines}$$

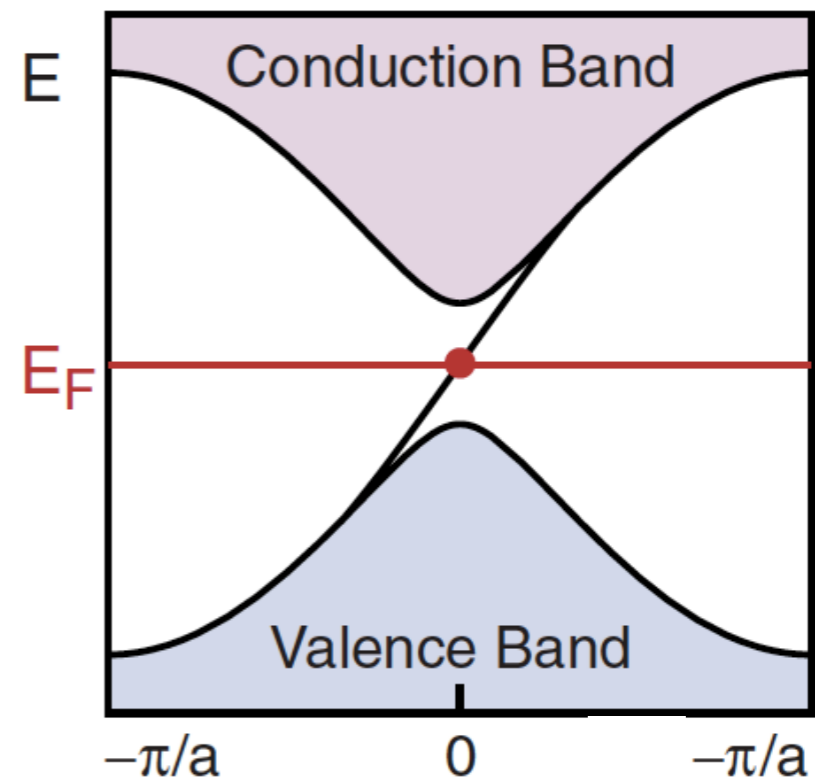
Recall: Chern insulator

A Chern insulator is a 2D insulator whose occupied bands cannot be deformed to an atomic insulator

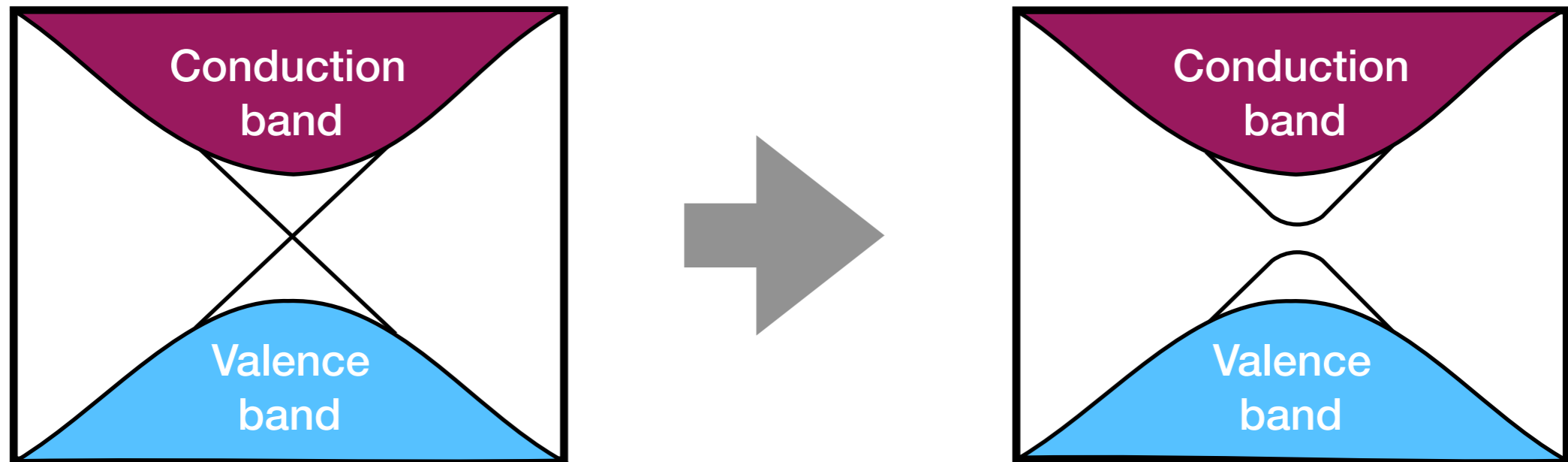
Topological invariant: Chern number



Bulk-edge correspondence



Surface states of bands with opposite Chern number generically gap



Unless protected by a symmetry:

Ex 1: spin conservation \Rightarrow quantum spin Hall

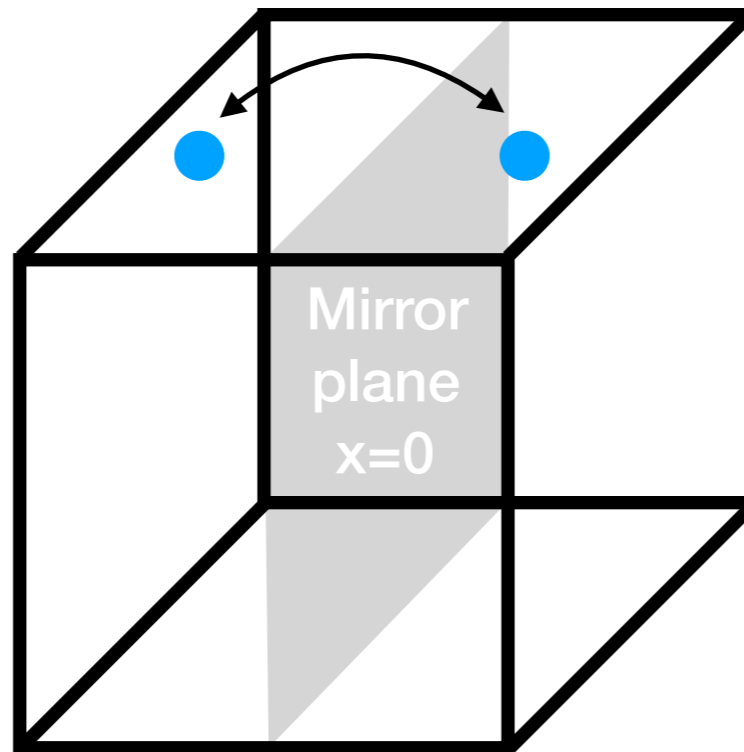
Ex 2: time-reversal symmetry \Rightarrow 2D TI

Crystal symmetry can also protect surface state crossings

Mirror Chern insulator: canonical TCI

Teo, Fu, Kane PRB 045426 (2008)

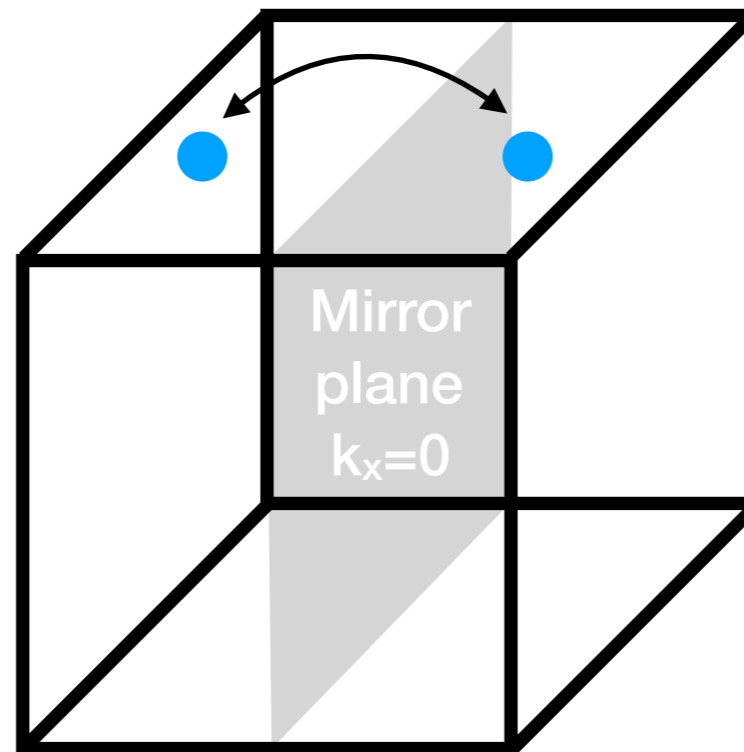
Mirror symmetry: $m_x : (x, y, z) \mapsto (-x, y, z)$



Mirror Chern insulator: canonical TCI

Teo, Fu, Kane PRB 045426 (2008)

Mirror symmetry: $m_x : (k_x, k_y, k_z) \mapsto (-k_x, k_y, k_z)$



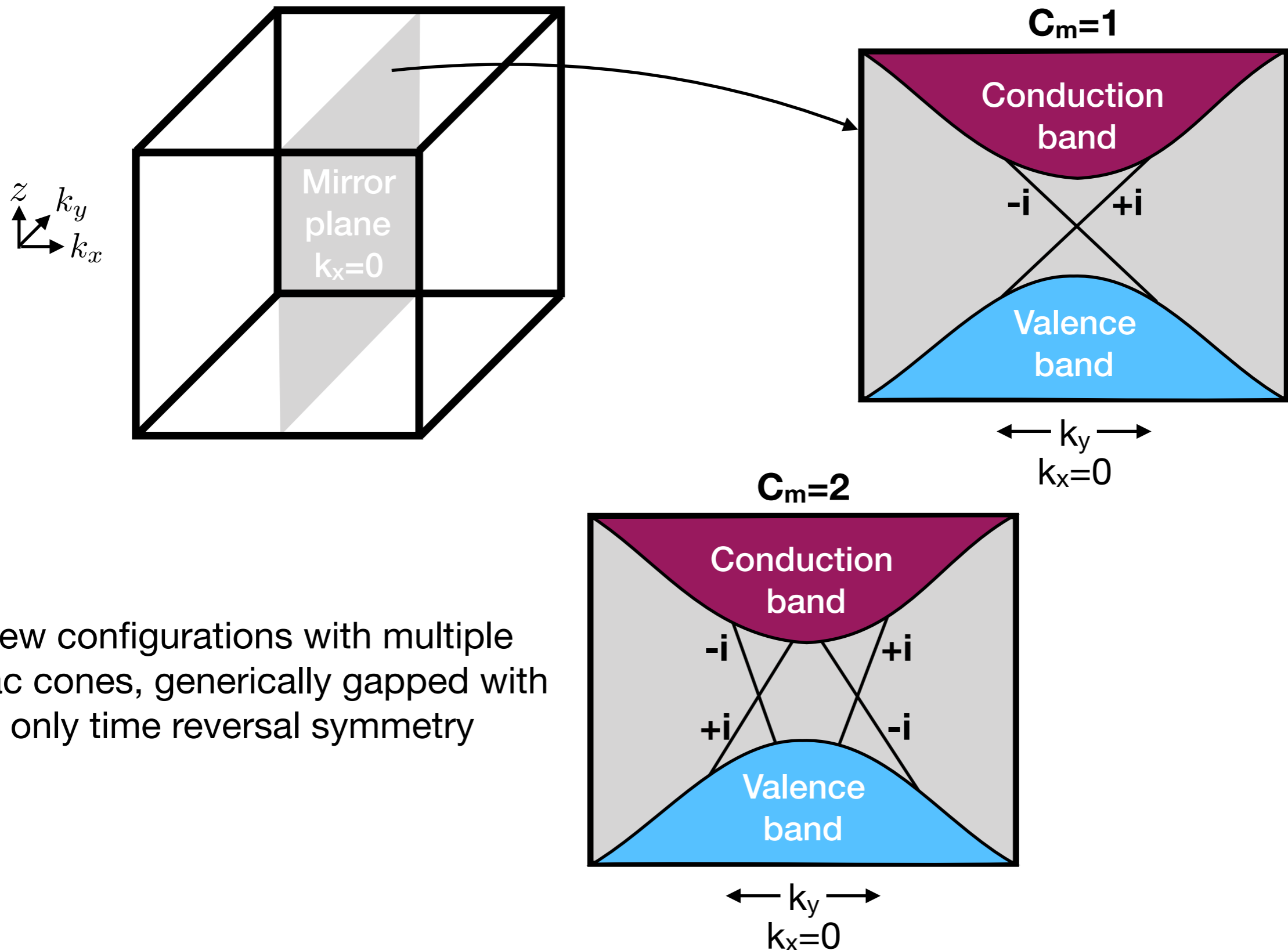
When $k_x=0$, m_x commutes with $H(k_x=0, k_y, k_z) \Rightarrow$ bands labelled by m_x eigenvalue: $\pm i$

Define Chern number for each mirror sector: C_{\pm}

Mirror Chern number: $C_m = \frac{1}{2}(C_+ - C_-)$

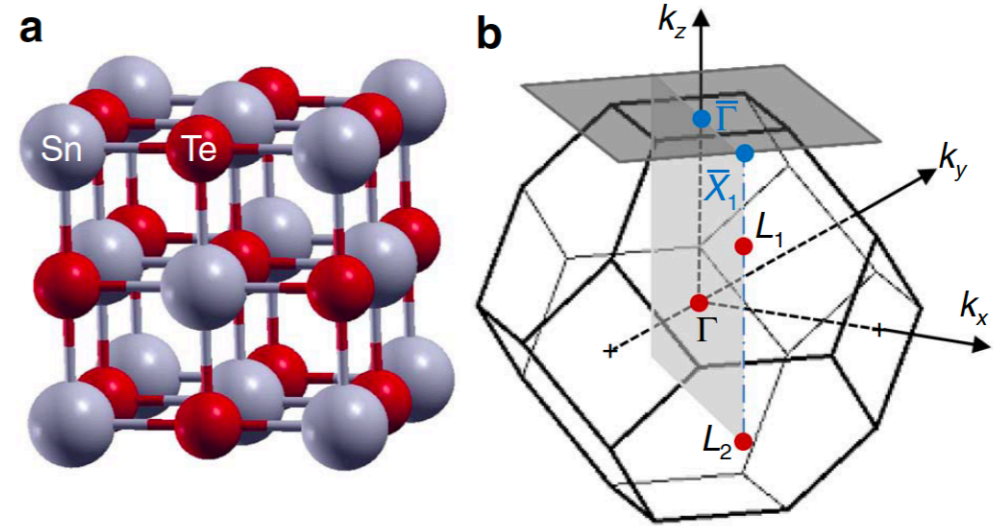
Surface states of mirror Chern insulator

Teo, Fu, Kane PRB 045426 (2008)



New configurations with multiple Dirac cones, generically gapped with only time reversal symmetry

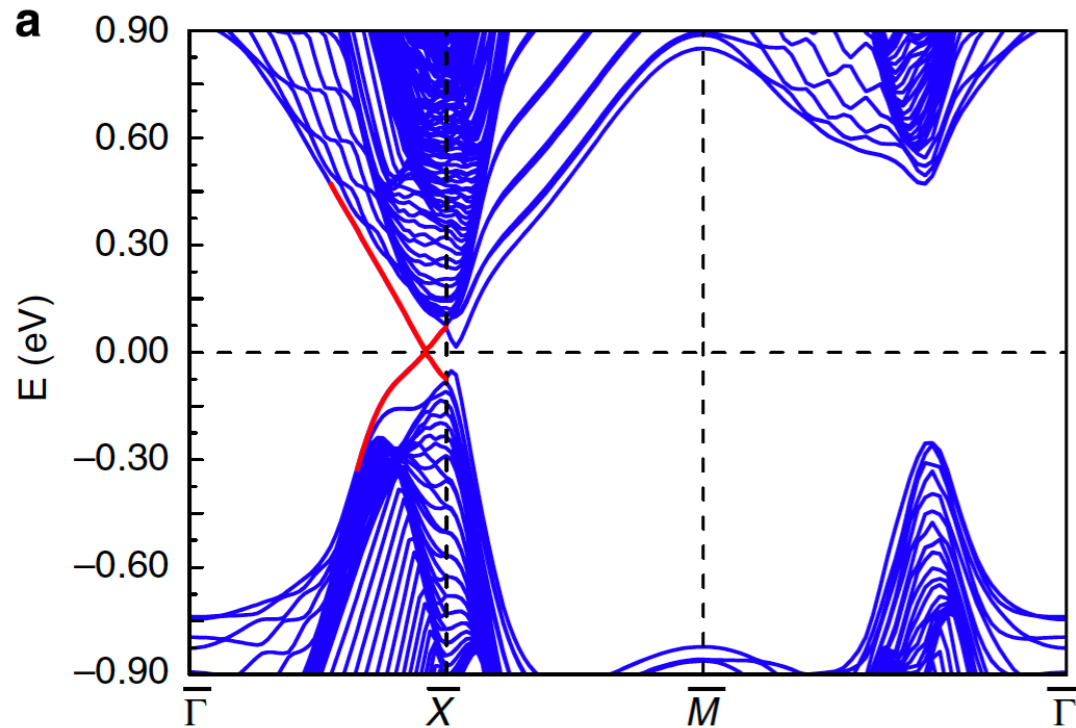
SnTe predicted/observed mirror Chern insulator



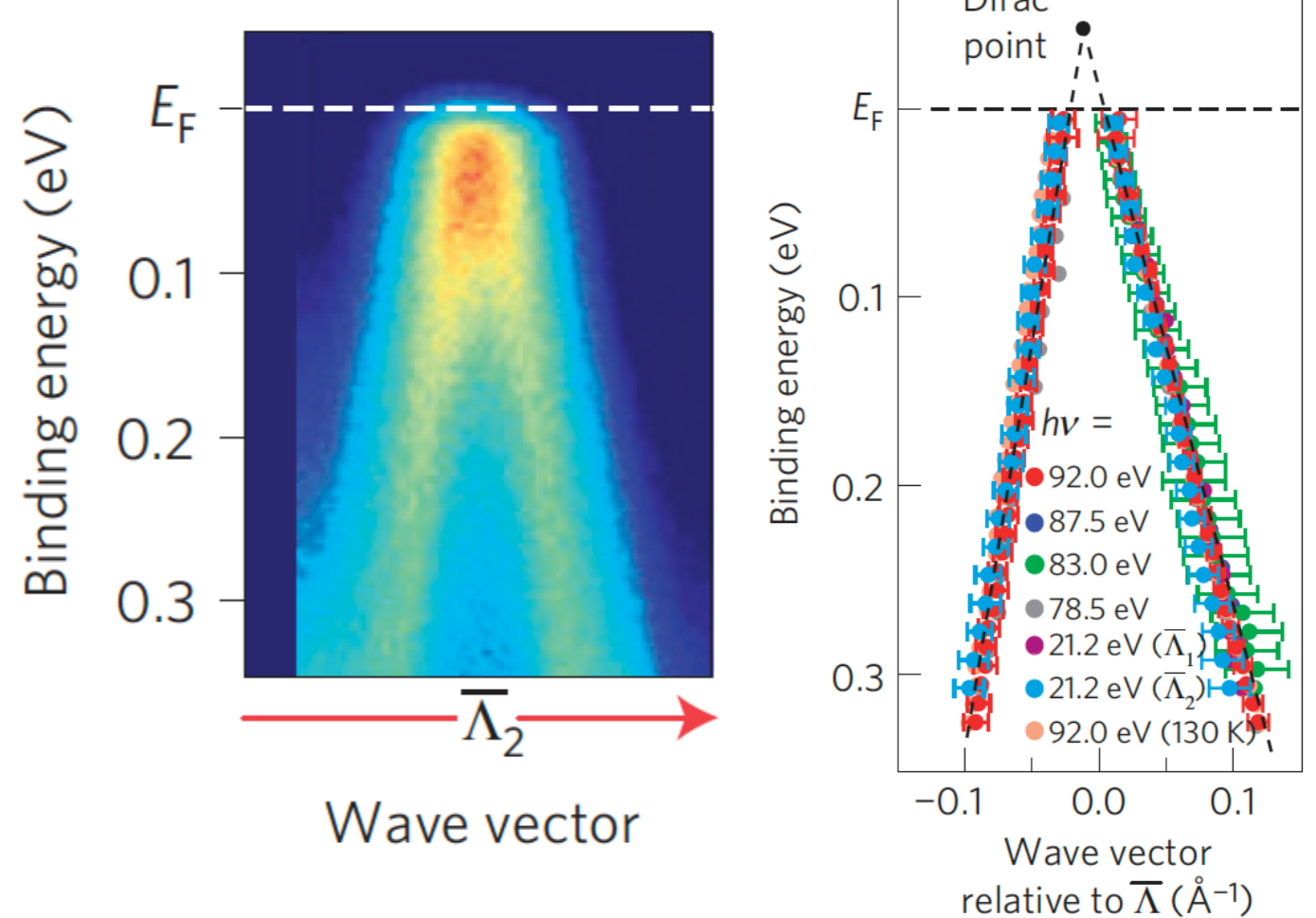
Prediction: Hsieh, et al,
Nat. Comm. 3, 982 (2012)

Observation: Tanaka, et al,
Nat. Phys. 8, 800 (2012), Ando group

$C_m=2$



ARPES



Topological insulators with inversion symmetry

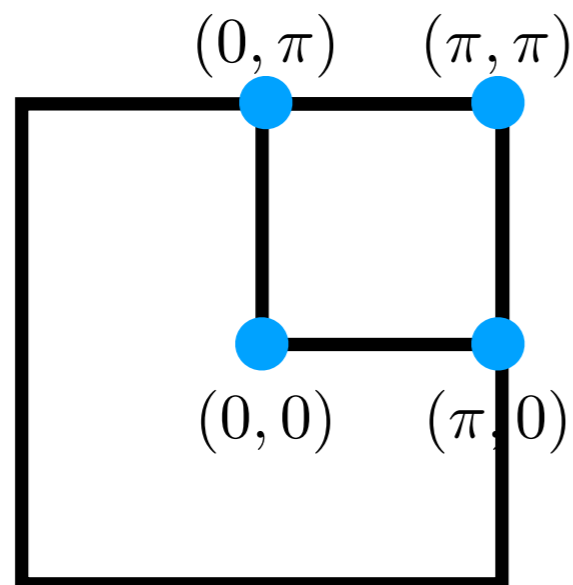
Inversion symmetry: $(x, y, z) \mapsto (-x, -y, -z)$

$$(k_x, k_y, k_z) \mapsto (-k_x, -k_y, -k_z)$$

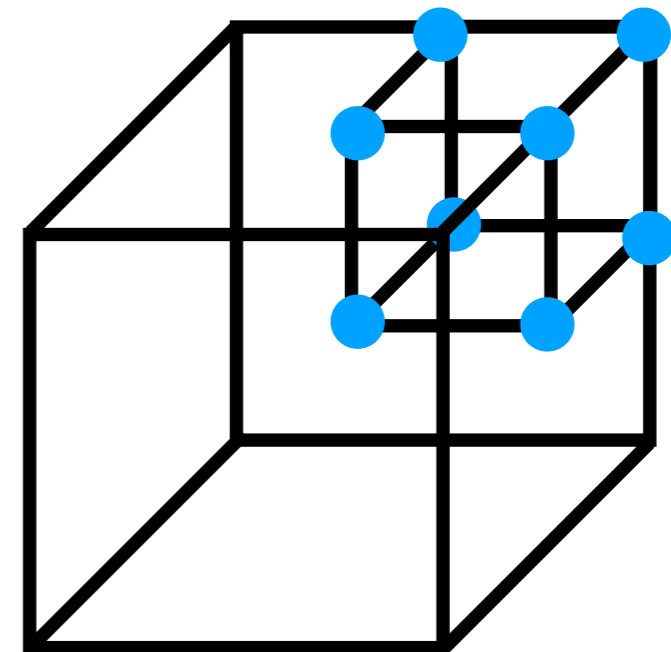
Inversion eigenvalues assigned at inversion-invariant points: $k_x, k_y, k_z = 0$ or π

“TRIMs” = time-reversal-invariant-momenta

4 TRIMs in 2D



8 TRIMs in 3D



(Number of TRIM points does not depend on lattice)

Topological insulators with inversion symmetry

Z_2 invariant is given by the product of inversion eigenvalues of occupied bands!

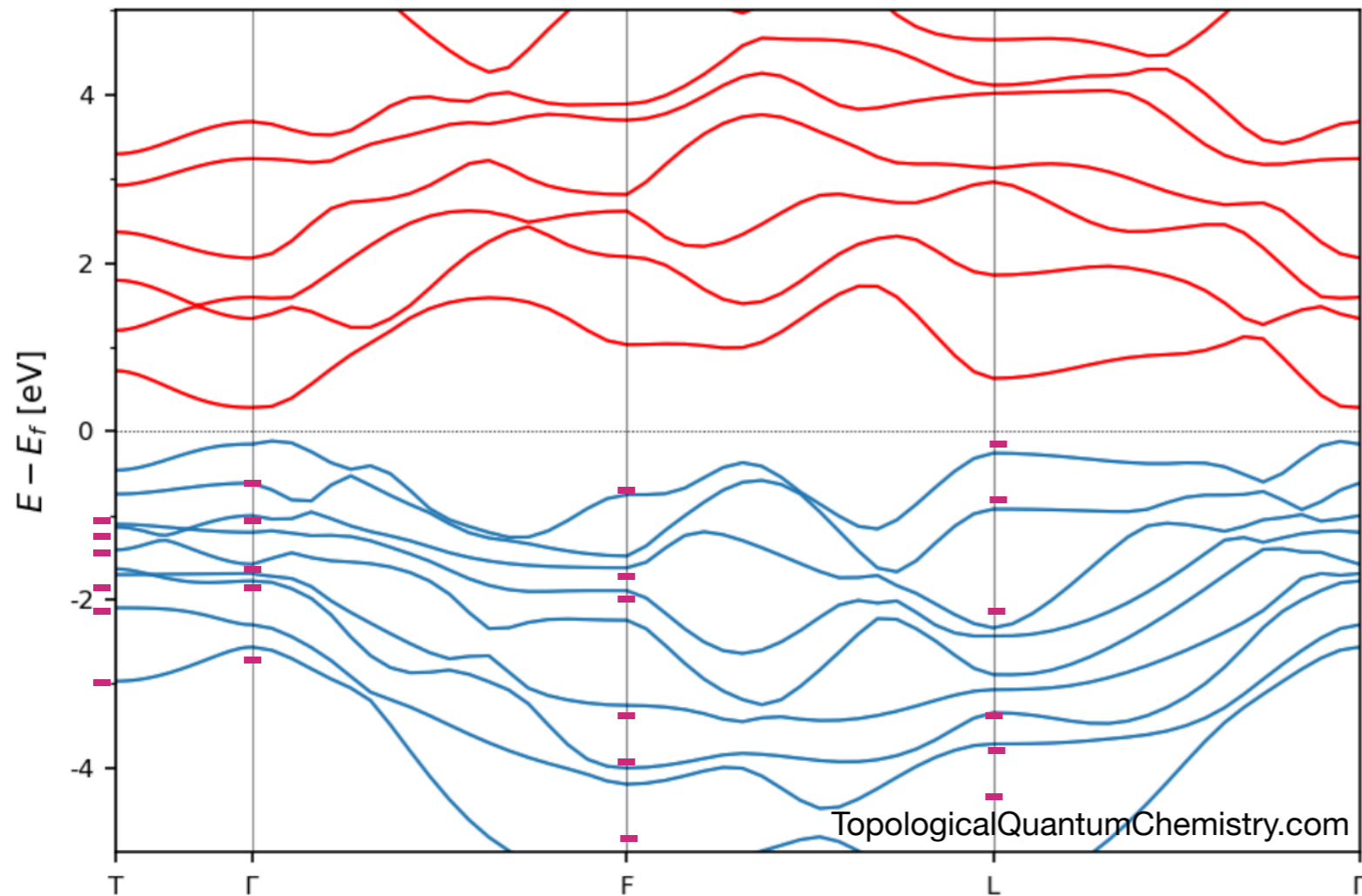
Fu and Kane PRB 76, 045302 (2007)

$$\delta_i = \prod_{m=1}^N \xi_{2m}(\Gamma_i) \quad \leftarrow \text{At each TRIM } (\Gamma_i), \text{ multiply one inversion eigenvalue from each Kramers pair}$$

$$(-1)^\nu = \prod_i \delta_i \quad \leftarrow \text{Multiply the results from all TRIMs}$$

Inversion symmetry identifies the Z_2 TI phase, but does not protect it!

Example of inversion eigenvalue formula: Bi_2Se_3



TRIM points:

$$\Gamma : (0, 0, 0)$$

$$L : (\pi, 0, 0), (0, \pi, 0), (0, 0, \pi)$$

$$F : (0, \pi, \pi), (\pi, 0, \pi), (\pi, \pi, 0)$$

$$T : (\pi, \pi, \pi)$$

$$\delta_i = \prod_{m=1}^N \xi_{2m}(\Gamma_i)$$

$$\delta_\Gamma = -1, \delta_L = \delta_F = \delta_T = +1$$

$$(-1)^\nu = \prod_i \delta_i$$

$$(-1)^\nu = -1 \Rightarrow \nu = -1$$

Glide symmetry can protect novel surface states

Wang, Alexandradinata, Cava, Bernevig Nature 532, 189 (2016)

Glide symmetry: mirror followed by fractional lattice translation

$$g_x : (x, y, z) \mapsto (-x, y, z + \frac{1}{2})$$

$$g_x : (k_x, k_y, k_z) \mapsto (-k_x, k_y, k_z)$$

When $k_x=0$ or $k_x=\pi$, bands labelled by g_x eigs

$$g_x^2 = -t_z \Rightarrow \text{eigs: } \pm i e^{-ik_z/2}$$

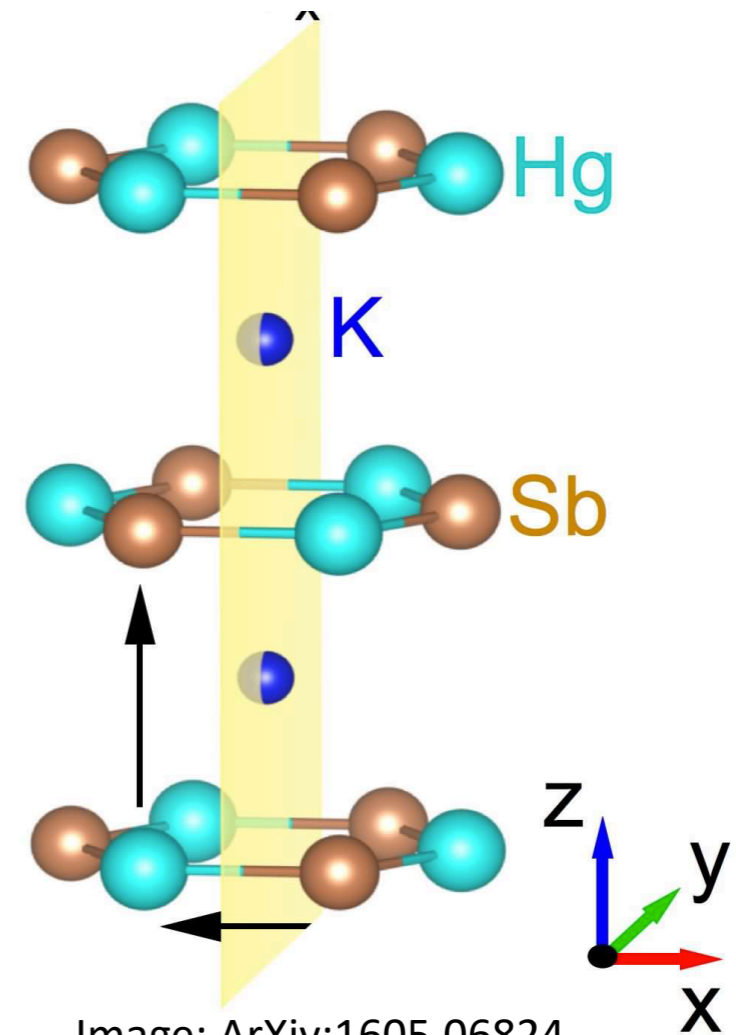


Image: ArXiv:1605.06824

Screw symmetry: mirror followed by fractional lattice translation

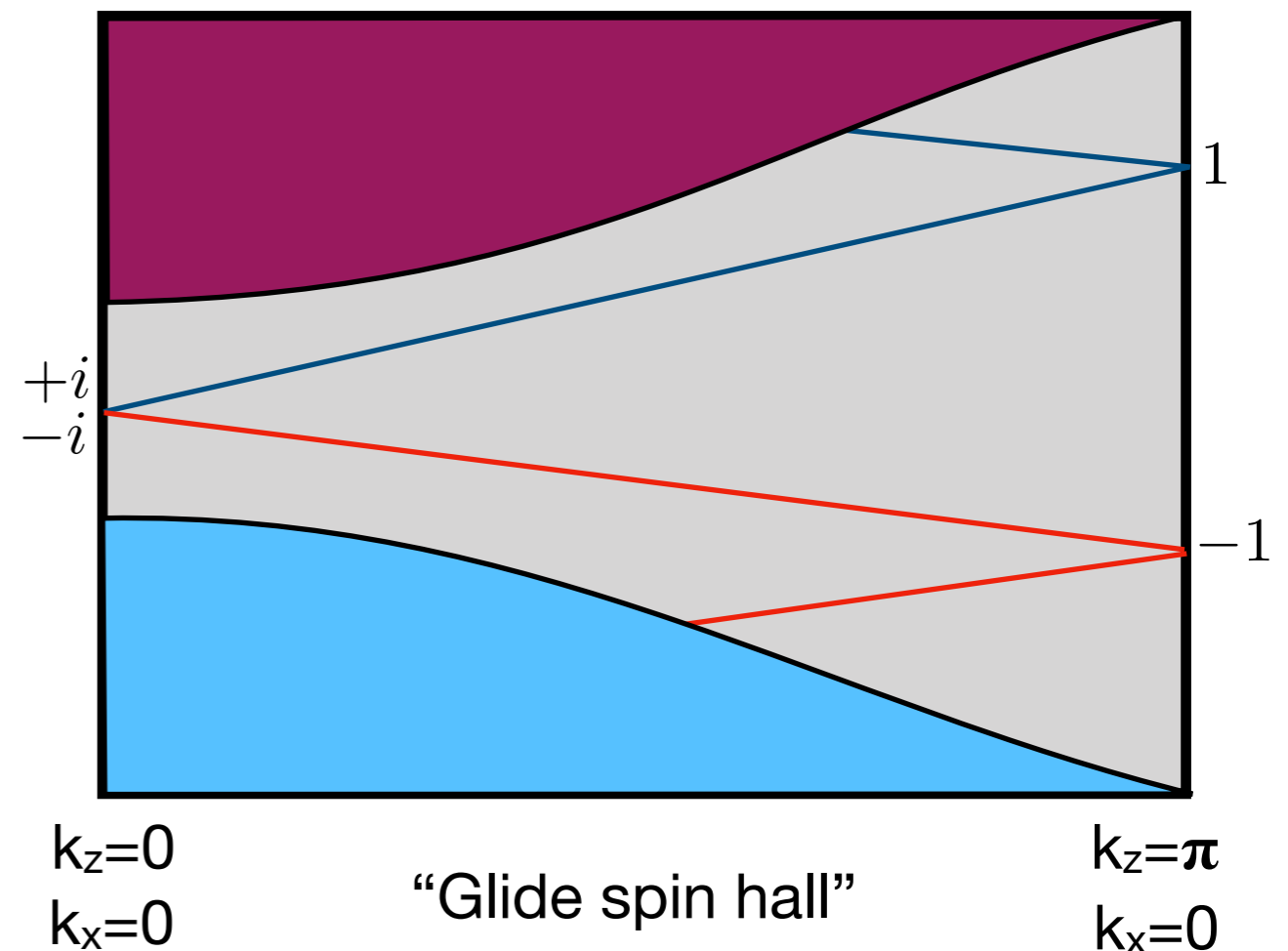
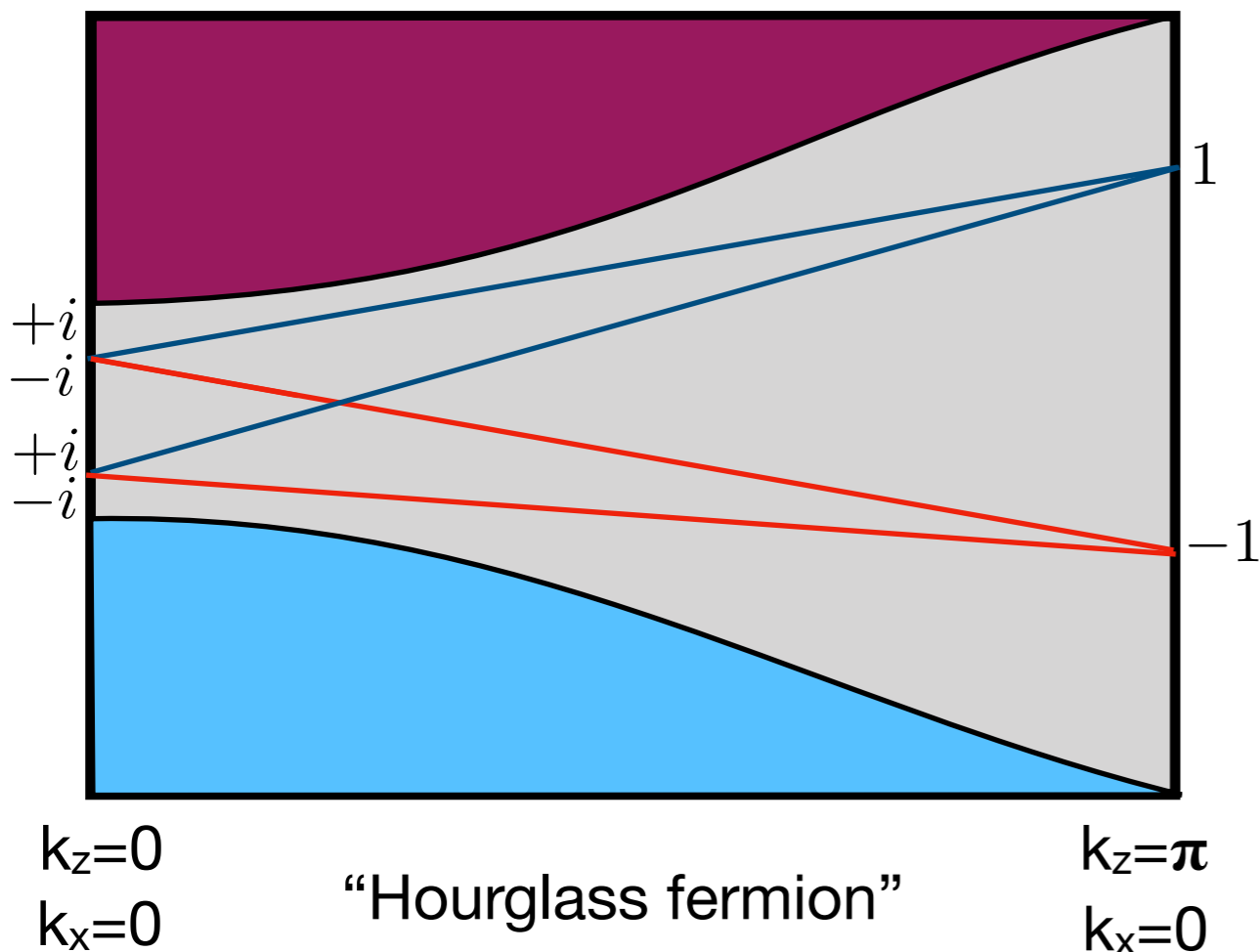
Space groups with a screw or glide symmetry are nonsymmorphic*

Glide symmetry can protect novel surface states

Wang, Alexandradinata, Cava, Bernevig Nature 532, 189 (2016)

What does the surface spectrum for $k_x=0$ plane look like?

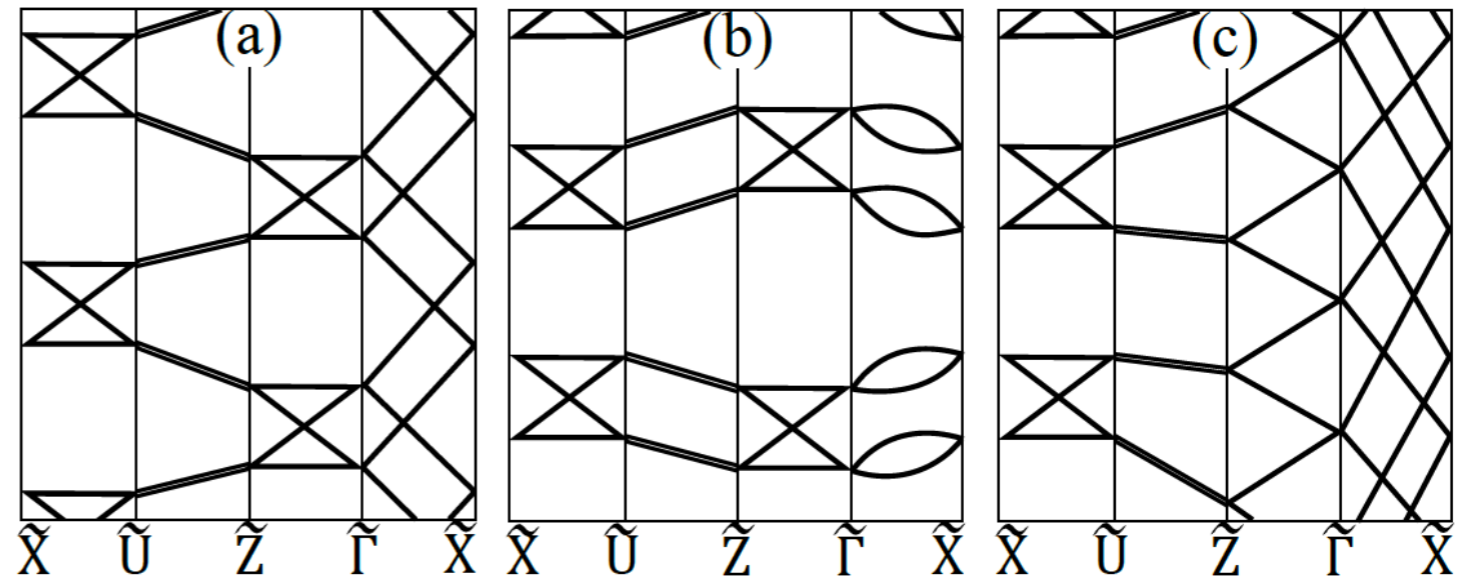
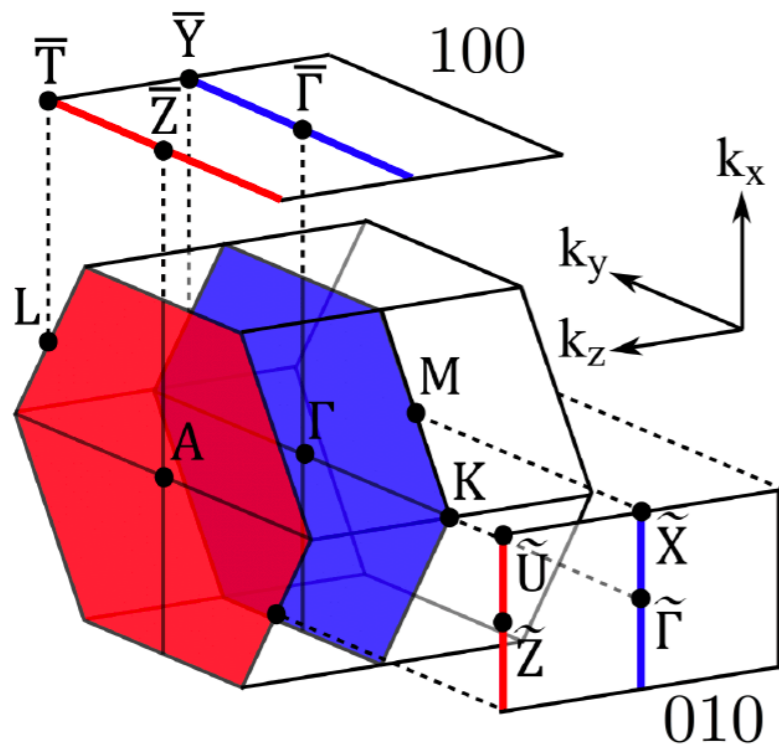
Use: $T^2=-1$ and g_x eigs: $\pm i e^{-ik_z/2}$



Glide symmetry can protect novel surface states

Wang, Alexandradinata, Cava, Bernevig Nature 532, 189 (2016)

Connectivity of bands in $k_x=0$ and $k_x=\pi$ planes can yield anomalous surface states



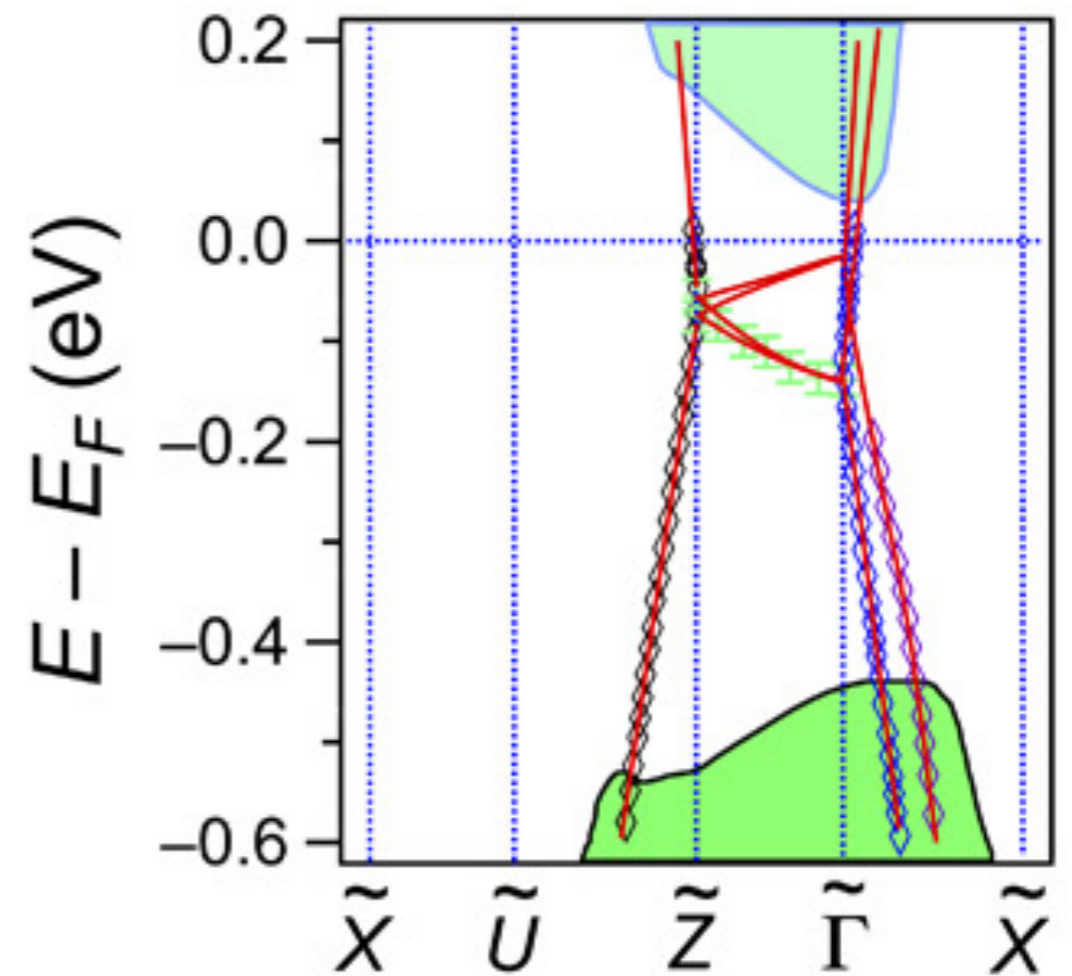
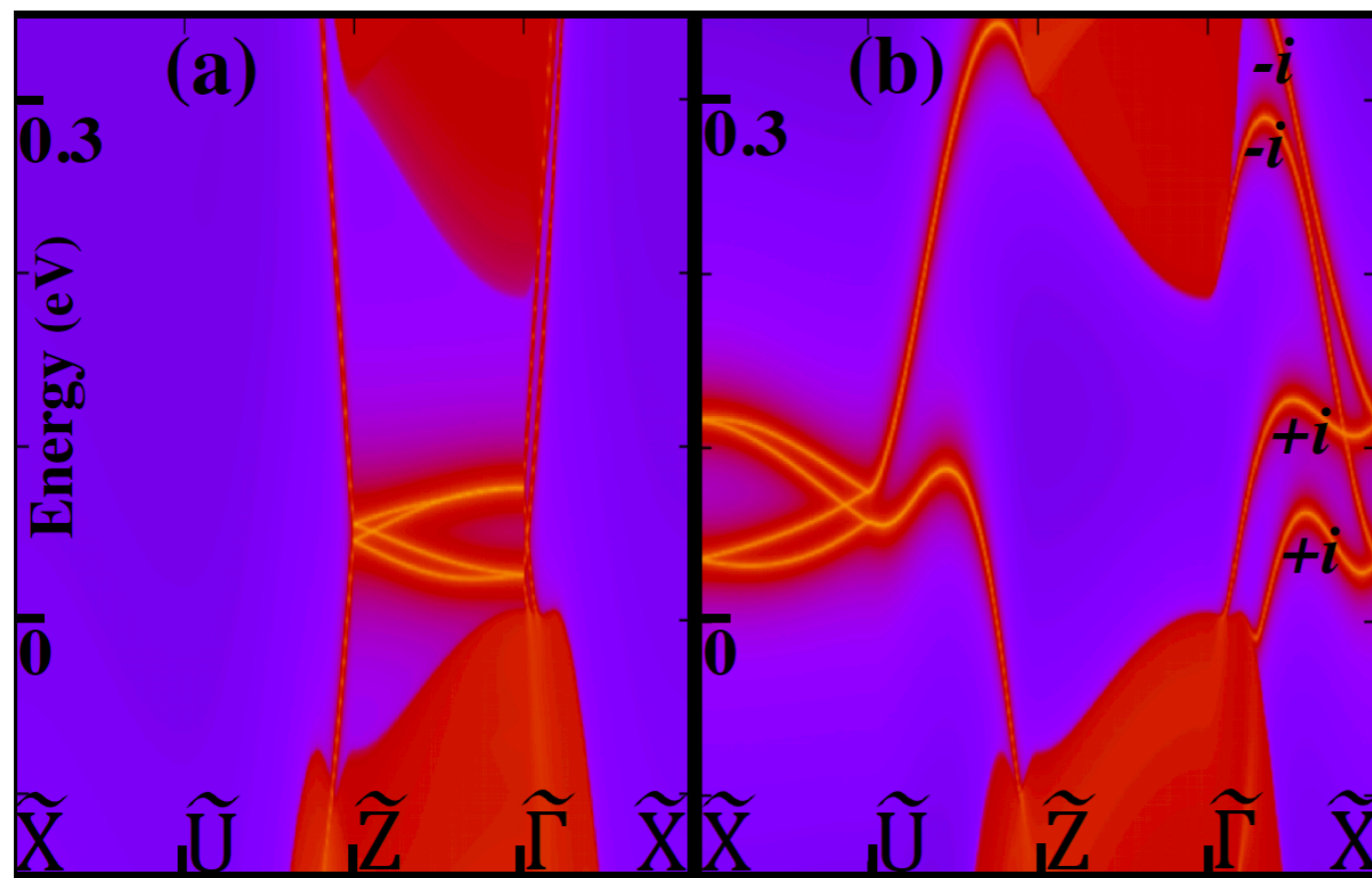
Z_4 invariant: Shiozaki, Sato, Gomi, PRB 93, 195413 (2016)

“Spectral flow”

KHgSb predicted/observed hourglass fermion

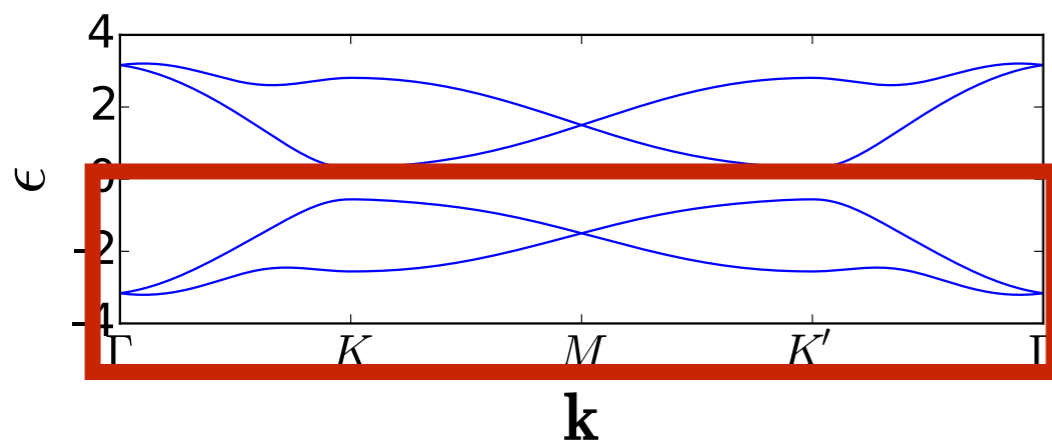
Prediction: Wang, Alexandradinata, Cava,
Bernevig Nature 532, 189 (2016)

Observation: Ma, et al, Sci.
Adv. (2017), Ding group

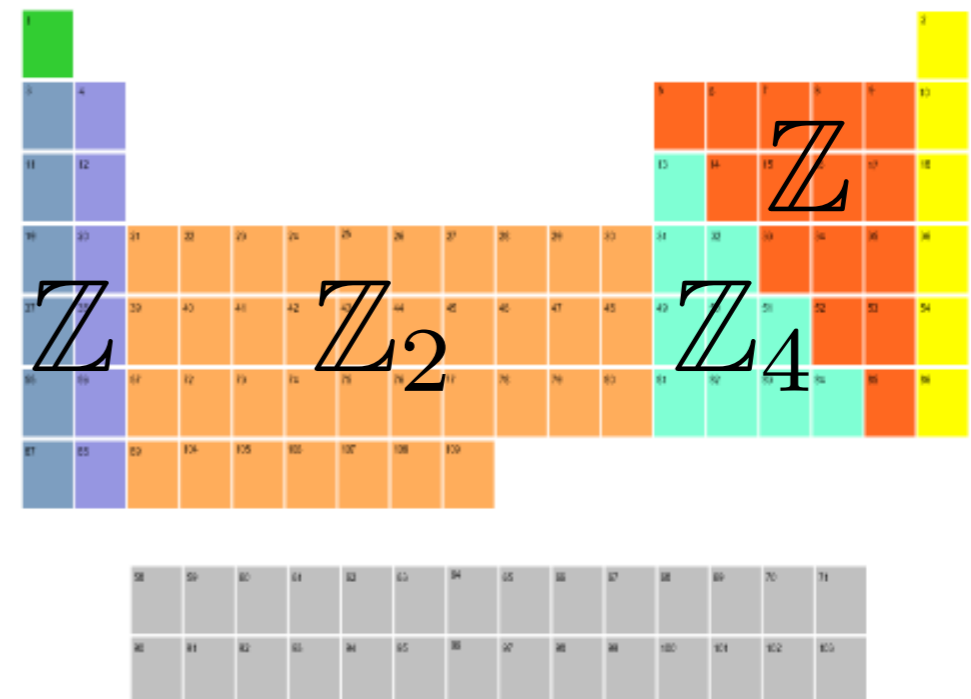


Ad hoc classification of topological crystalline insulators leaves open questions:

1. Given a space group, what are the possible topological indices? How do topological indices corresponding to different symmetries combine?
2. Topological indices are formulated in momentum space, but crystals are classified in real space.... How can we find topological materials?!



?





Insight from recent advances in topological band theory of space groups

Topological quantum chemistry diagnoses and predict topological materials

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

Symmetry indicators classify stable topological phases in each space group

Po, Vishwanath, Watanabe, Nat. Comm. 8, 50 (2017)

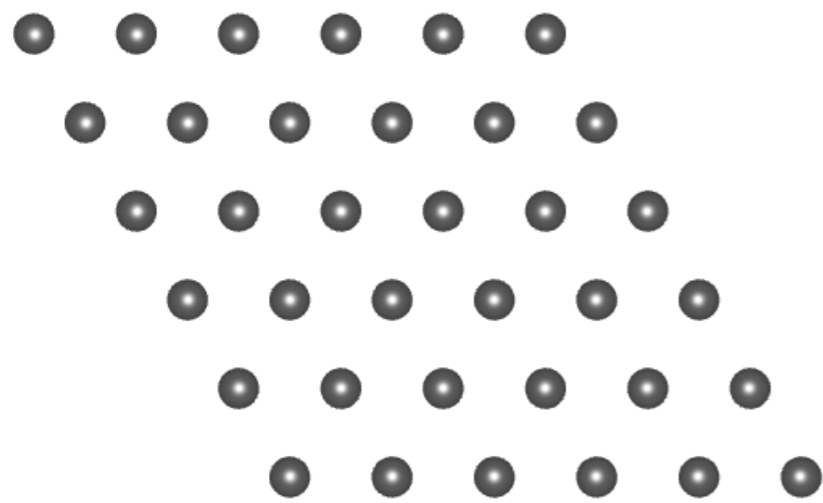
Key: topological bands are not deformable to an atomic limit

1. Identify all atomic limits by their symmetry eigenvalues
2. Bands whose symmetry eigenvalues do not match atomic limit are topological

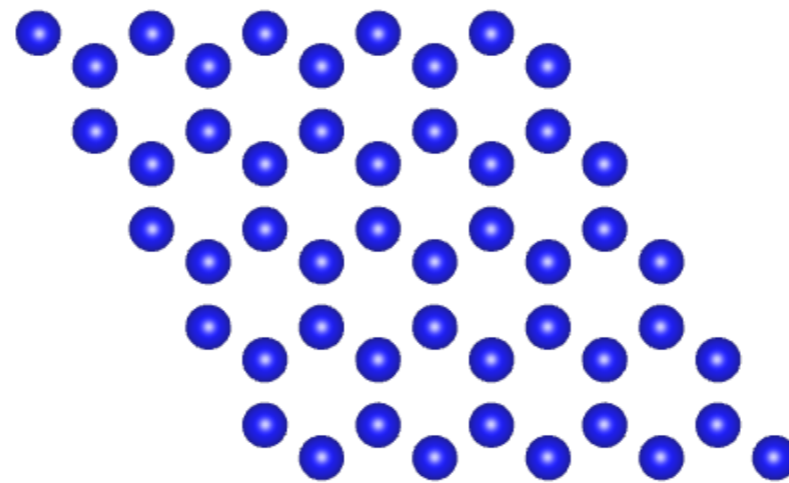
How to identify all atomic limits?

Within one space group, many ways to arrange atoms

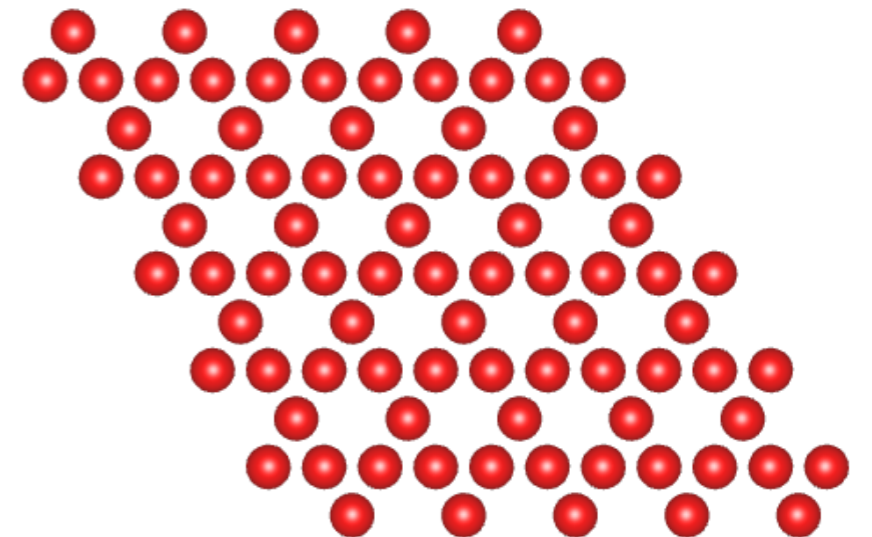
“Wyckoff positions”



1 atom/unit cell
(triangular)



2 atoms/unit cell
(honeycomb)

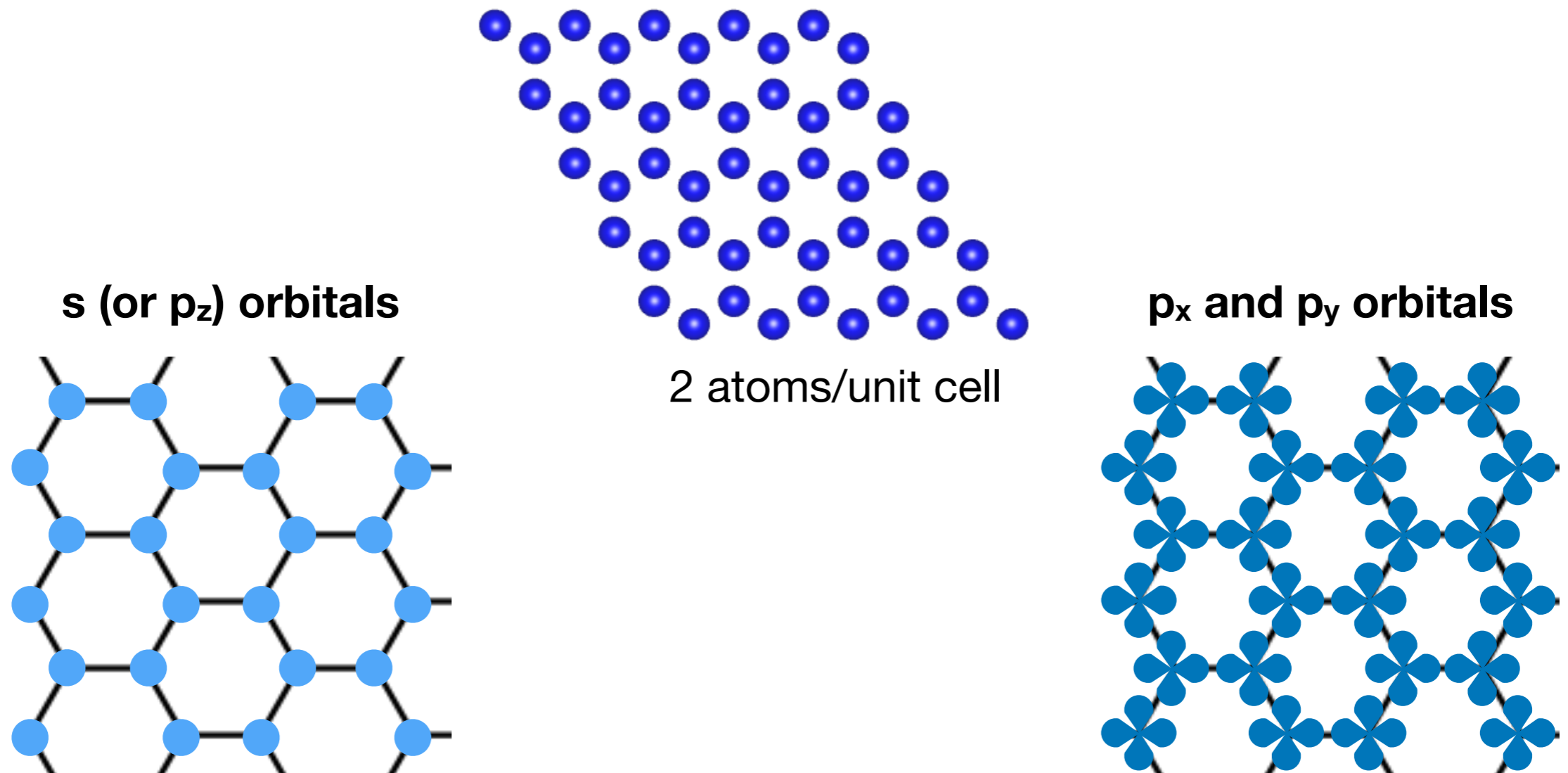


3 atoms/unit cell
(kagome)

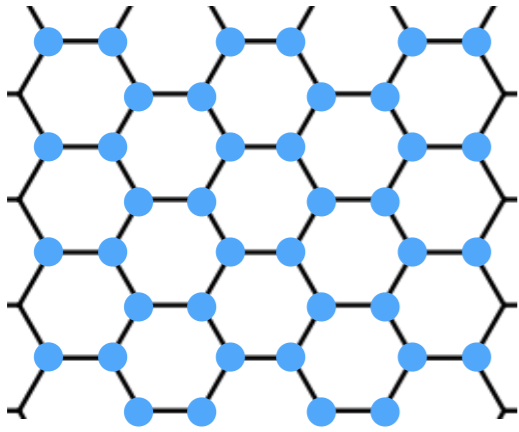
All atoms are related by symmetry

How to identify all atomic limits?

Within one arrangement, many choices of orbitals



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

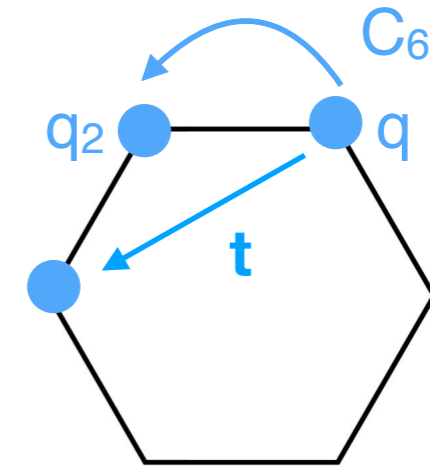
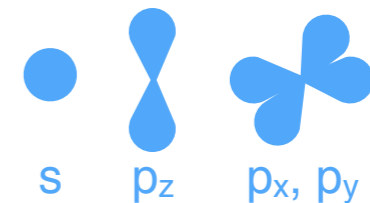


Symmetry of a single site determines symmetry of entire lattice

Identify “site-symmetry group”:
 G_q = symmetries that leave q invariant

C_3, m_y

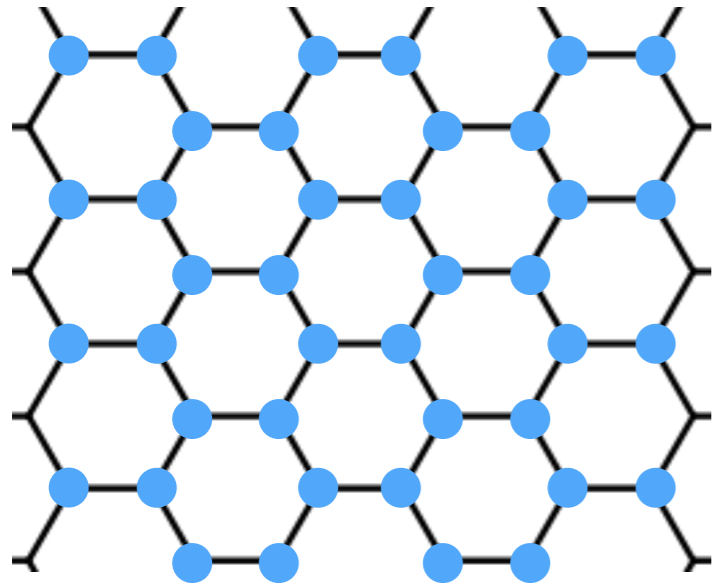
Orbitals at q transform under a rep, $\rho(g)$, of G_q



Elements of space group that do not leave q invariant tile the lattice

C_6, t, \dots

Mathematically: symmetry of single site determines representation of entire space group



“Band representation”

Zak PRL 1980, PRB 1981, 1982

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

$$\text{Ind}_{G_q}^G \rho$$

How to construct a band representation:

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

	q	q ₂	q ₃	q ₄	...
q	[Diagonal block]		[Off-diagonal block]		
q ₂					
q ₃			[Off-diagonal block]		
q ₄					
...					

The symmetry irreps of a band representation in the Brillouin zone are completely determined

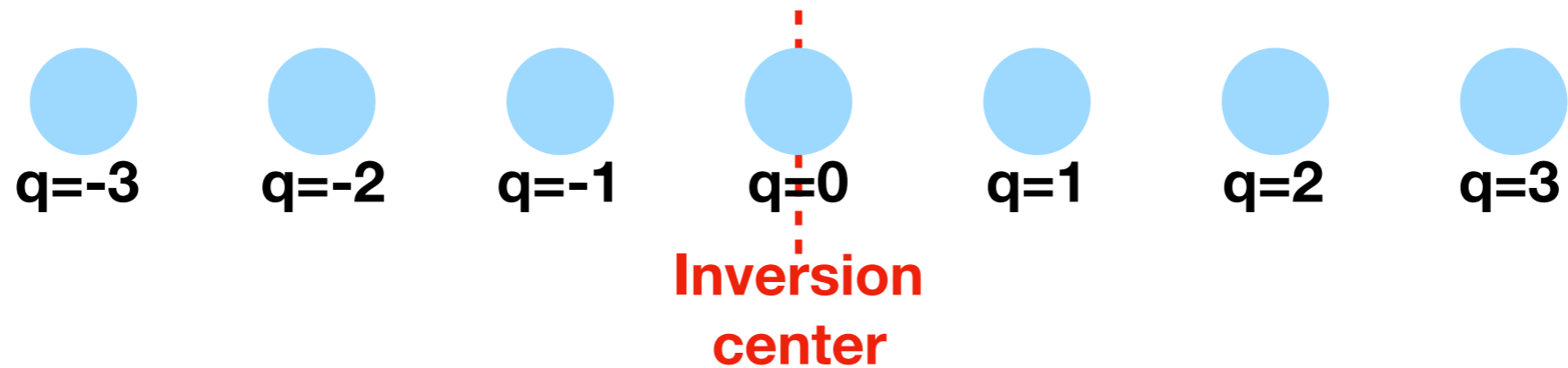
Zak PRL 1980, PRB 1981, 1982

Fourier transforming matrix gives irreps at any k point



Diagonal blocks form representation of “little group of k ”
 $gk = k + K$

Example: band representation of 1D lattice of s orbitals with inversion symmetry



Space group generators:

Identity

...	-2	-1	0	1	2	...
-2	1					
-1		1				
0			1			
1				1		
2					1	
...						

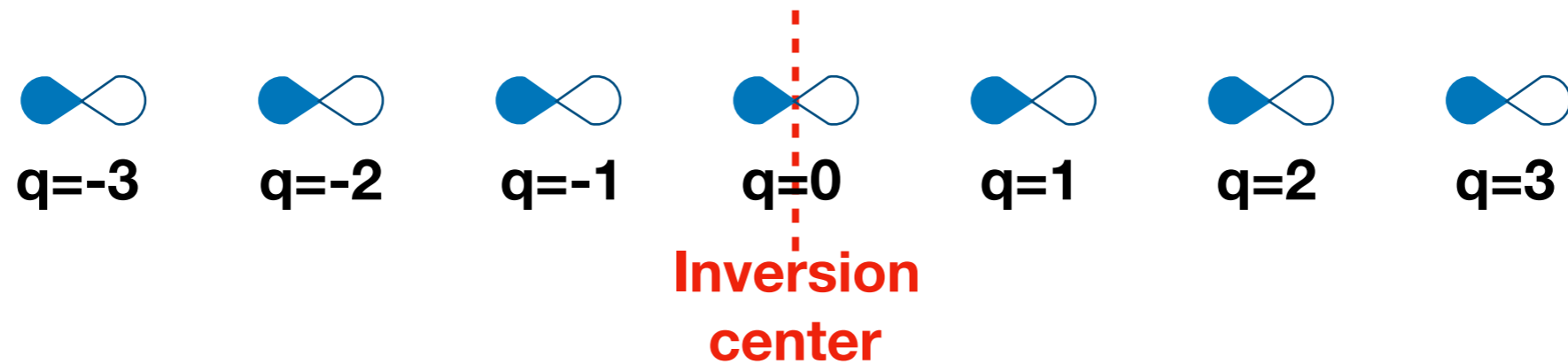
Inversion

...	-2	-1	0	1	2	...
-2					1	
-1				1		
0			1			
1		1				
2	1					
...						

translation by 1

...	-2	-1	0	1	2	...
-2						
-1	1					
0		1				
1			1			
2				1		
...					1	

Example: band representation of 1D lattice of p orbitals with inversion symmetry



Space group generators:

Identity

...	-2	-1	0	1	2	...
-2	1					
-1		1				
0			1			
1				1		
2					1	
...						

Inversion

...	-2	-1	0	1	2	...
-2					-1	
-1				-1		
0			-1			
1		-1				
2	-1					
...						

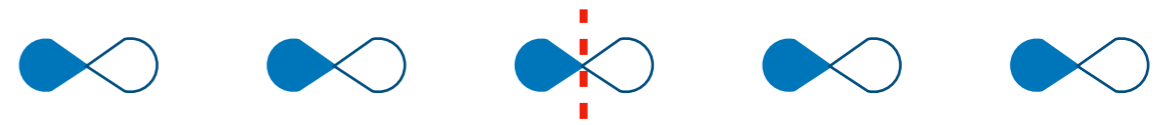
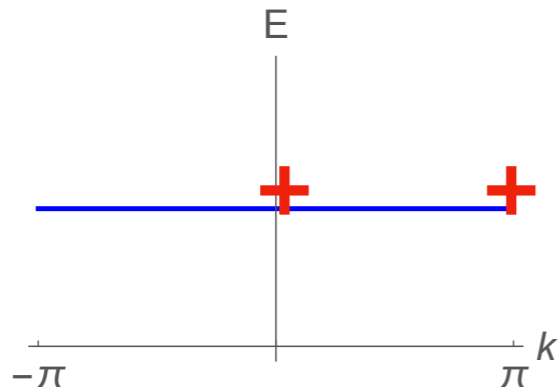
translation by 1

...	-2	-1	0	1	2	...
-2						
-1	1					
0		1				
1			1			
2				1		
...					1	

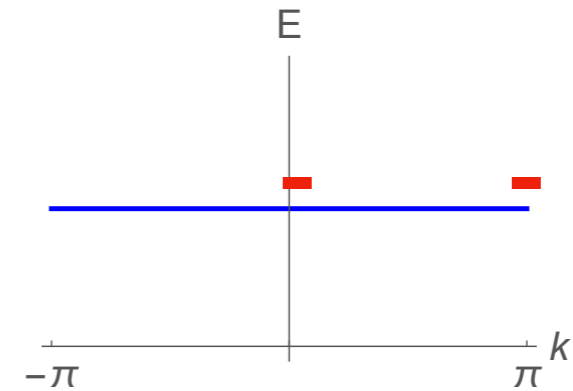
Fourier transform yields inversion eigenvalues at $k=0$ and $k=\pi$



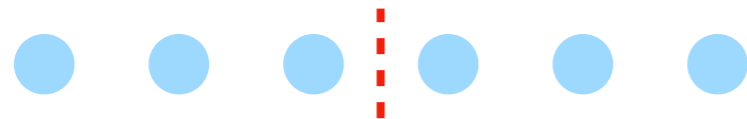
Atomic limit s orbitals:



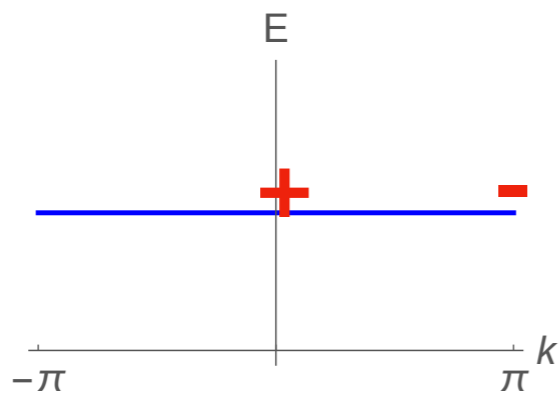
Atomic limit p orbitals:



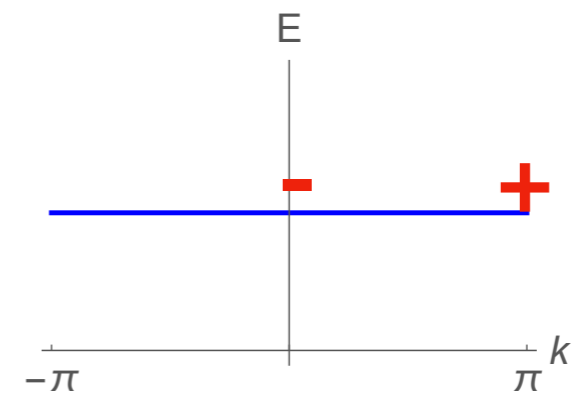
Repeat with atoms shifted by half a unit cell:



Atomic limit s orbitals:



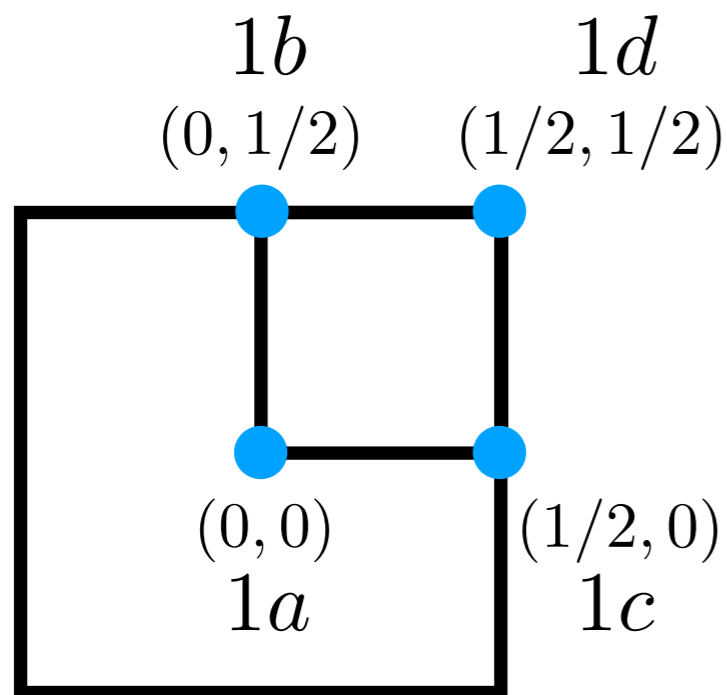
Atomic limit p orbitals:



These four “atomic limits” capture all possible inversion eigenvalues *in 1D!*

What are the inversion eigenvalues of all possible atomic limits in 2D?

Atom positions:



Negative inversion eigenvalues appear at pairs of TRIMs!

Inversion eigenvalues for s orbitals

	$(0,0)$	$(0,\pi)$	$(\pi,0)$	(π,π)
$1a$	+	+	+	+
$1b$				
$1c$				
$1d$				

Inversion eigenvalues for p orbitals

	$(0,0)$	$(0,\pi)$	$(\pi,0)$	(π,π)
$1a$	-	-	-	-
$1b$	-	+	-	+
$1c$	-	-	+	+
$1d$	-	+	+	-

A band structure with an odd number of negative inversion eigenvalues is not an atomic limit phase \Rightarrow must be topological

Goal: compute all atomic limit phases for all space groups

(Why? So that we can identify topological crystalline insulators in any space group)

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 maximal site-symmetry groups

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

\Rightarrow **Finitely many EBRs**

How many EBRs are there?

Large but finite number, estimate:

$$(230 \text{ space groups}) \times (3 \text{ max Wyckoff pos.}) \times (3 \text{ irreps}) = 2070$$

Actual:	no TR	TR
Single-valued irreps (spinless)	3383	3141
Double-valued irreps (spinful)	2263	1616

⇒ 10,403 total EBRs

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

bilbao crystallographic server

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

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

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

Bilbao Crystallographic Server → BANDREP

Help

Band representations of the Double Space Groups

Band Representations

This program calculates the band representations (BR) induced from the irreps of the site-symmetry group of a given Wyckoff position.

Alternatively, it gives the set of elementary BRs of a Double Space Group.

In both cases, it can be chosen to get the BRs with or without time-reversal symmetry.

The program also indicates if the elementary BRs are decomposable or indecomposable. If it is decomposable, the program gives all the possible ways to decompose it.

References. For more information about this program see the following articles:

- Bradlyn *et al.* "Topological quantum chemistry" *Nature* (2017). **547**, 298-305. doi:10.1038/nature23268
- Vergniory *et al.* "Graph theory data for topological quantum chemistry" *Phys. Rev. E* (2017). **96**, 023310. doi:10.1103/PhysrevE.96.023310
- Elcoro *et al.* "Double crystallographic groups and their representations on the Bilbao Crystallographic Server" *J. of Appl. Cryst.* (2017). **50**, 1457-1477. doi:10.1107/S1600576717011712

If you are using this program in the preparation of an article, please cite at least one of the above references.

Please, enter the sequential number of group as given in the *International Tables for Crystallography*, Vol. A

choose it

1. Get the elementary BRs without time-reversal symmetry
2. Get the elementary BRs with time-reversal symmetry
3. Get the BRs without time-reversal symmetry from a Wyckoff position
4. Get the BRs with time-reversal symmetry from a Wyckoff position

Elementary

Elementary TR

Wyckoff

Wyckoff TR

Each column is elementary band representation

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 $\rho \uparrow G$, 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

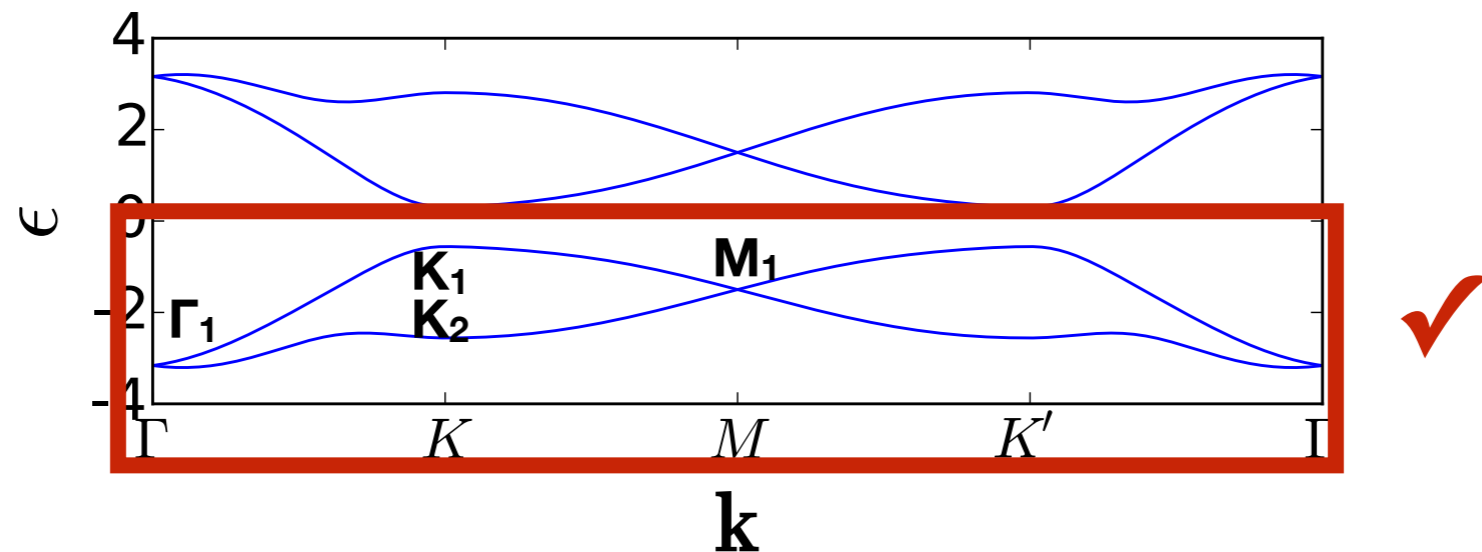
Wyckoff pos.	1a(6mm)	1a(6mm)	1a(6mm)	1a(6mm)	1a(6mm)	1a(6mm)	2b(3m)
Band-Rep.	$A_1 \uparrow G(1)$	$A_2 \uparrow G(1)$	$B_1 \uparrow G(1)$	$B_2 \uparrow G(1)$	$E_1 \uparrow G(2)$	$E_2 \uparrow G(2)$	$A_1 \uparrow G(2)$
Decomposable \\ Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable
$\Gamma:(0,0,0)$	$\Gamma_1(1)$	$\Gamma_2(1)$	$\Gamma_4(1)$	$\Gamma_3(1)$	$\Gamma_6(2)$	$\Gamma_5(2)$	$\Gamma_1(1) \oplus \Gamma_4(1)$
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

We can now identify topological bands

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



Smooth deformations cannot change symmetry labels

Topological bands are not a “sum” of elementary band representations

See also: Po, Vishwanath, Watanabe, Nature Comm. 8, 50 (2017),
Shiozaki, Sato, Gomi, PRB 95, 235425 (2017)

Steps for materials search:

For every known chemical compound:

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

Topological Materials Database
24905 Materials: 4339 Topological Insulators, 10061 Semi-Metals

Search About

Compound Contains Only these elements Exclude ICSD Number

e.g. Bi1 Se2 Ge eg. 01 N - or - eg. 123456 Search

Show Advanced Search

TopologicalQuantumChemistry.com

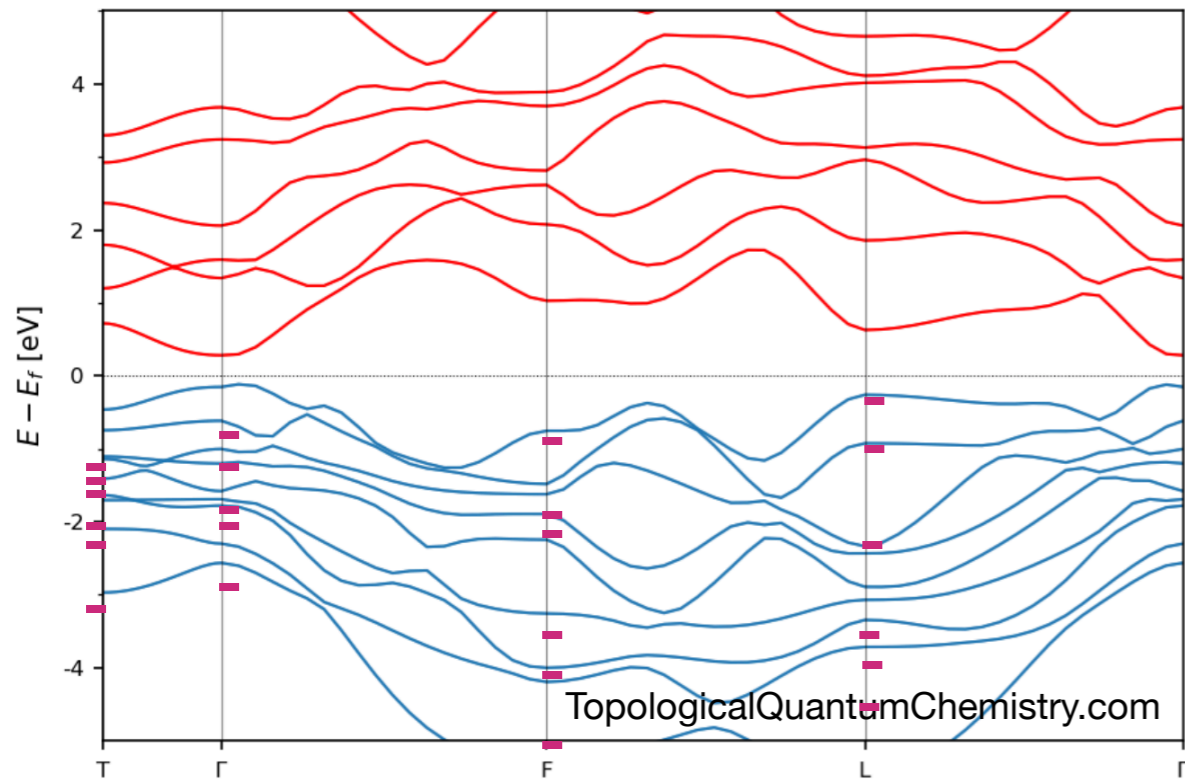
Vergniory, Elcoro, Felser, Regnault, Bernevig, Wang *Nature* 566, 480 (2019)

See also: Materiae <http://materiae.iphy.ac.cn>

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

3 Li	4 Be															9 F	10 Ne
11 Na	12 Mg															17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn

Summary



Crystal symmetry can protect and identify topological phases

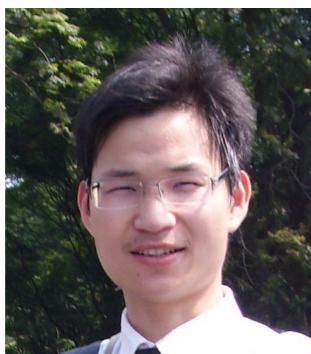
Exs: mirror Chern, inversion eigenvalue formula, hourglass fermion, ...

All symmetry indicators — generalizations of inversion eigenvalue invariant — can be determined from elementary band reps

Collaborators



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