# Topological Crystalline Insulators and Topological Quantum Chemistry

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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:*

| 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 | $\mathbb{Z}$ | ⋯ |

no symmetry →

Integer quantum Hall/ Chern insulator

*real case:*

| 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 | $2\mathbb{Z}$ | ⋯ |

fermions w/ time-reversal →

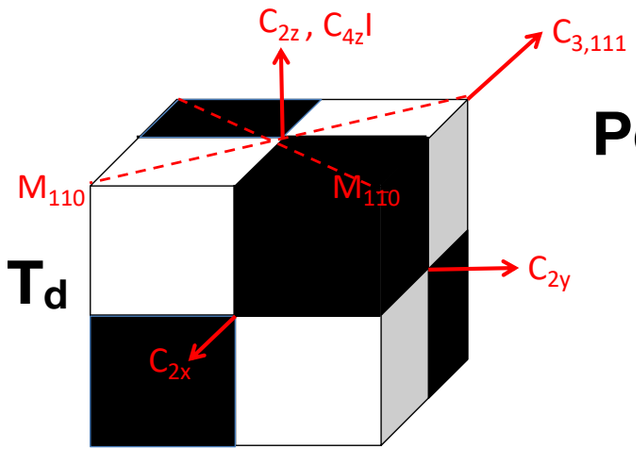
2d and 3d topological insulators
(weak index not captured)

# 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

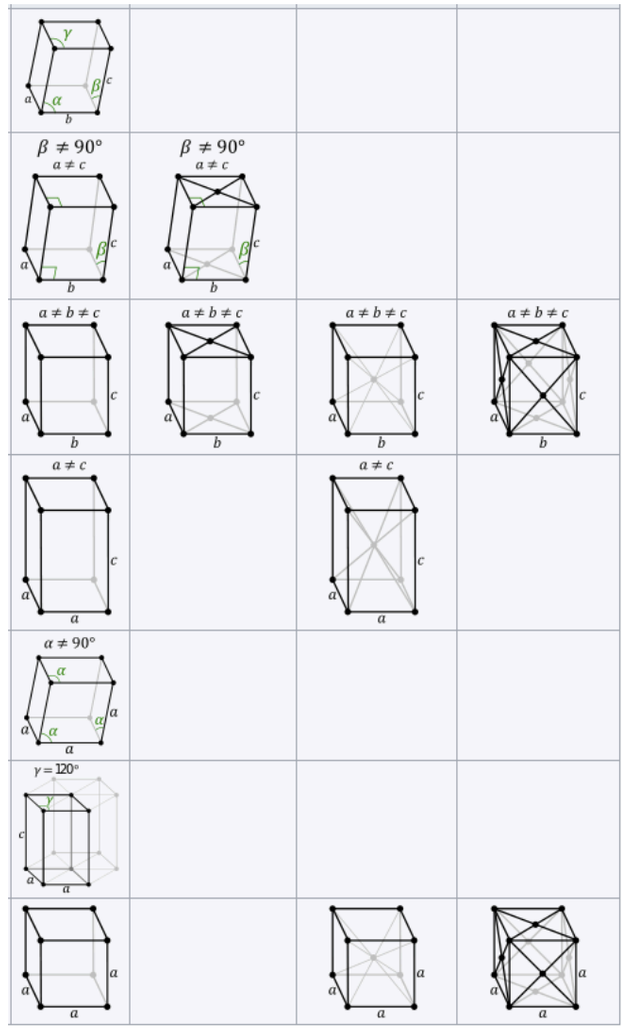
# What are crystal symmetries?




**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?

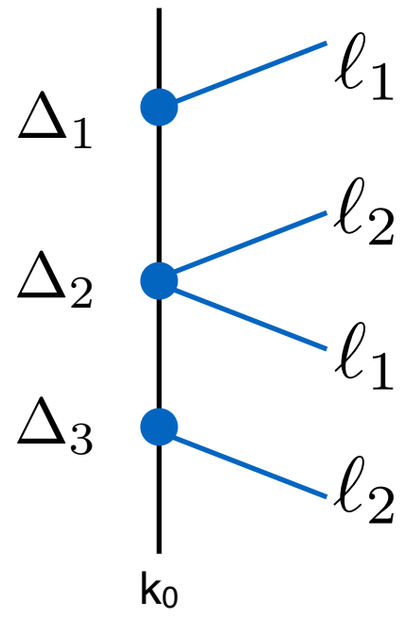
Fourier-transformed Hamiltonian: $\boxed{\Delta(\mathcal{G})}H(\mathbf{k})\Delta(\mathcal{G})^{-1} = H(\mathcal{G}\mathbf{k})$

matrix representative of symmetry operation

"Little group" of $k_0$: $\mathcal{G}\mathbf{k}_0 = \mathbf{k}_0$

Eigenstates transform under little group irreps

Irreps at $k_0$ determine irreps along lines emanating from $k_0$



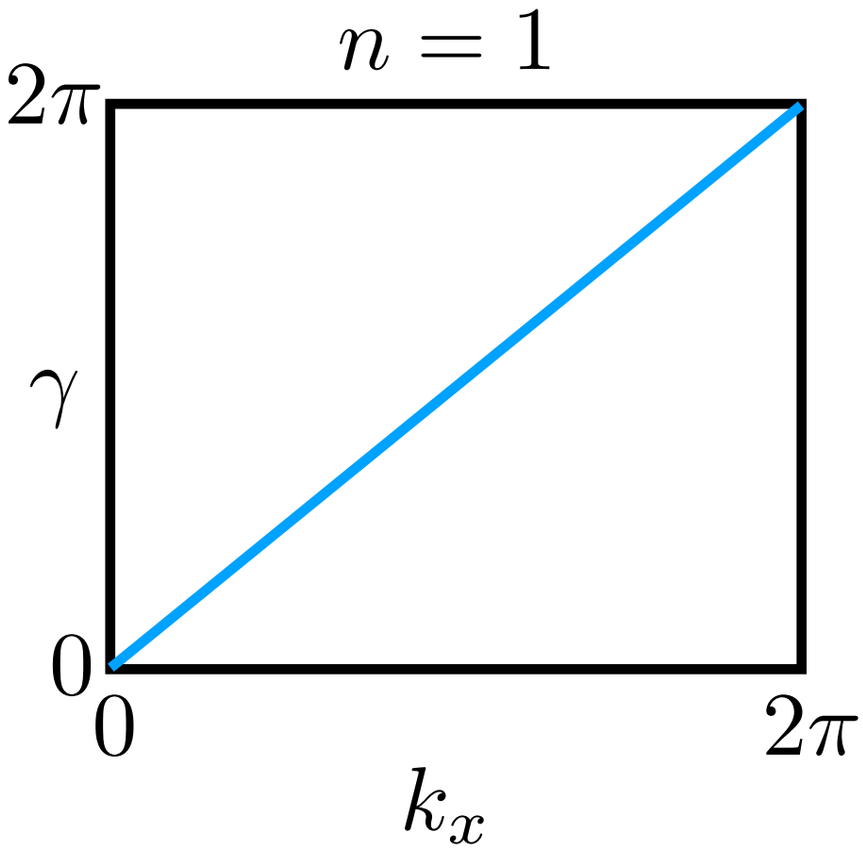

$$\left.\begin{aligned}\Delta_1 &\to \ell_1\\ \Delta_2 &\to \ell_1 \oplus \ell_2\\ \Delta_3 &\to \ell_2\end{aligned}\right\}$$

*Compatibility relations*
between points and lines

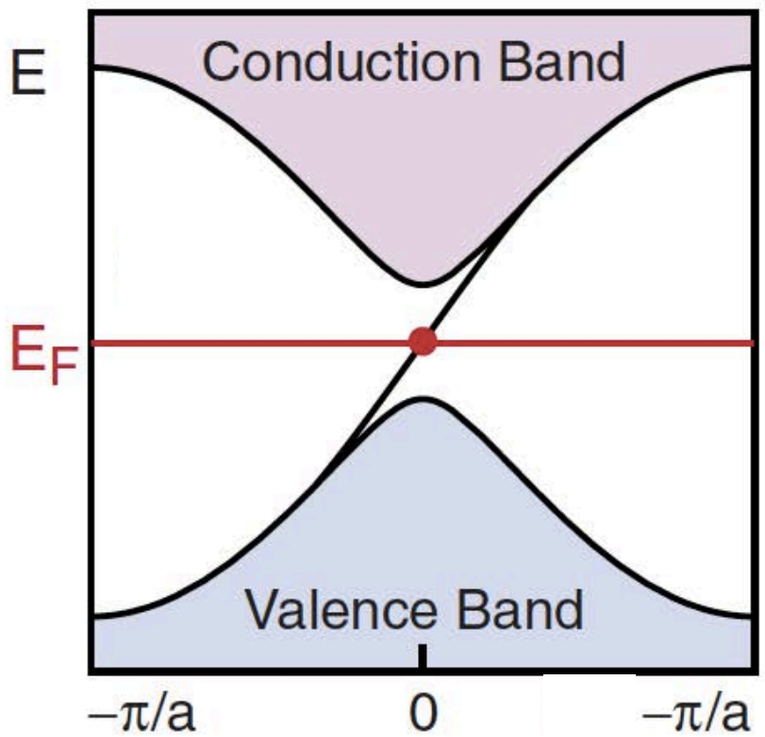
# Recall: Chern insulator

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

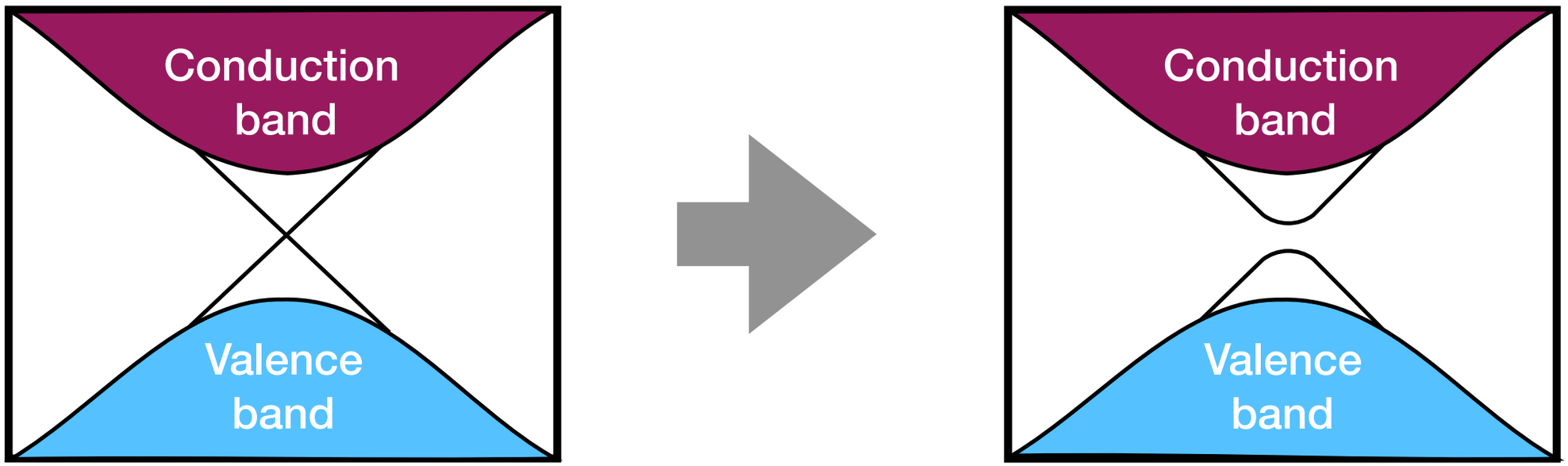
Topological invariant: Chern number




Bulk-edge correspondence



# Surface states of bands with opposite Chern number generically gap




<u>Unless protected by a symmetry:</u>

Ex 1: spin conservation ⇒ quantum spin Hall

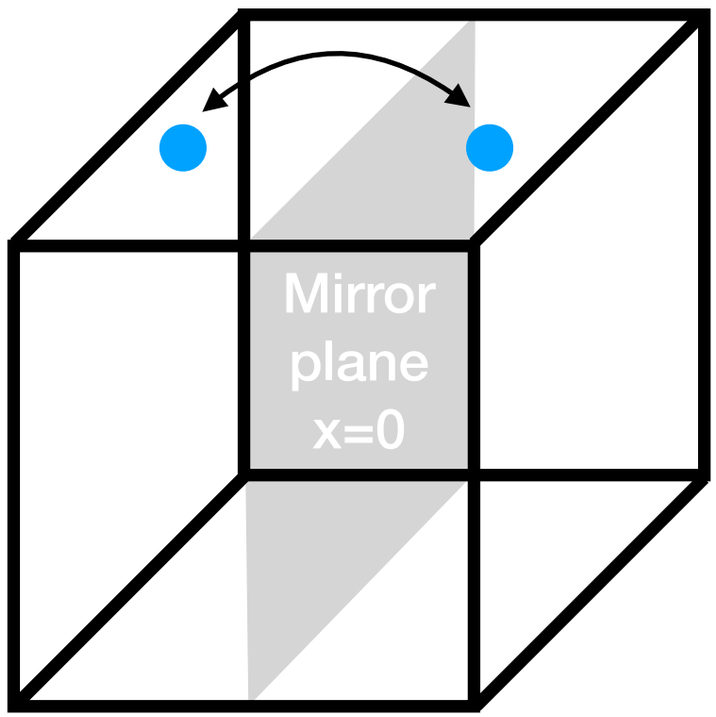
Ex 2: time-reversal symmetry ⇒ 2D TI

Crystal symmetry can also protect surface state crossings

# Mirror Chern insulator: canonical TCI

Teo, Fu, Kane PRB 045426 (2008)

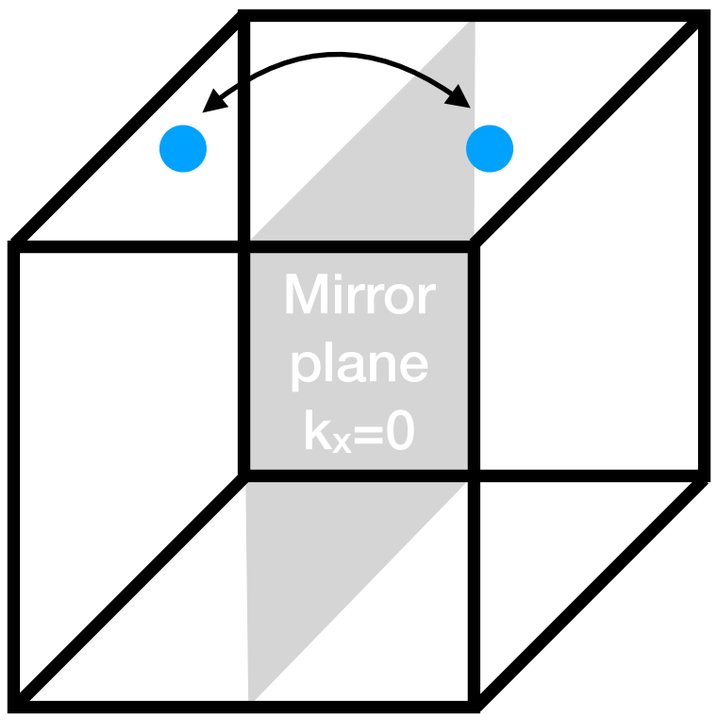
Mirror symmetry: $m_x : (x, y, z) \mapsto (-x, y, z)$



# Mirror Chern insulator: canonical TCI

Teo, Fu, Kane PRB 045426 (2008)

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



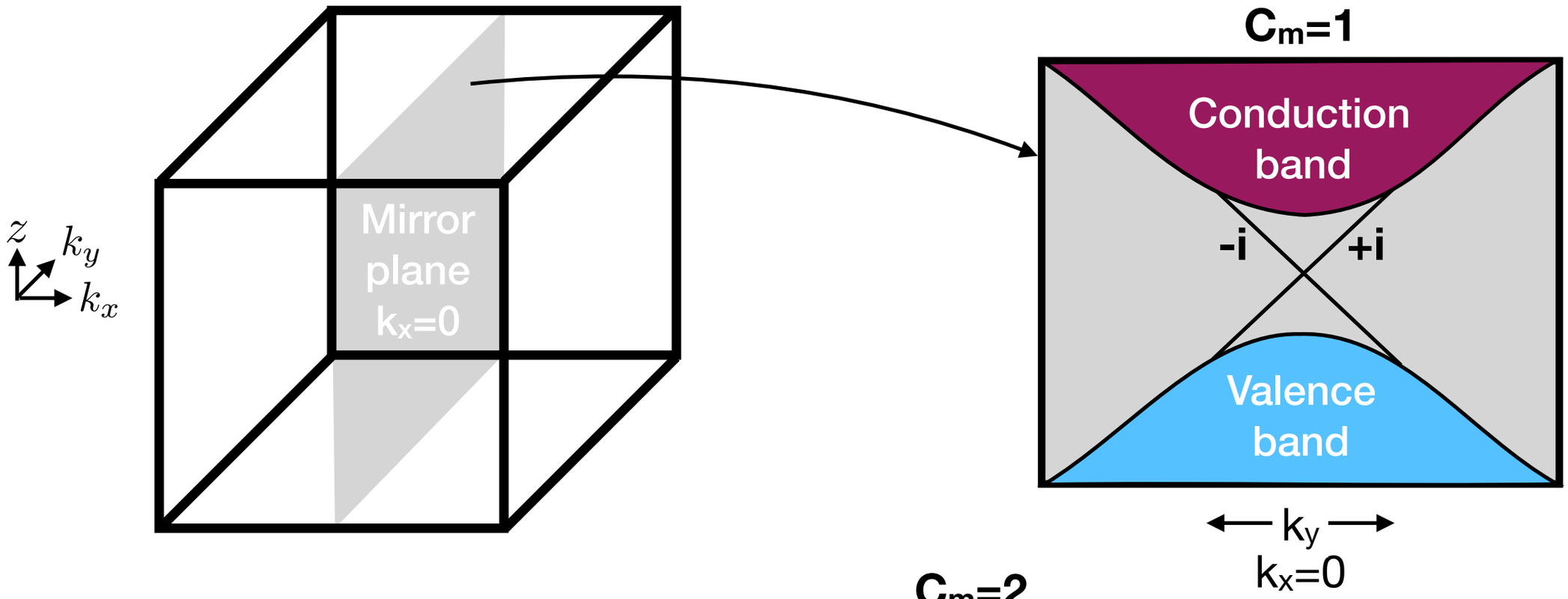

When $k_x$=0, $m_x$ commutes with H($k_x$=0, $k_y$, $k_z$) ⇒ bands labelled by $m_x$ eigenvalue: +/- i

Define Chern number for each mirror sector: C±

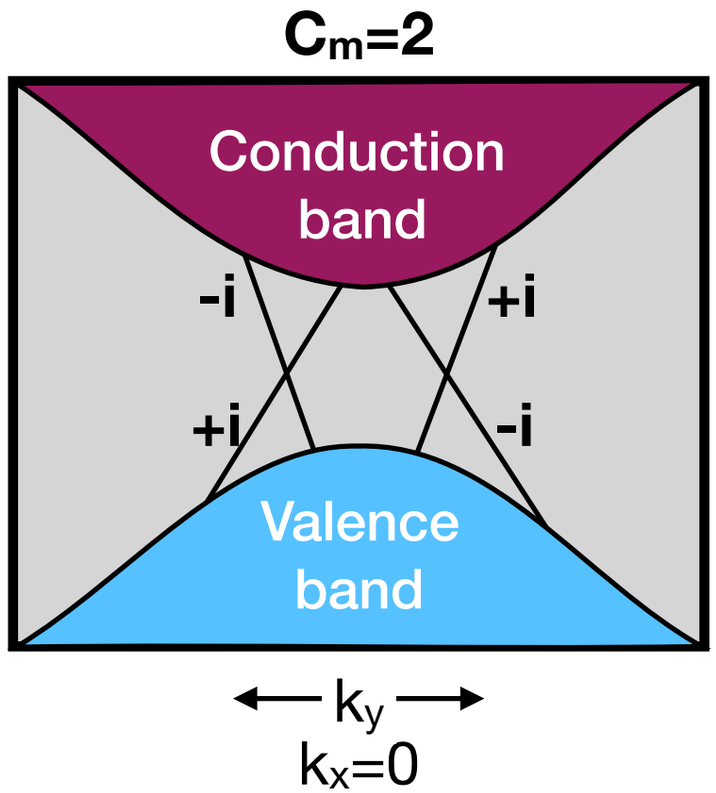
Mirror Chern number: $C_m = \frac{1}{2}(C_+ - C_-)$

# Surface states of mirror Chern insulator

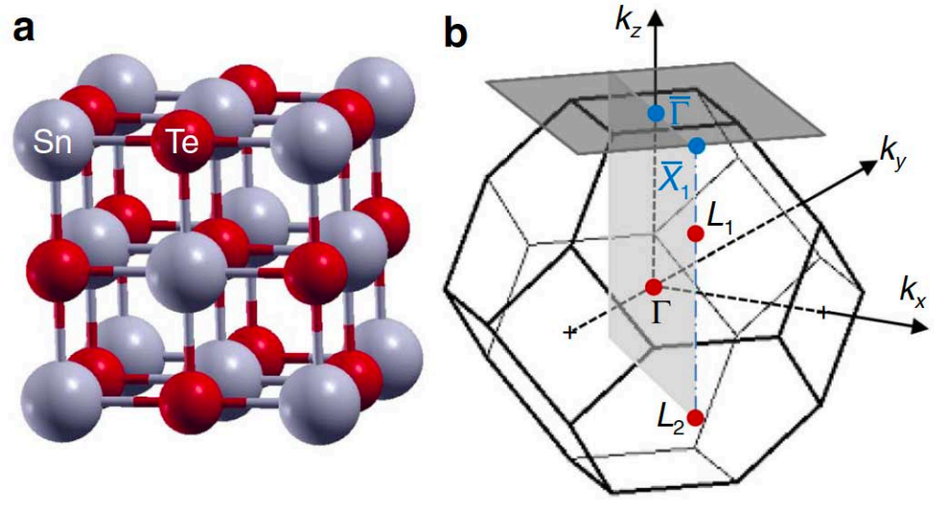
Teo, Fu, Kane PRB 045426 (2008)




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



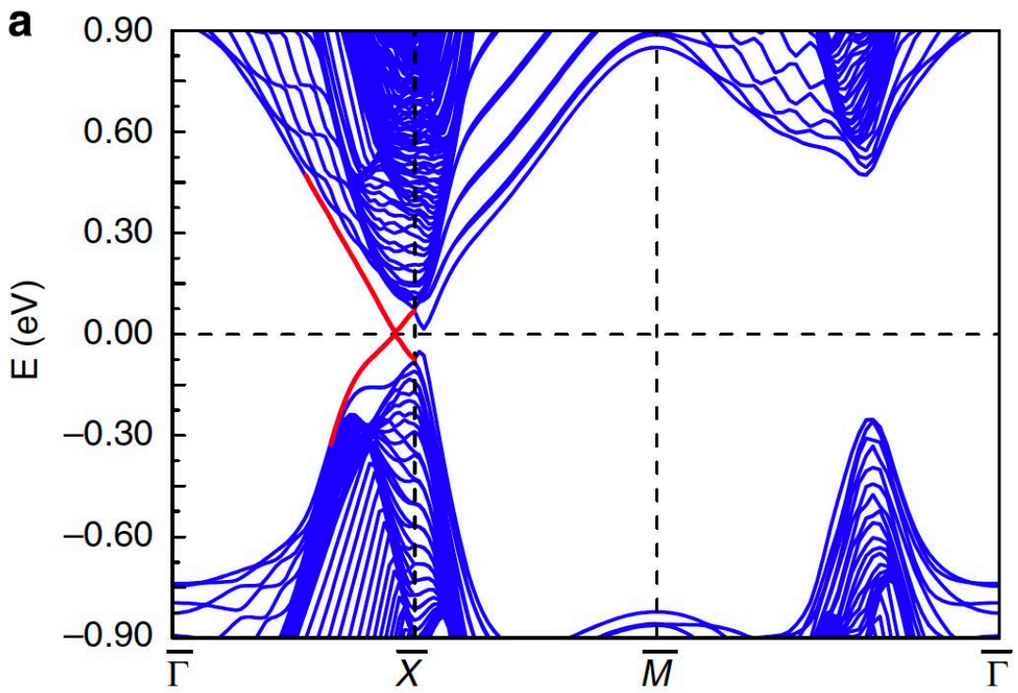
# SnTe predicted/observed mirror Chern insulator



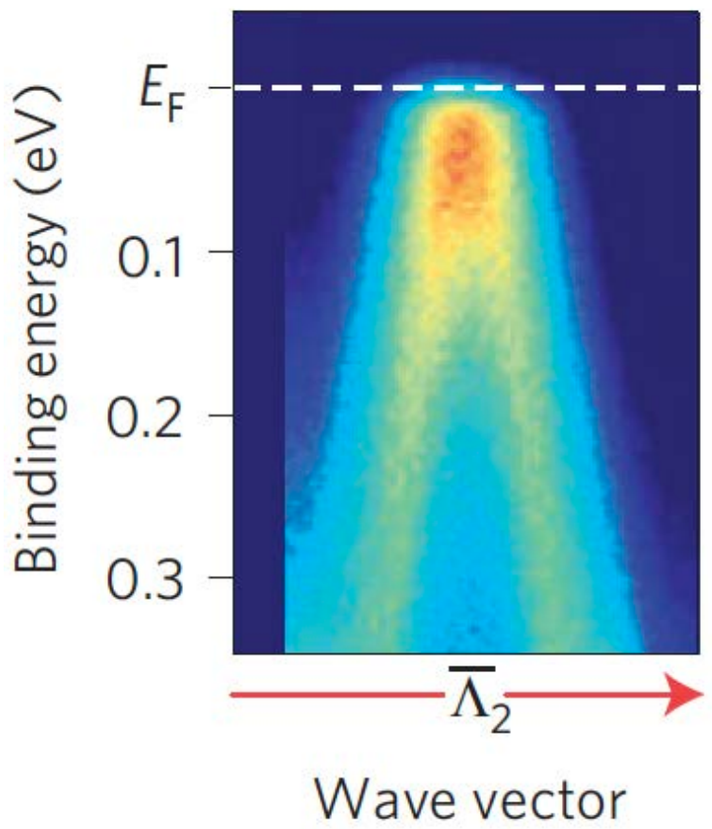

Prediction: Hsieh, et al,
Nat. Comm. 3, 982 (2012)

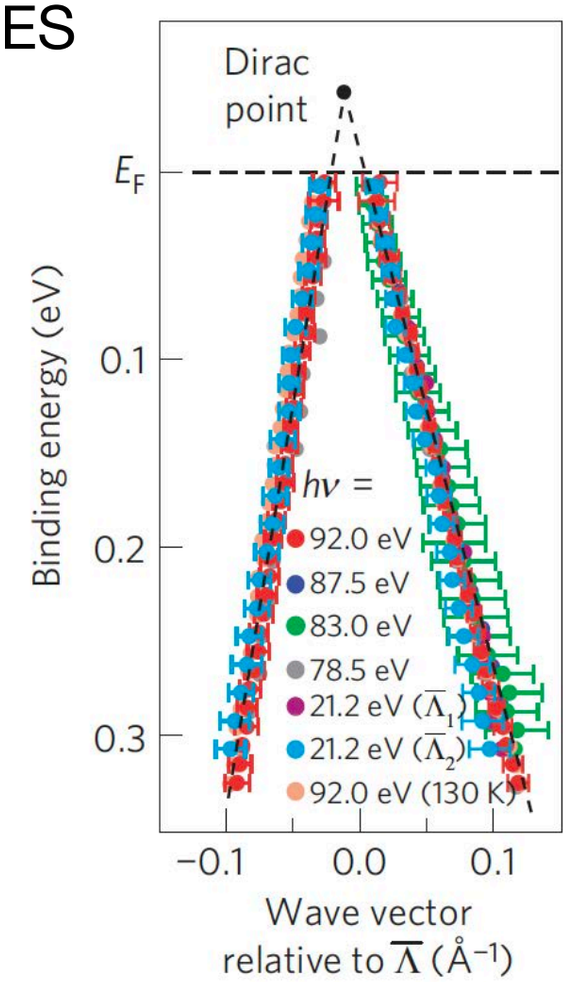
Observation: Tanaka, et al,
Nat. Phys. 8, 800 (2012), Ando group

$C_m$=2




ARPES



# Topological insulators with inversion symmetry

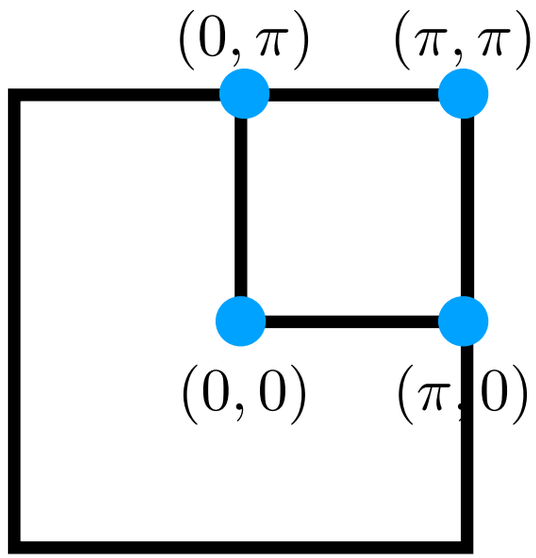
Inversion symmetry: $(x, y, z) \mapsto (-x, -y, -z)$

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

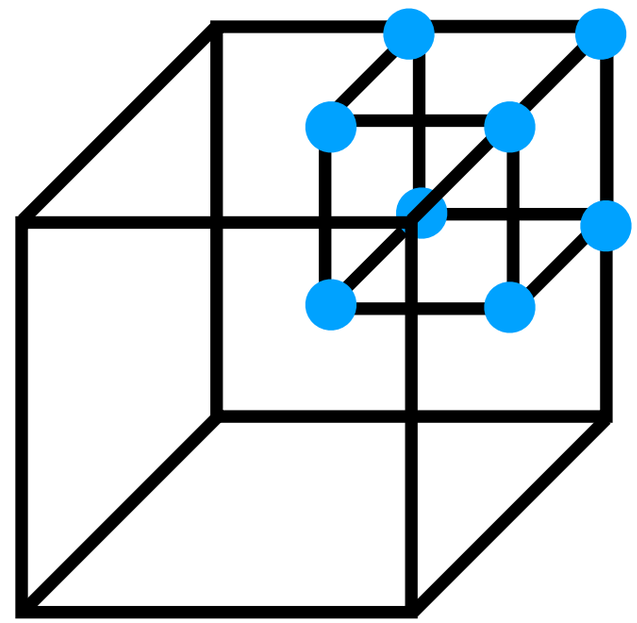
Inversion eigenvalues assigned at inversion-invariant points: $k_x, k_y, k_z = 0 \text{ or } \pi$

“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!

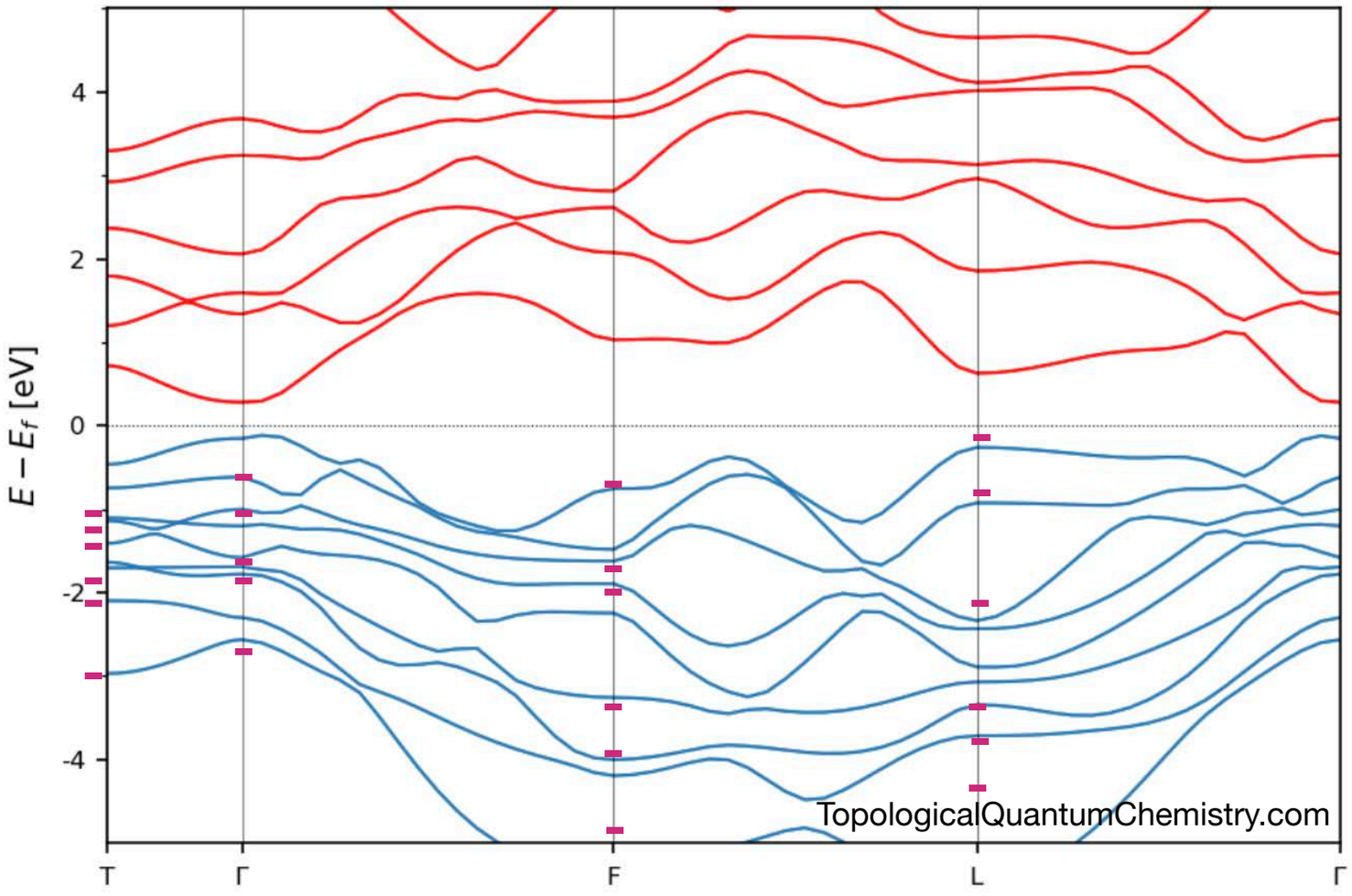
Fu and Kane PRB 76, 045302 (2007)

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

$$(-1)^{\nu} = \prod_{i} \delta_i$$ ← 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:**

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

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

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

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

$$\delta_i = \prod_{m=1}^{N} \xi_{2m}(\Gamma_i) \qquad \delta_\Gamma = -1, \delta_L = \delta_F = \delta_T = +1$$

$$(-1)^\nu = \prod_i \delta_i \qquad (-1)^\nu = -1 \Rightarrow \boxed{\nu = -1}$$

# 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 $k_x$=$\boldsymbol{\pi}$, bands labelled by $g_x$ eigs

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

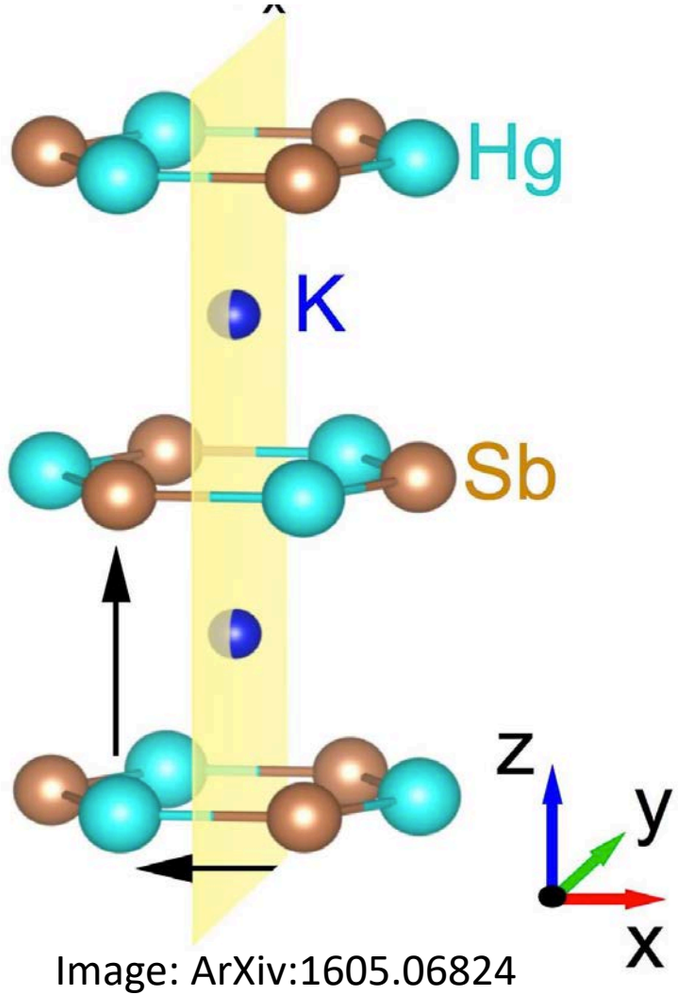



Image: ArXiv:1605.06824

**Screw symmetry:** mirror followed by fractional lattice translation

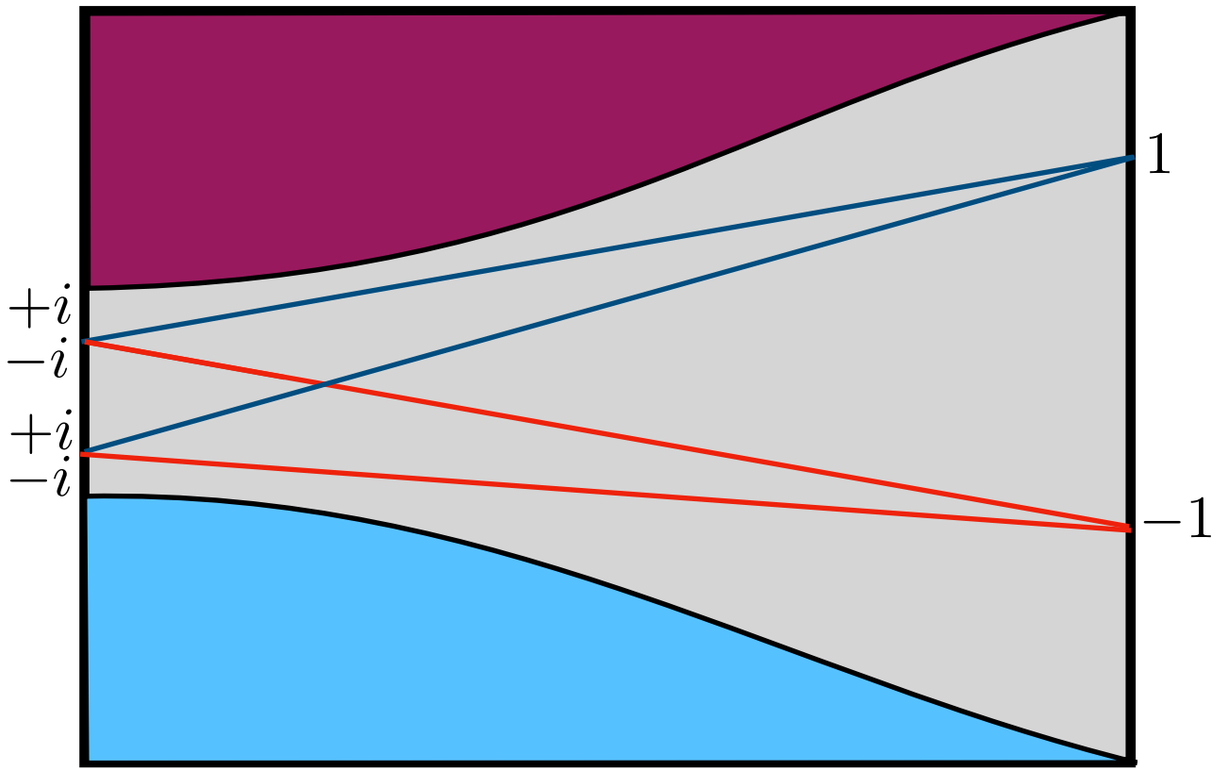
**Space groups with a screw or glide symmetry are nonsymmorphic***

# Glide symmetry can protect novel surface states

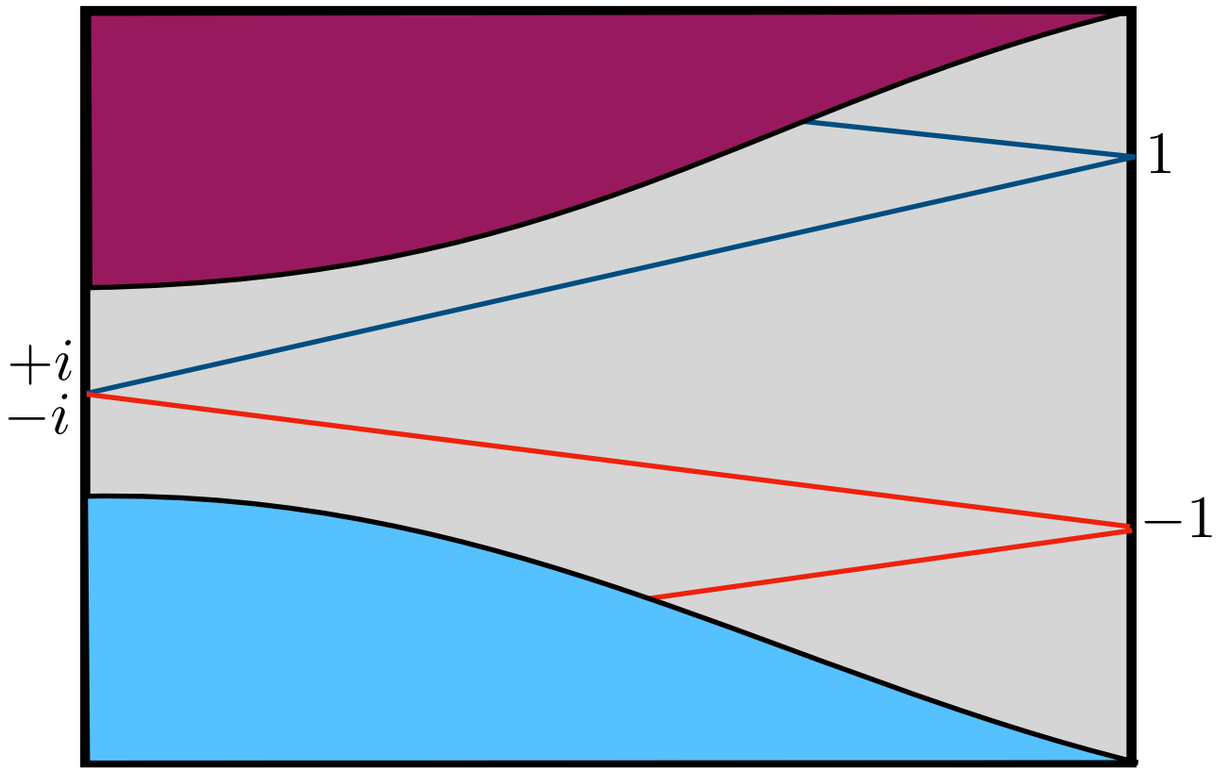
Wang, Alexandradinata, Cava, Bernevig Nature 532, 189 (2016)

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

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




"Hourglass fermion"

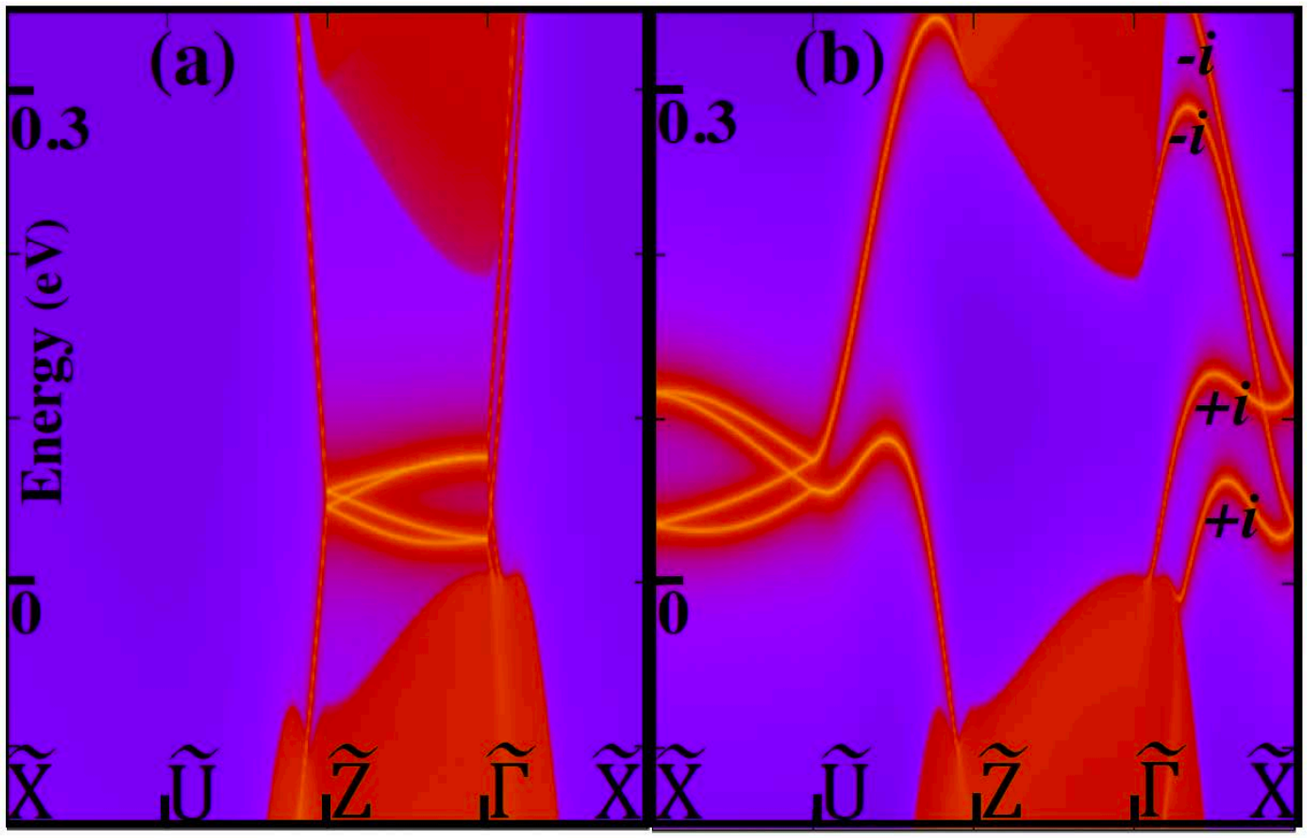


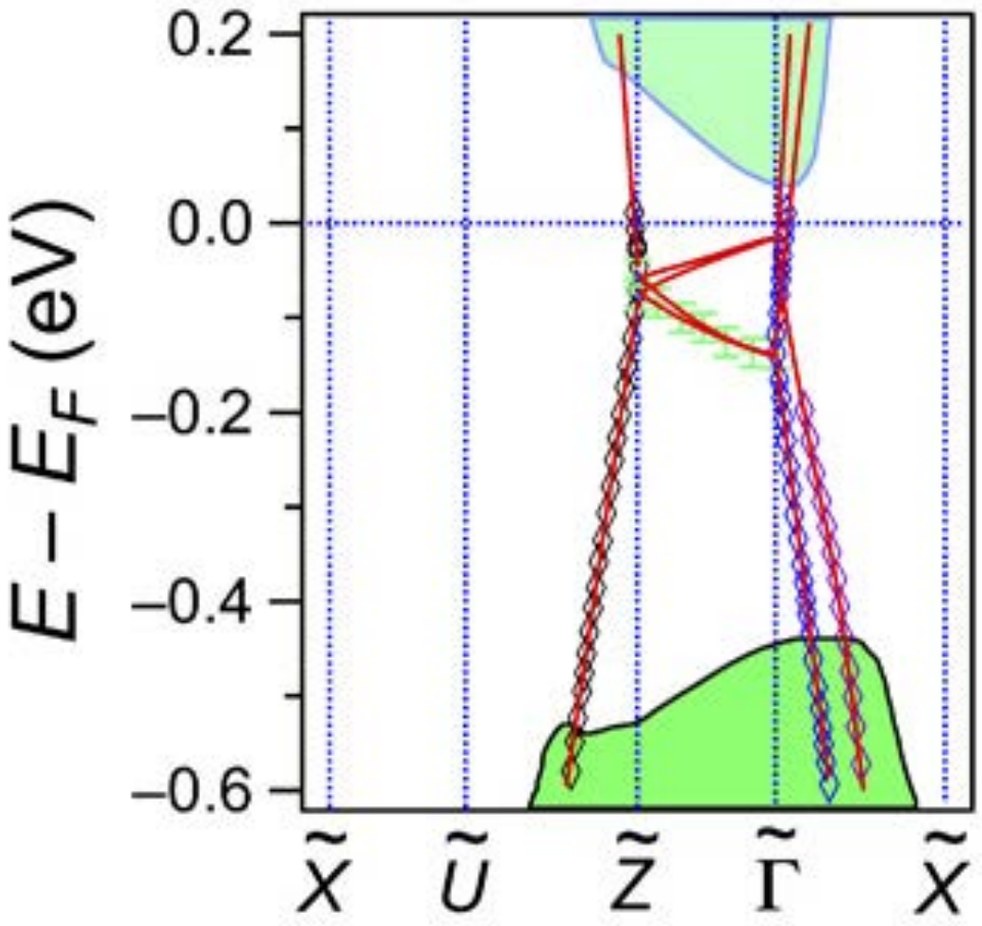

"Glide spin hall"

# KHgSb predicted/observed hourglass fermion

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

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

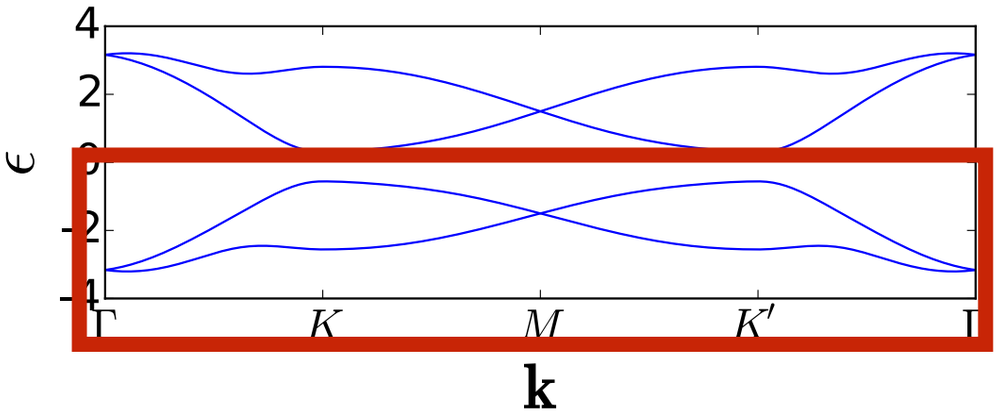


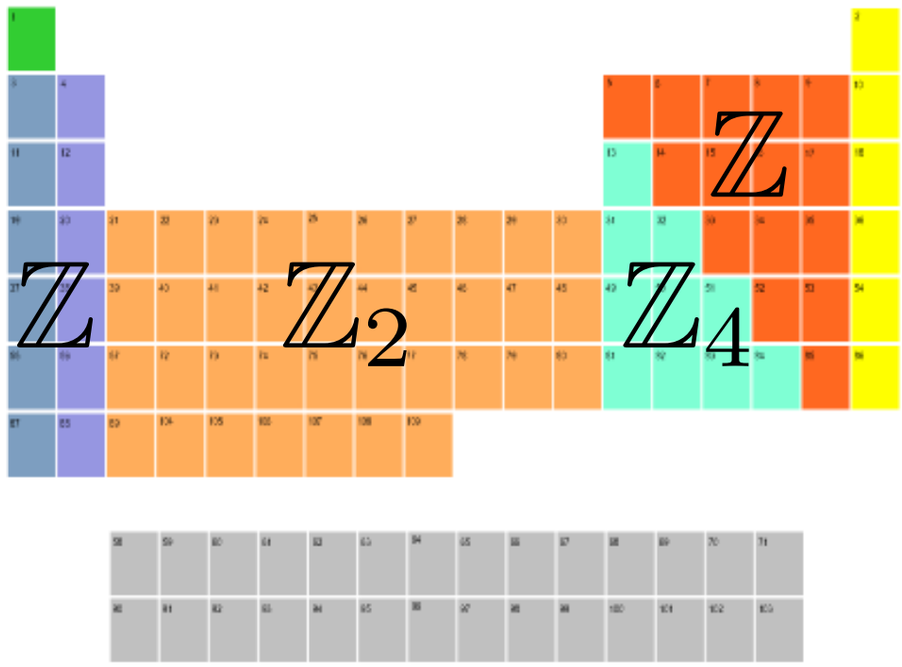
# Ad hoc classification of topological crystalline insulators leaves open questions:

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?!




?




# Recent insights from topological band theory

**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)

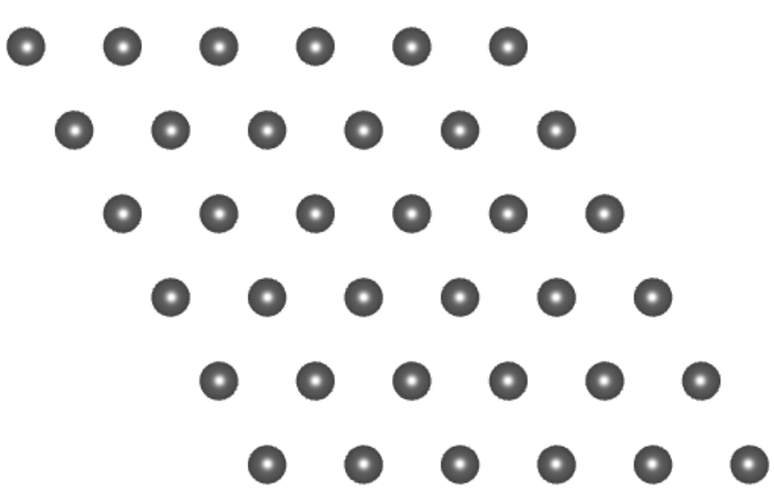
## Key: topological bands are not deformable to an atomic limit

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

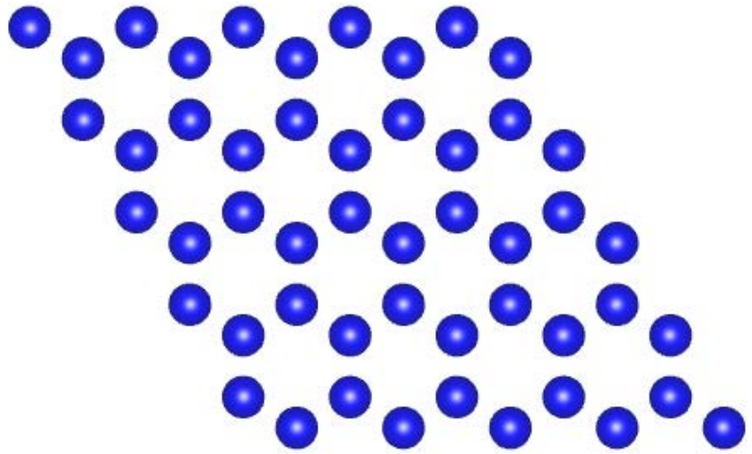
# How to identify all atomic limits?

**Within one space group, many ways to arrange atoms**

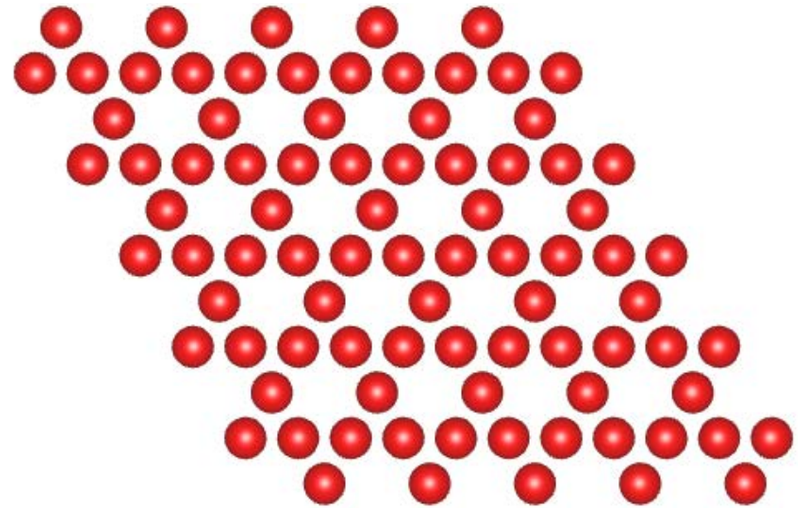
**“Wyckoff positions”**



1 atom/unit cell
(triangular)



2 atoms/unit cell
(honeycomb)

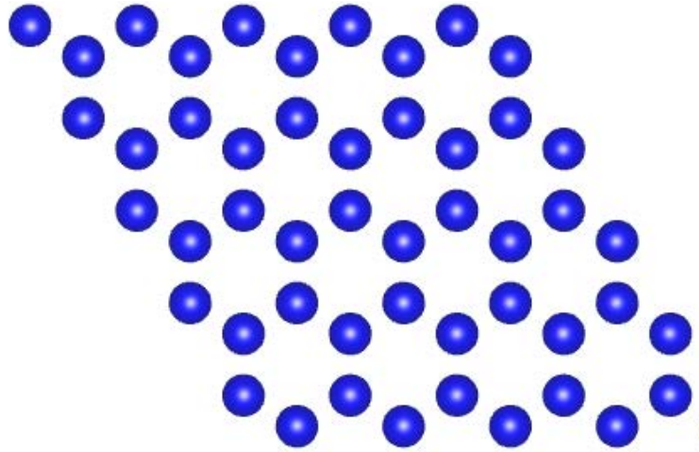


3 atoms/unit cell
(kagome)

All atoms are related by symmetry

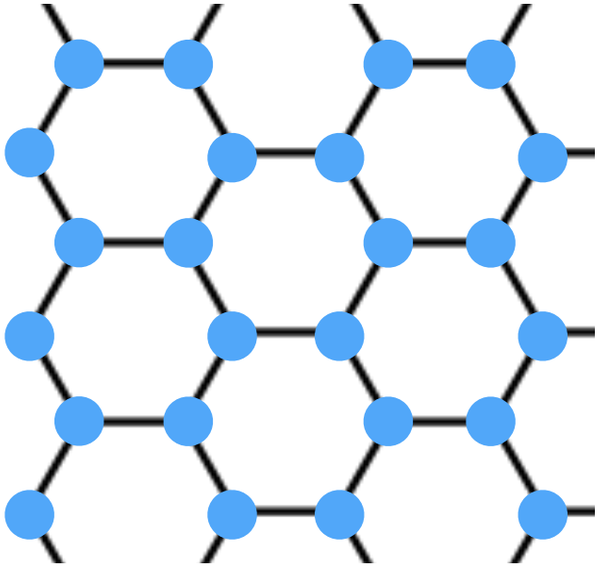
# How to identify all atomic limits?

## Within one arrangement, many choices of orbitals

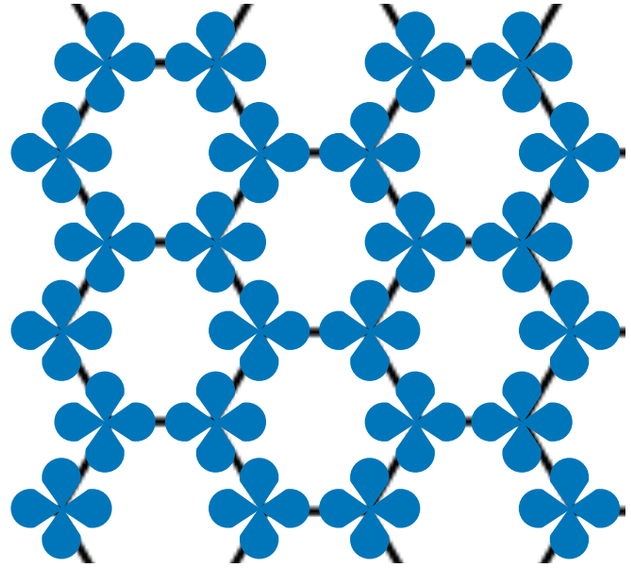


2 atoms/unit cell

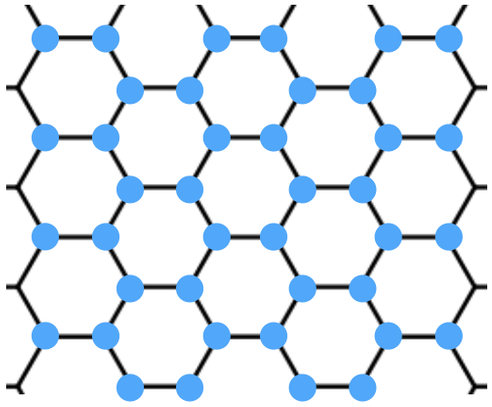
**s (or $p_z$) orbitals**



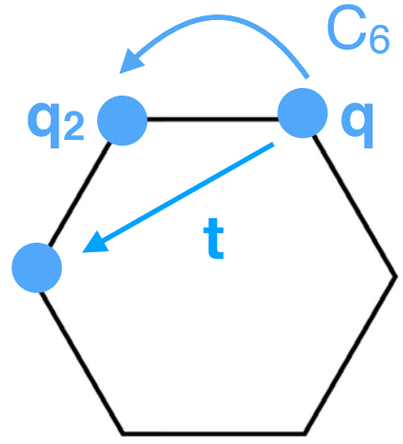
**$p_x$ and $p_y$ orbitals**



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



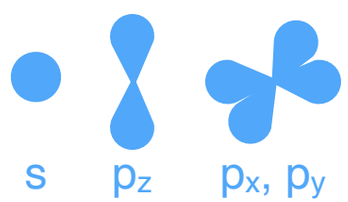
# Symmetry of a single site determines symmetry of entire lattice




Identify "**site-symmetry group**":
$G_q$ = symmetries that leave **q** invariant

$C_3$, $m_y$

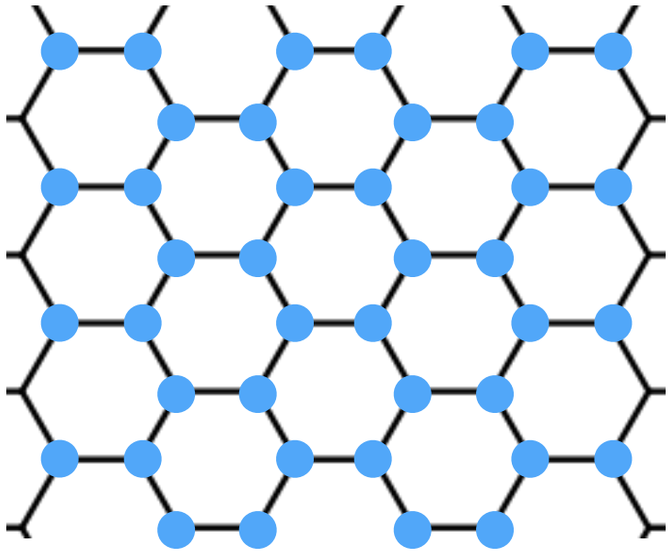
Orbitals at **q** transform under a rep, $\rho(g)$, of $G_q$




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

$C_6$, t, …

# 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

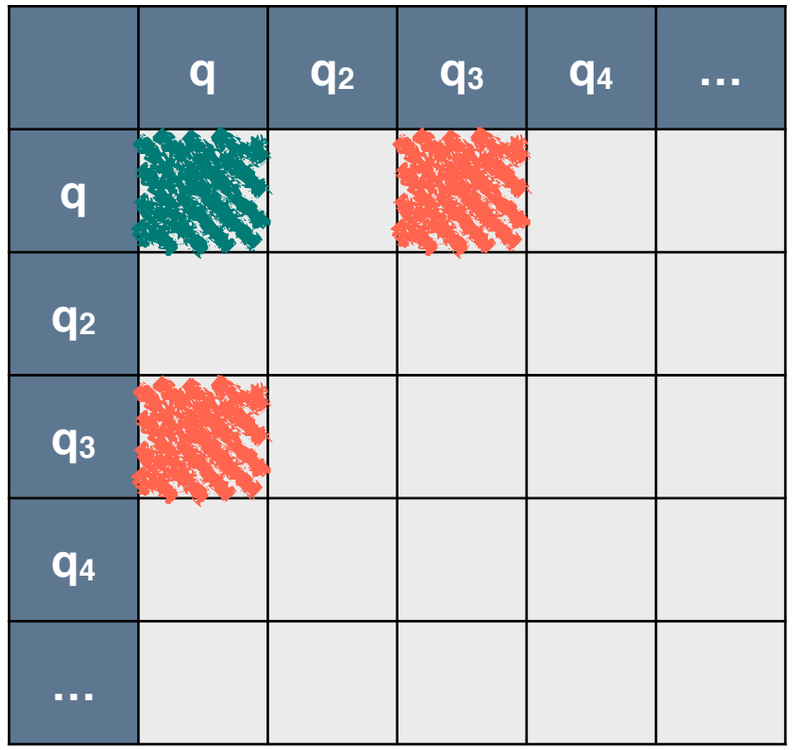
$$\mathrm{Ind}_{G_q}^{G}\rho$$

How to construct a band representation:

Each symmetry operation represented by BIG matrix

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

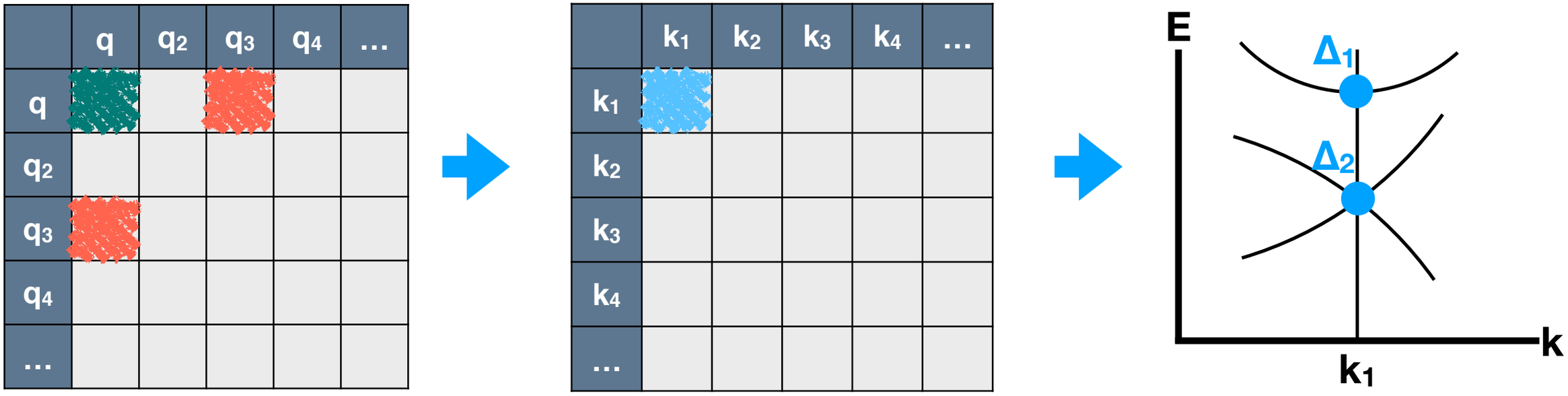
Off-diagonal block if g interchanges sites



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

Zak PRL 1980, PRB 1981, 1982

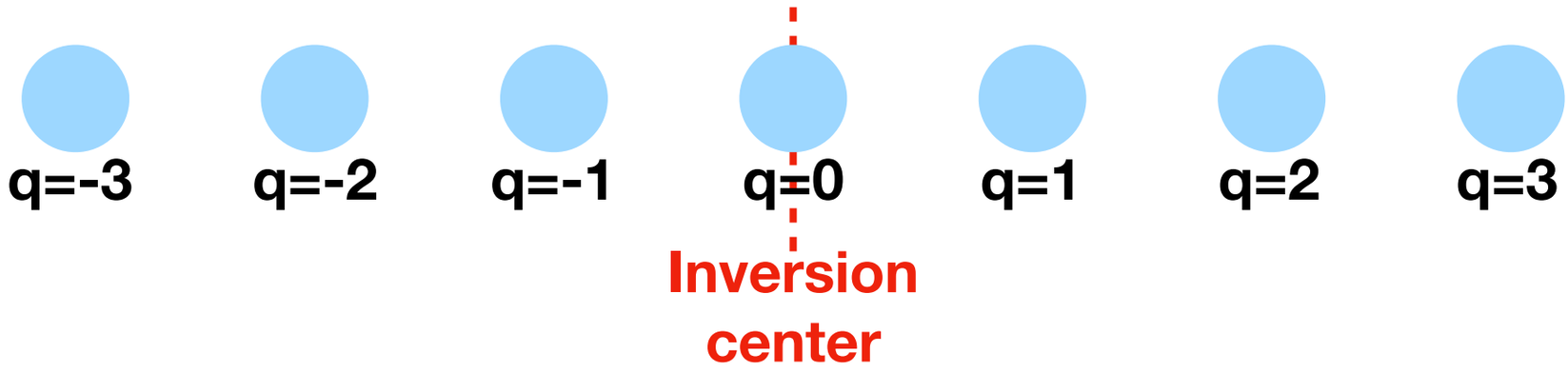
Fourier transforming matrix gives irreps at any k point




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:

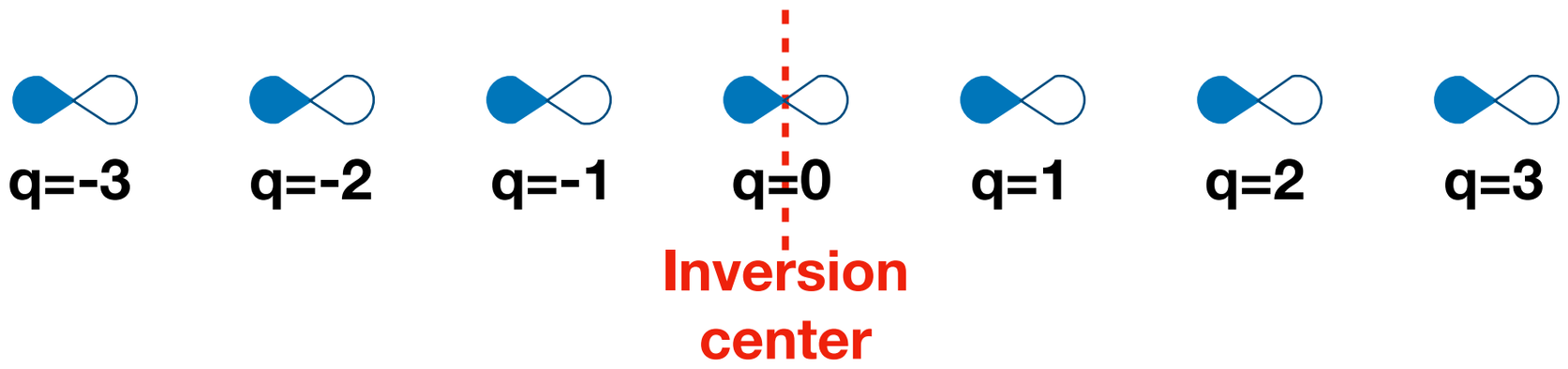
### Inversion

| … | -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:

### Inversion

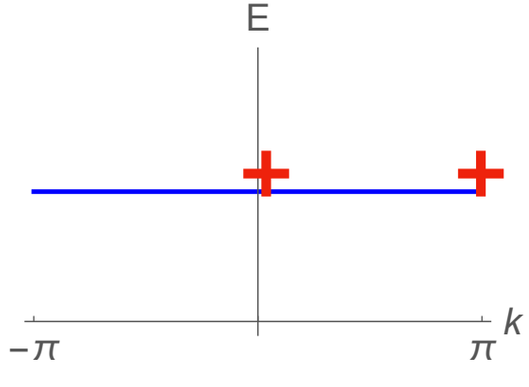
| … | -2 | -1 | 0 | 1 | 2 | … |
|---|---|---|---|---|---|---|
| -2 | | | | | -1 | |
| -1 | | | | -1 | | |
| 0 | | | -1 | | | |
| 1 | | -1 | | | | |
| 2 | -1 | | | | | |
| … | | | | | | |

### translation by 1

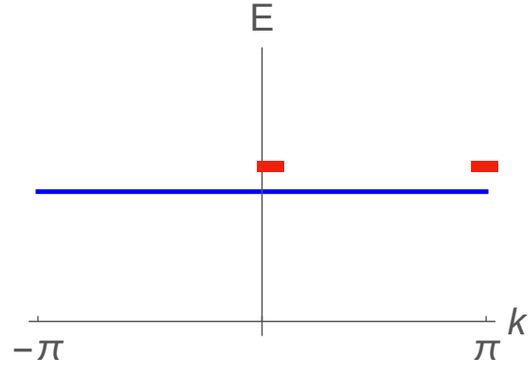
| … | -2 | -1 | 0 | 1 | 2 | … |
|---|---|---|---|---|---|---|
| -2 | | | | | | |
| -1 | 1 | | | | | |
| 0 | | 1 | | | | |
| 1 | | | 1 | | | |
| 2 | | | | 1 | | |
| … | | | | | 1 | |

# Fourier transform yields inversion eigenvalues at k=0 and k=π

Atomic limit s orbitals:

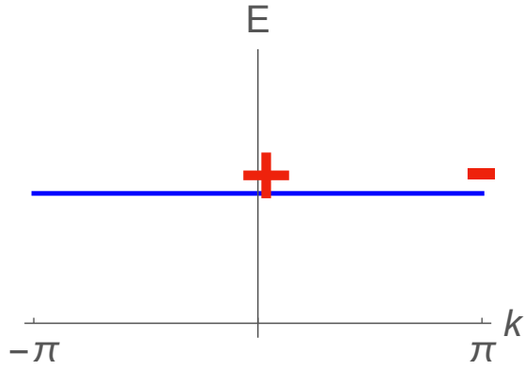



Atomic limit p orbitals:

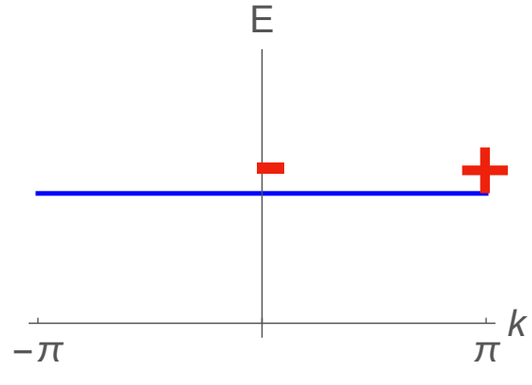



## Repeat with atoms shifted by half a unit cell:

Atomic limit s orbitals:



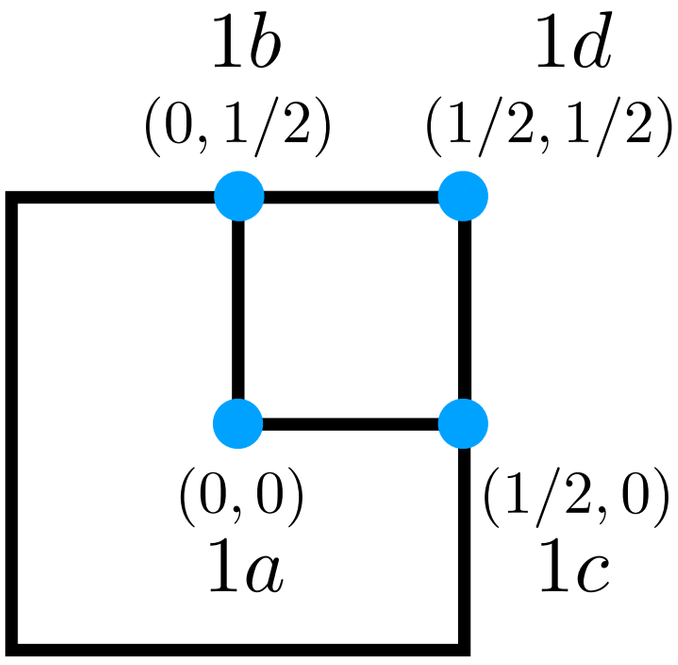

Atomic limit p orbitals:




## 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:




**Always an even number of negative inversion eigenvalues!**

Inversion eigenvalues for *s* orbitals

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

Inversion eigenvalues for *p* orbitals

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

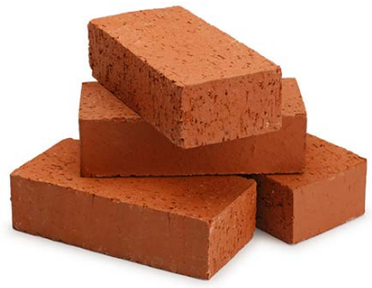
**A band structure with an odd number of negative inversion eigenvalues is not an atomic limit phase ⇒ must be topological**

# Goal: compute <u>all</u> atomic limit phases for <u>all</u> 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 <u>maximal</u> site-symmetry groups

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

⇒ Finitely many EBRs

# How many EBRs are there?

Large but finite number, estimate:

(230 space groups) x (3 max Wyckoff pos.) x (3 irreps) = 2070

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

**⇒ 10,403 total EBRs**

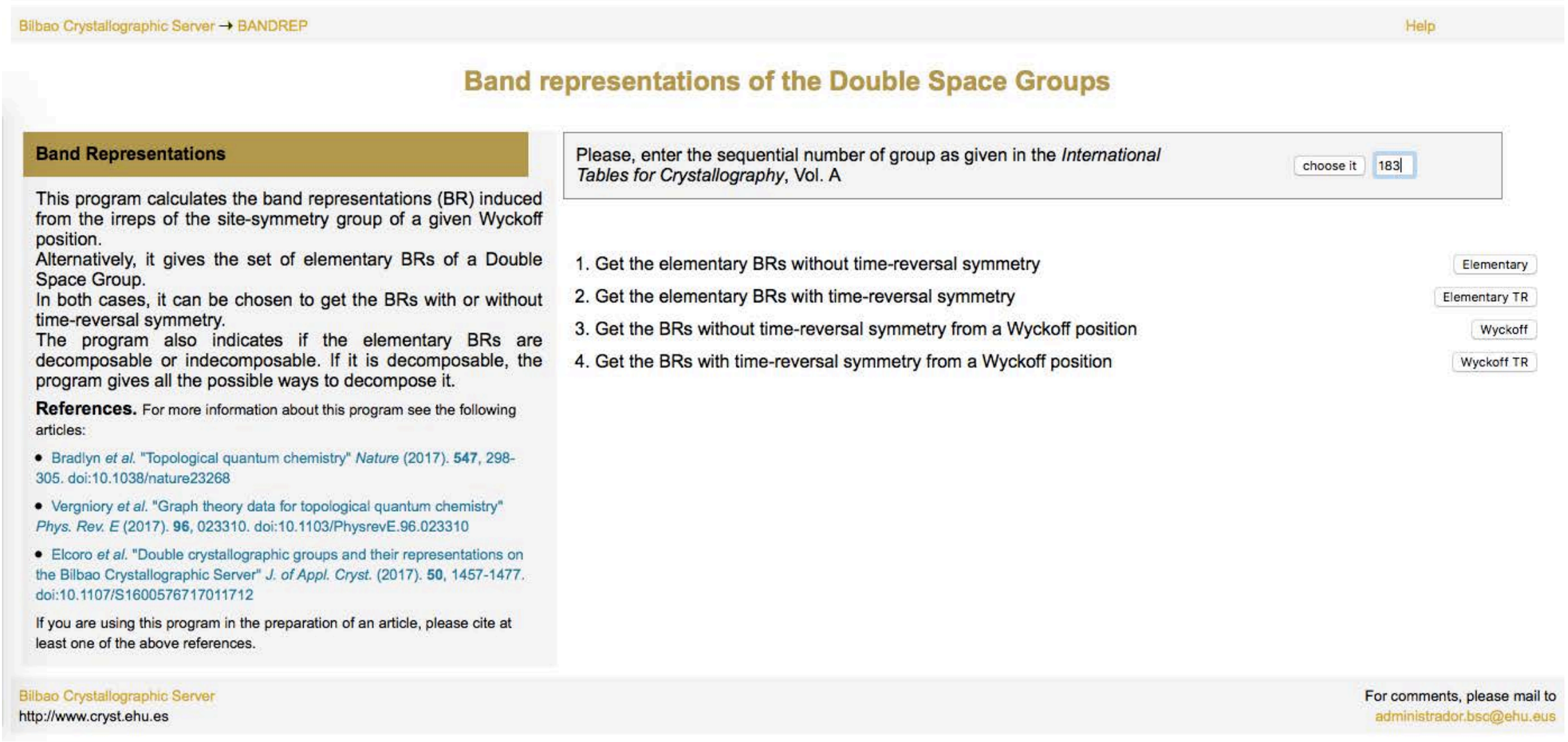
# Symmetry labels for all EBRs are enumerated on the Bilbao Crystallographic Server

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)



# 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) | $L_1(1)$ | $L_2(1)$ | $L_4(1)$ | $L_3(1)$ | $L_3(1) \oplus L_4(1)$ | $L_1(1) \oplus L_2(1)$ | $L_1(1) \oplus L_4(1)$ | |

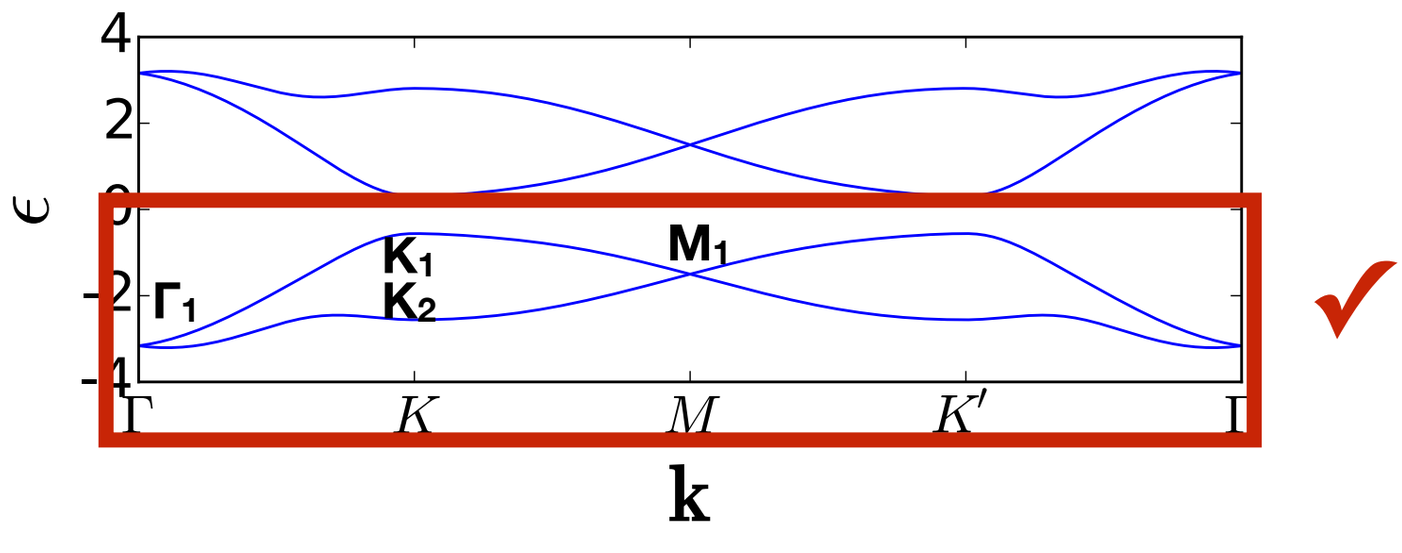
Atom arrangement

Orbital

High-symmetry points

# 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

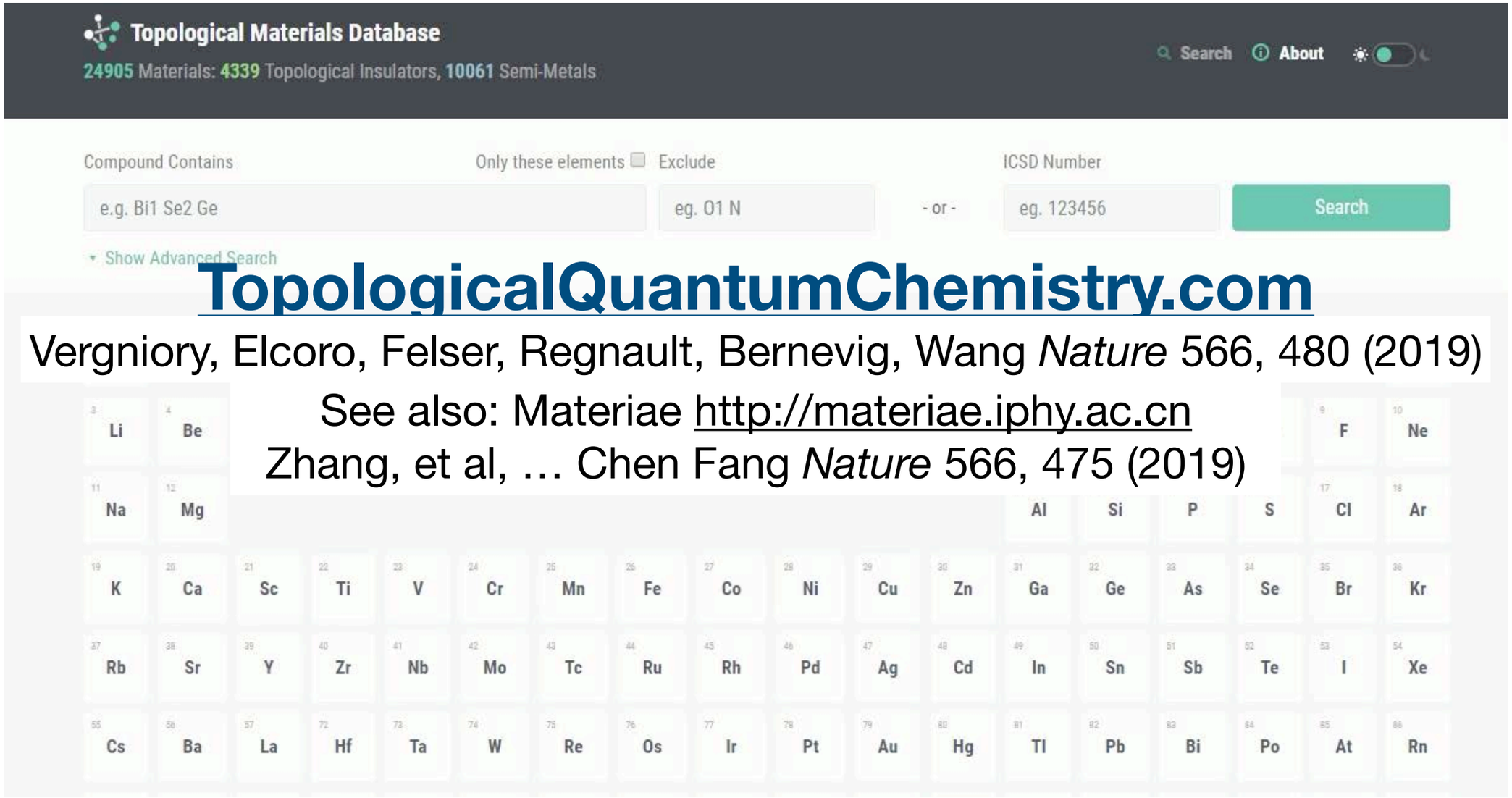
Topological bands are not a “sum” of elementary band representations

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

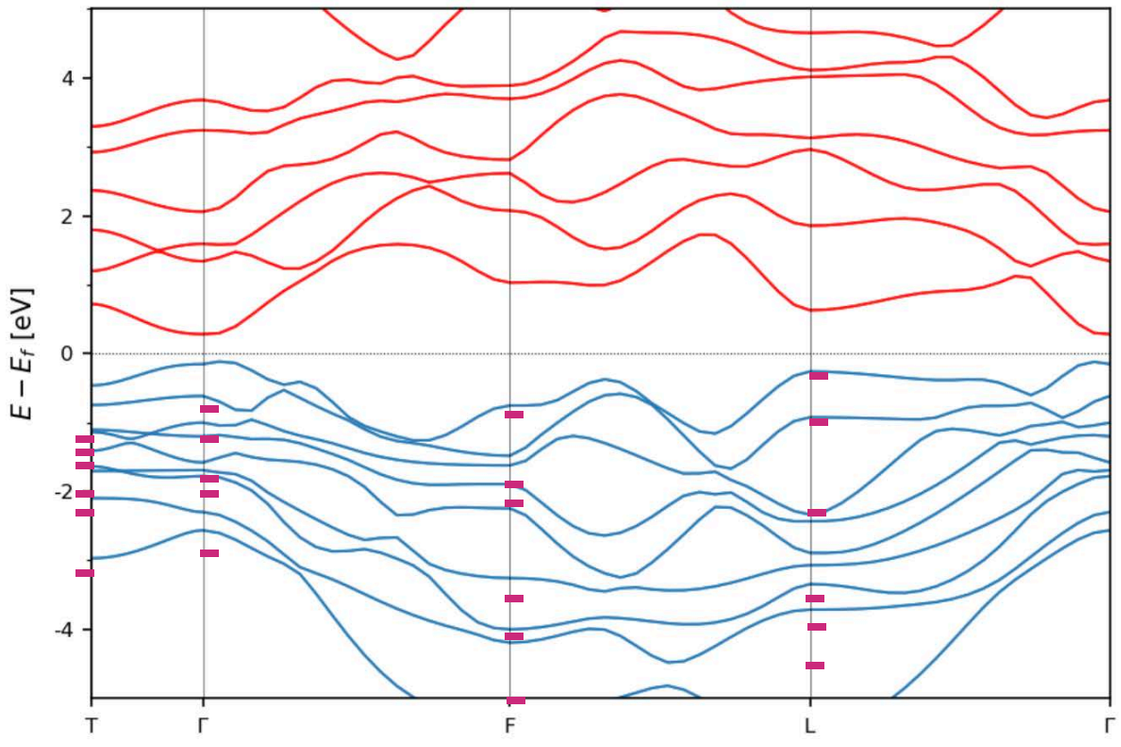



Vergniory, Elcoro, Felser, Regnault, Bernevig, Wang *Nature* 566, 480 (2019)

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

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

# Summary




Crystal symmetry can protect and identify topological phases

Exs: mirror Chern, inversion index, hourglass, …

Symmetry indicators can be determined from elementary band representations

Materials: TopologicalQuantumChemistry.com

Review article: **JC** & Bradlyn, ArXiv: 2006.04890

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Princeton