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	$\cdots$
A	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\cdots$
AIII	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	$\cdots$

no symmetry →

Integer quantum Hall/ Chern insulator

real case:

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

fermions w/ time-reversal →

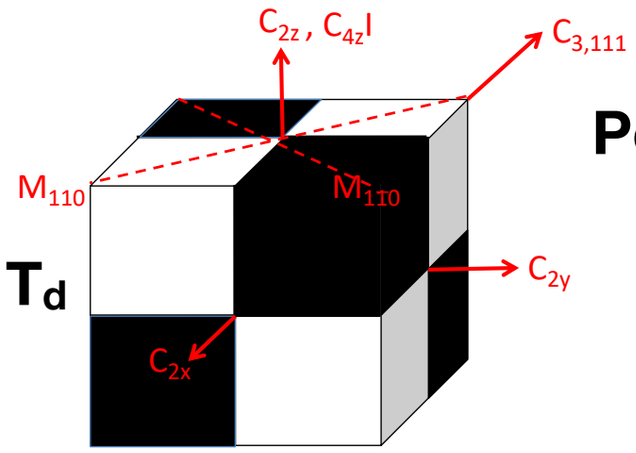
2d and 3d topological insulators
(weak index not captured)

Crystal symmetries refine the classification of topological phases

Outline:

- What are the possible crystal symmetries?
- Examples of topological phases with crystal symmetry
- Classification of band structures by symmetry irreps
  - Topological quantum chemistry/symmetry indicators

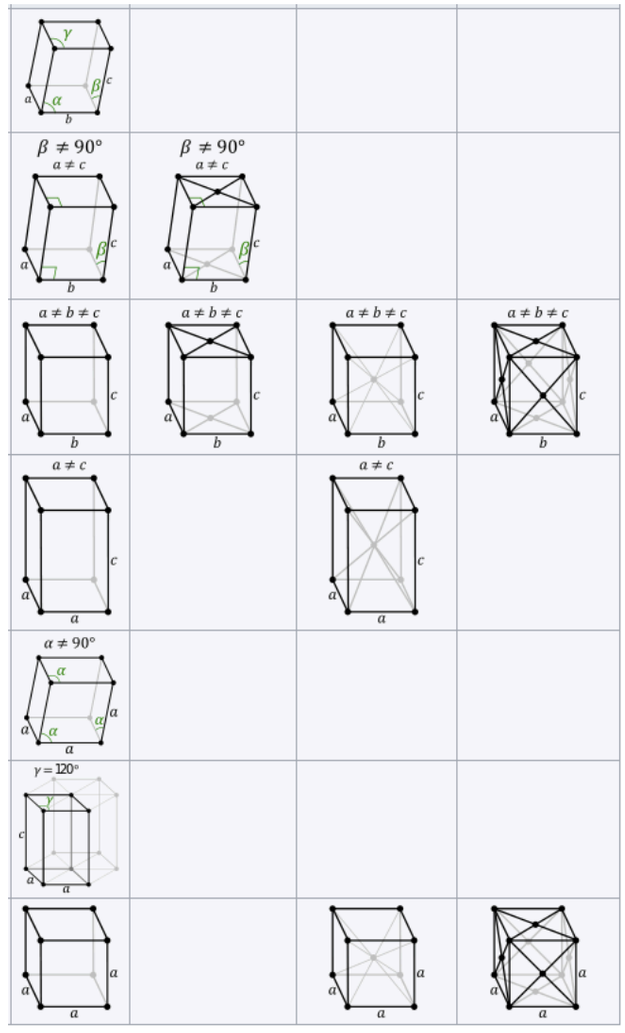
What are crystal symmetries?



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?

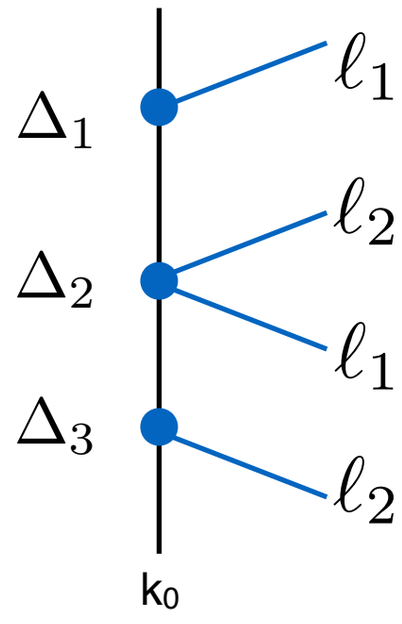
Fourier-transformed Hamiltonian: $\Delta(\mathcal{G})H(\mathbf{k})\Delta(\mathcal{G})^{-1} = H(\mathcal{G}\mathbf{k})$

matrix representative of symmetry operation

"Little group" of 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



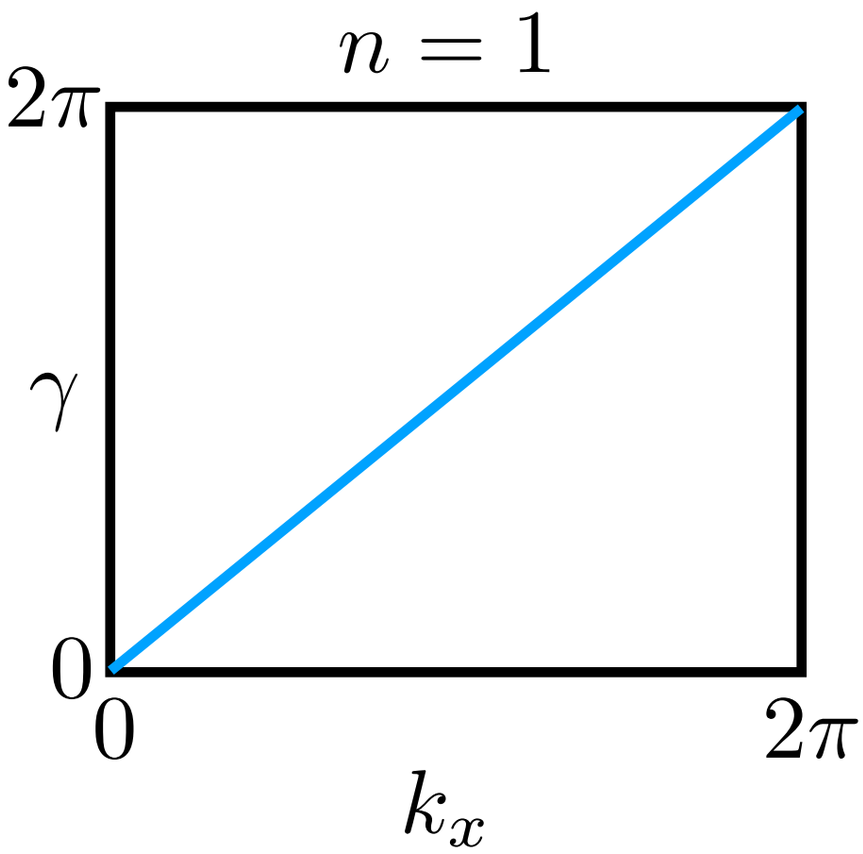
$$\left.\begin{aligned} \Delta_1 &\to \ell_1 \\ \Delta_2 &\to \ell_1 \oplus \ell_2 \\ \Delta_3 &\to \ell_2 \end{aligned}\right\}$$

Compatibility relations between points and lines

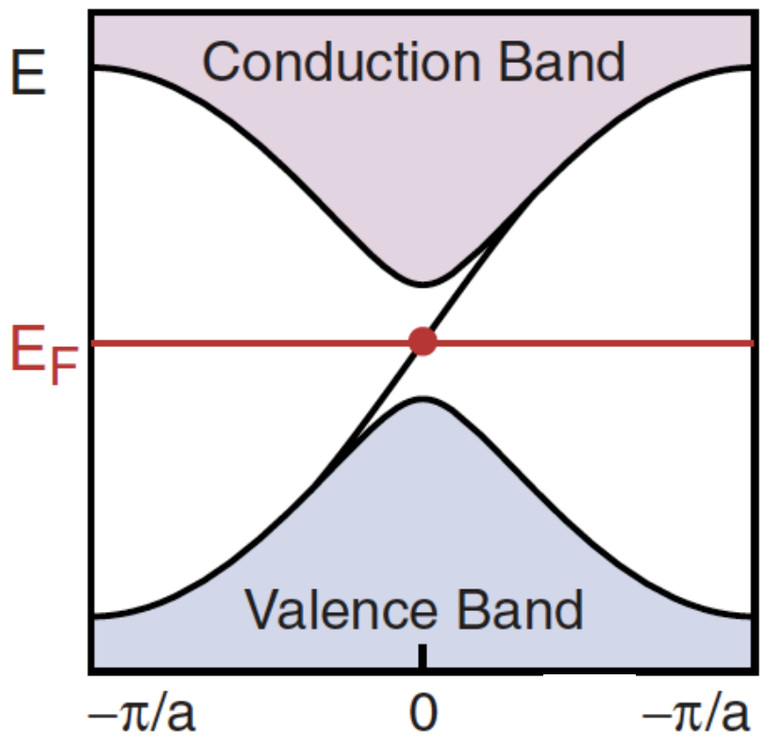
“Chern insulator” is a building block for topological crystalline insulators

A Chern insulator is a 2D topological insulator that does not require symmetry

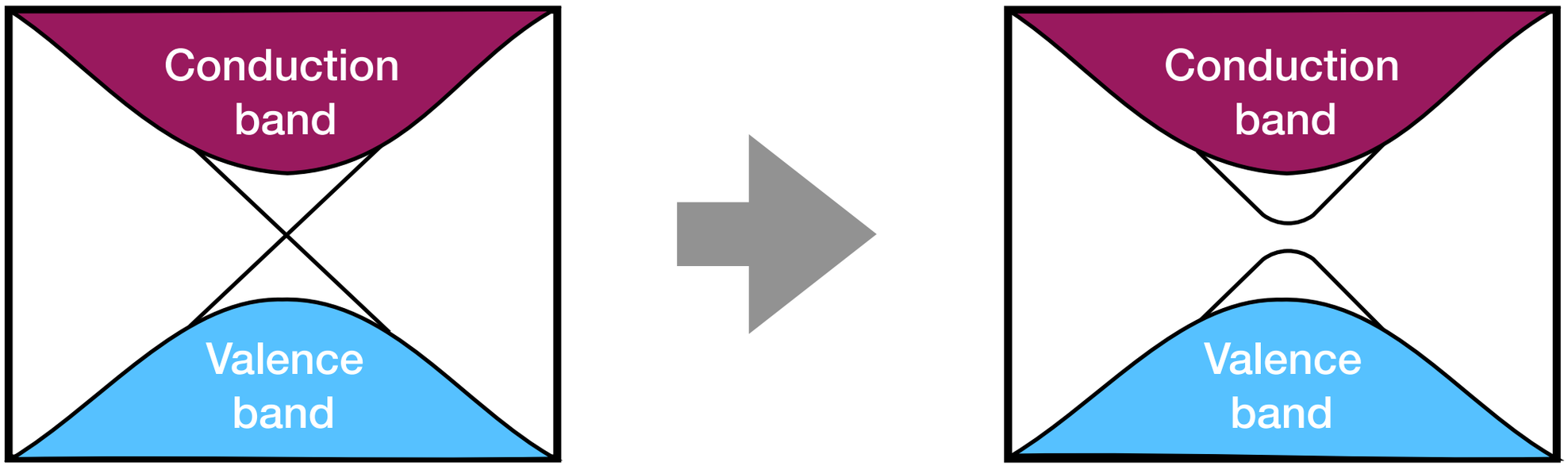
Topological invariant: Chern number



Bulk-edge correspondence



Surface states of bands with opposite Chern number generically gap



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

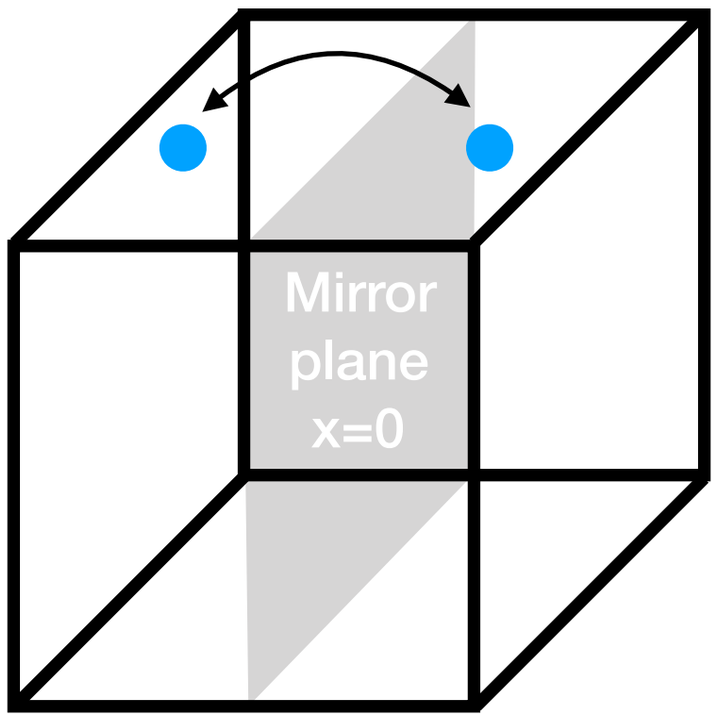
Ex 1: spin conservation ⇒ quantum spin Hall

Ex 2: time-reversal symmetry ⇒ 2D TI

Mirror Chern insulator: canonical TCI

Teo, Fu, Kane PRB 045426 (2008)

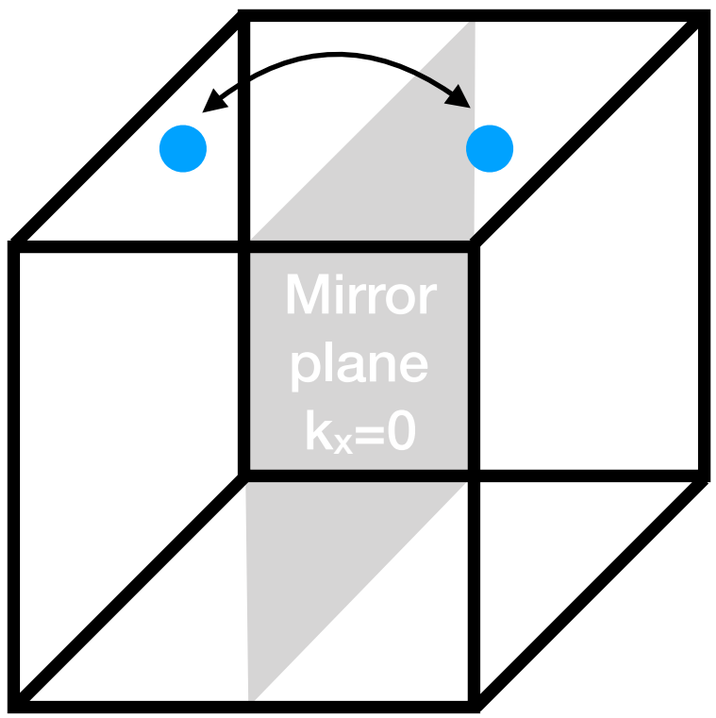
Mirror symmetry: $m_x : (x, y, z) \mapsto (-x, y, z)$



Mirror Chern insulator: canonical TCI

Teo, Fu, Kane PRB 045426 (2008)

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



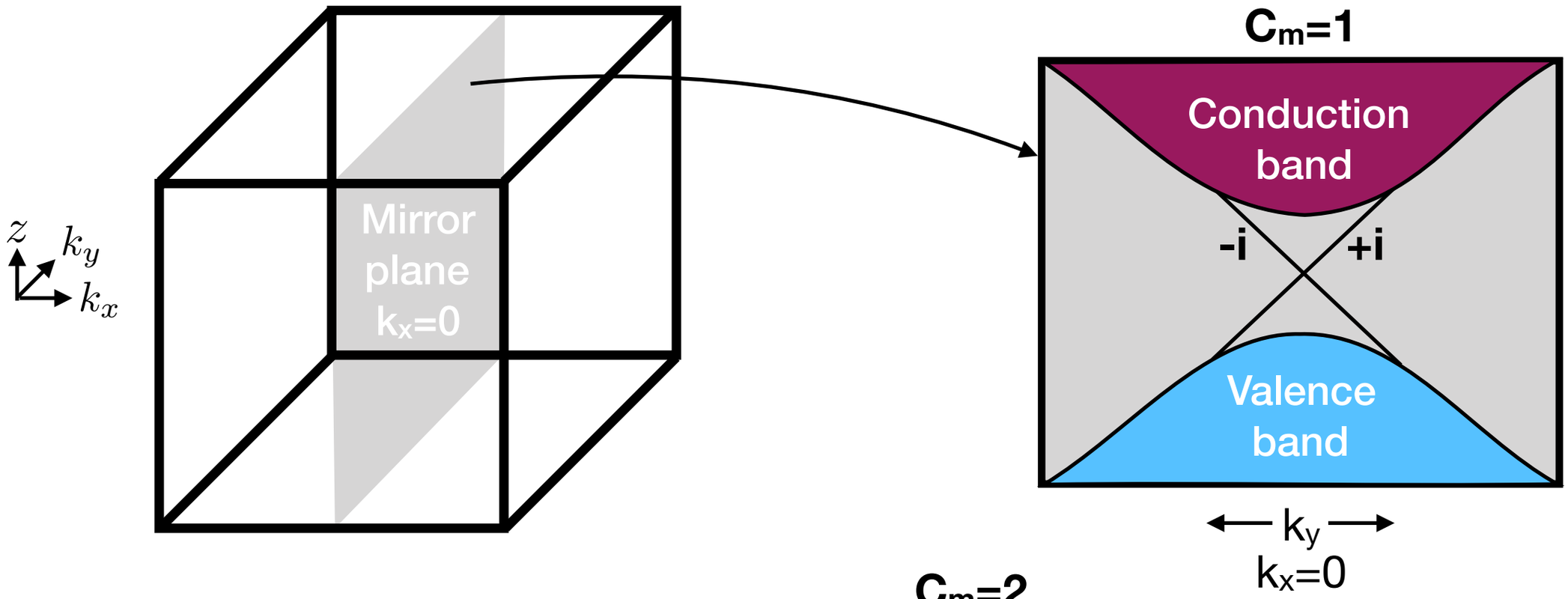
When k_x=0, m_x commutes with H(k_x=0, k_y, k_z) ⇒ bands labelled by m_x eigenvalue: +/- i

Define Chern number for each mirror sector: C±

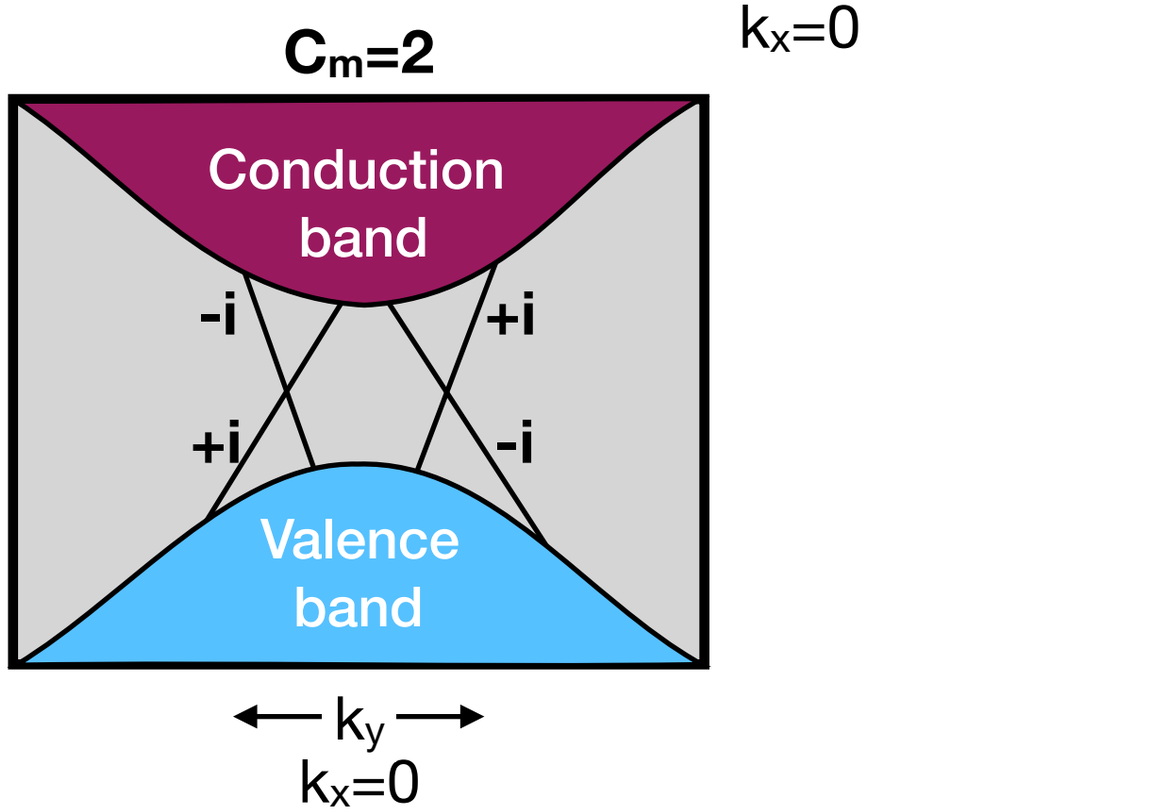
Mirror Chern number: $C_m = \frac{1}{2}(C_+ - C_-)$

Surface states of mirror Chern insulator

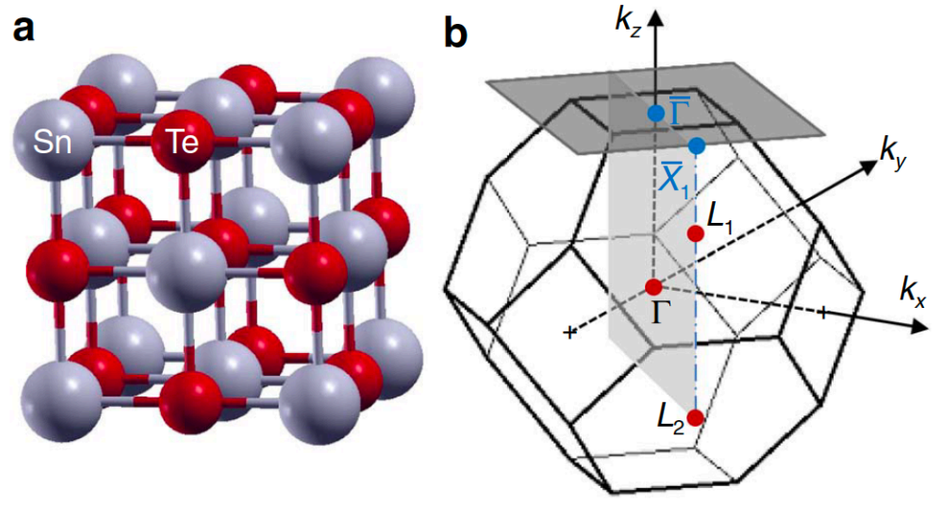
Teo, Fu, Kane PRB 045426 (2008)



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



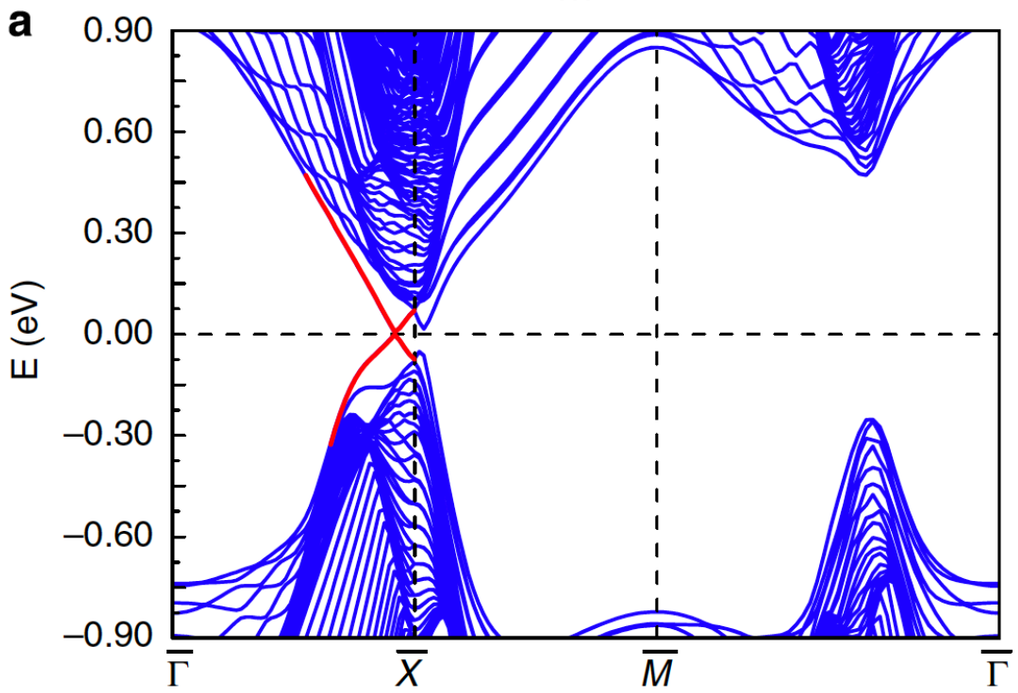
SnTe predicted/observed mirror Chern insulator



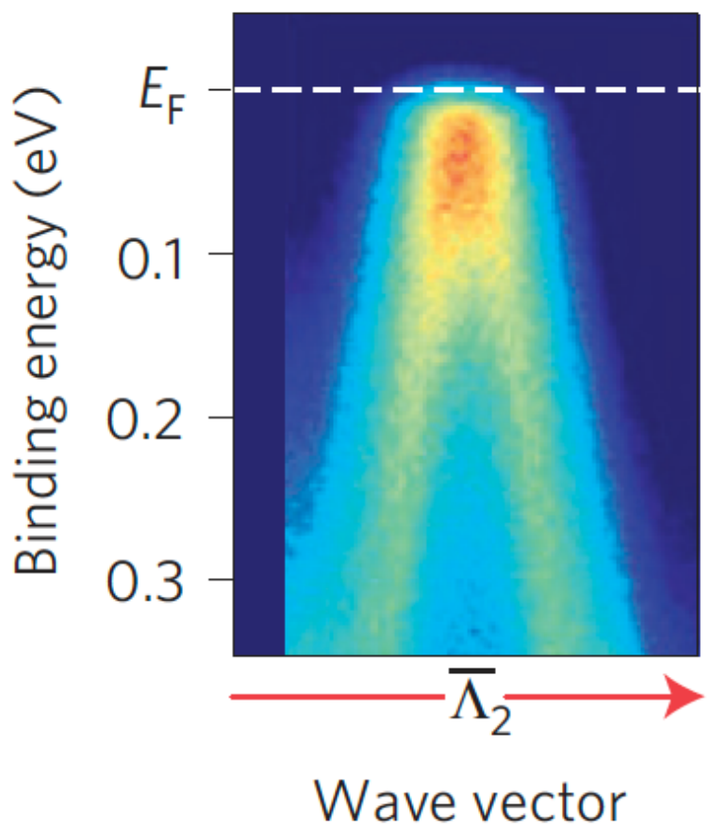
Prediction: Hsieh, et al,
Nat. Comm. 3, 982 (2012)

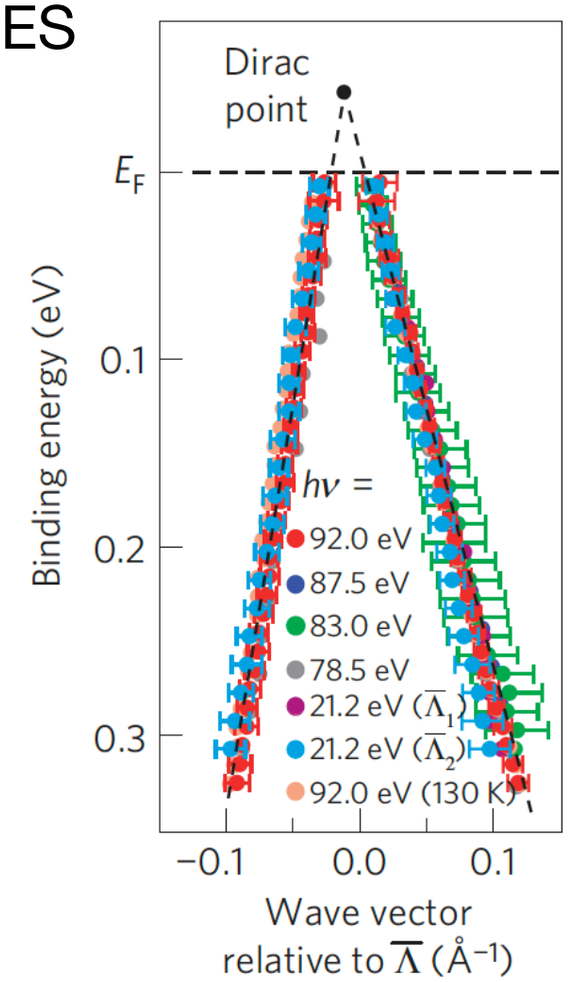
Observation: Tanaka, et al,
Nat. Phys. 8, 800 (2012), Ando group

C_m=2



ARPES





Topological insulators with inversion symmetry

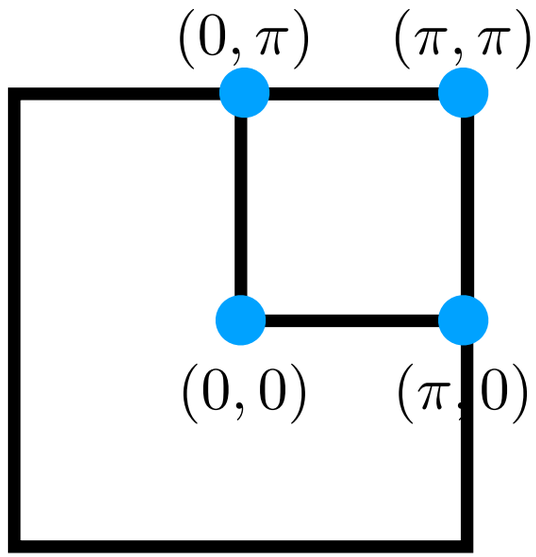
Inversion symmetry: $(x, y, z) \mapsto (-x, -y, -z)$

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

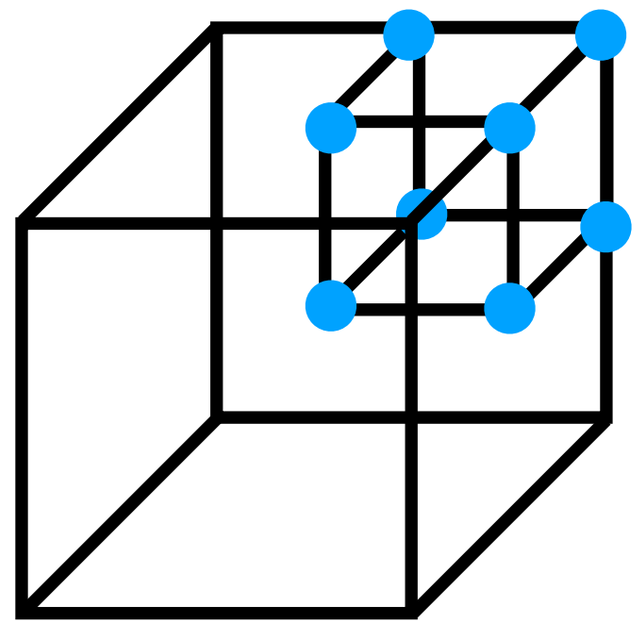
Inversion eigenvalues assigned at inversion-invariant points: $k_x, k_y, k_z = 0 \text{ or } \pi$

“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!

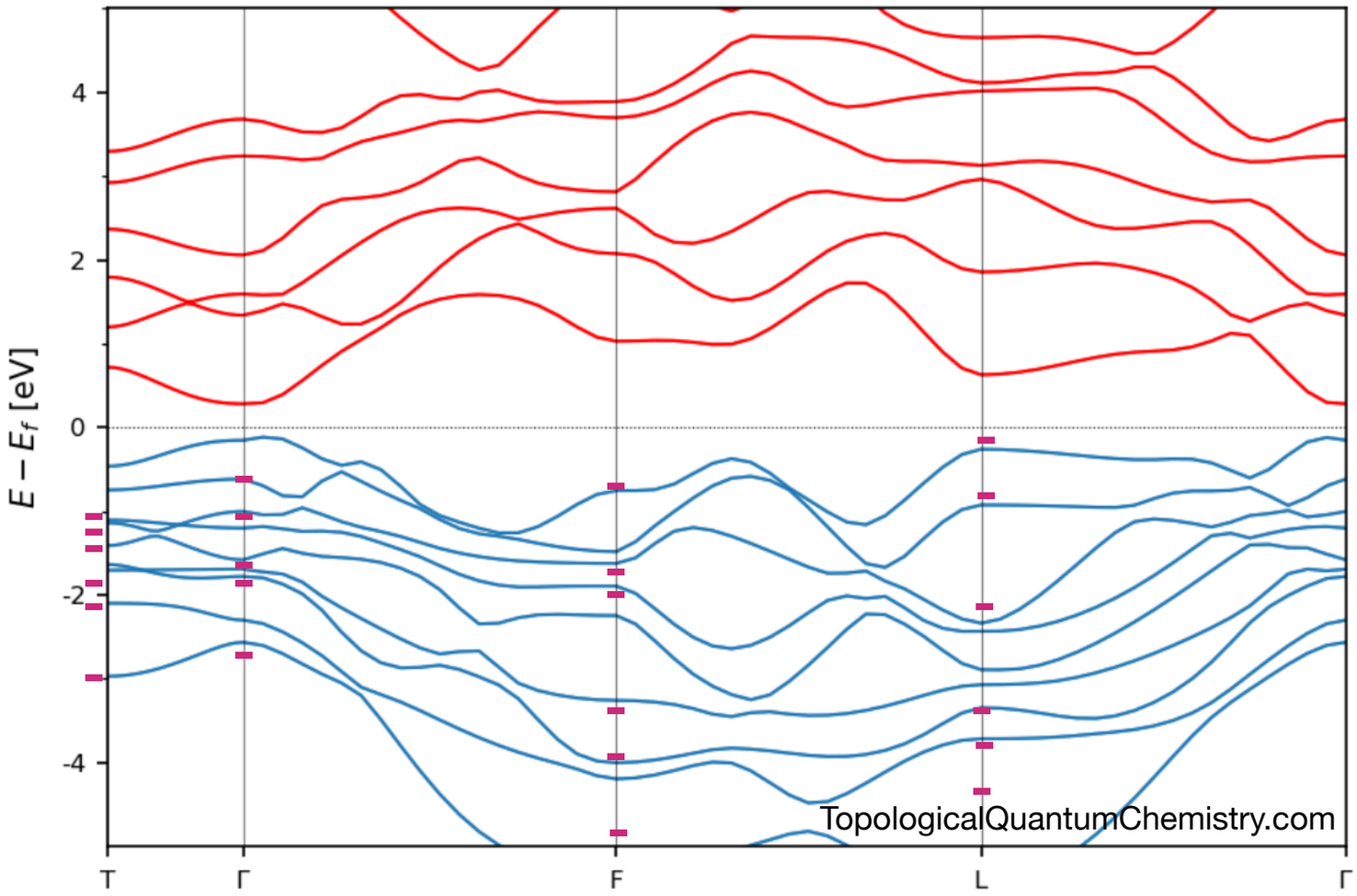
Fu and Kane PRB 76, 045302 (2007)

$$\delta_i = \prod_{m=1}^{N} \xi_{2m}(\Gamma_i)$$ ← At each TRIM (Γ_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:

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

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

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

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

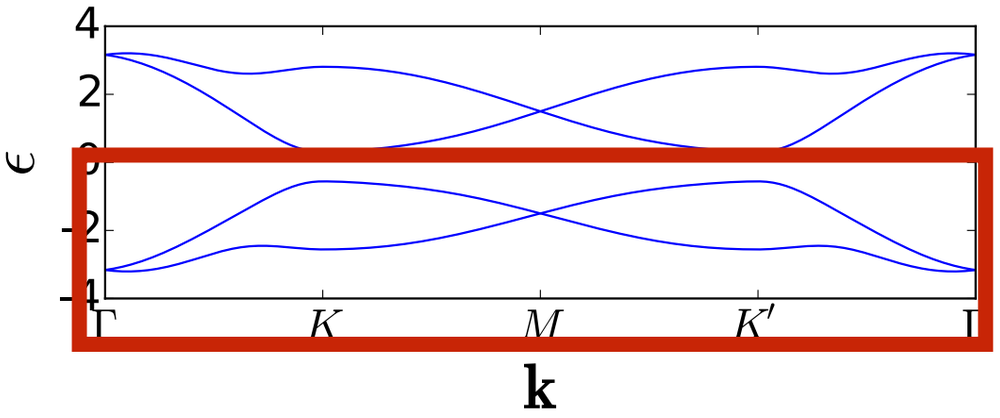
$$\delta_i = \prod_{m=1}^{N} \xi_{2m}(\Gamma_i) \qquad \delta_\Gamma = -1, \delta_L = \delta_F = \delta_T = +1$$

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

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?!



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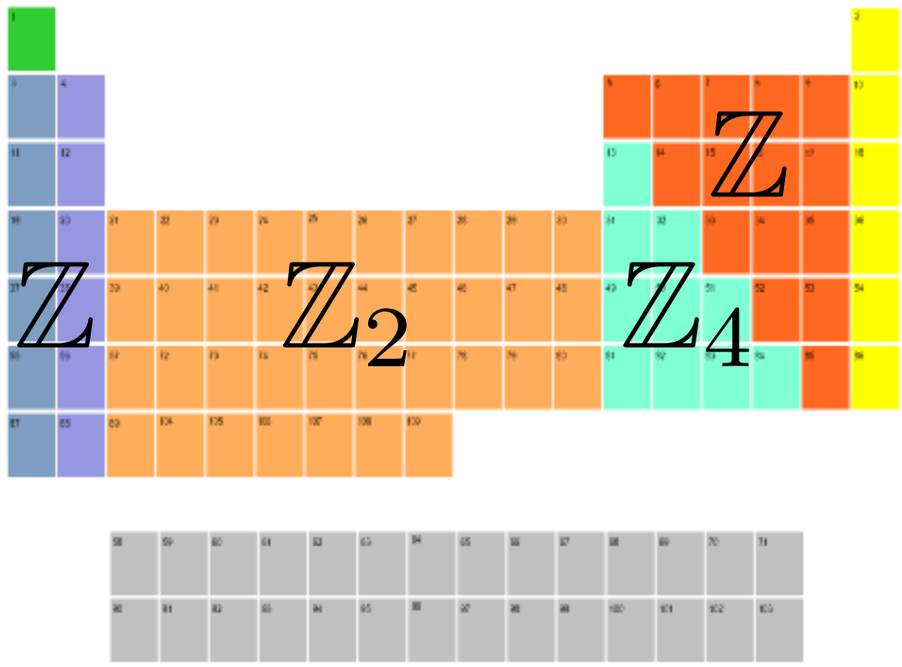


Insight from recent advances in topological band theory of space groups

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)

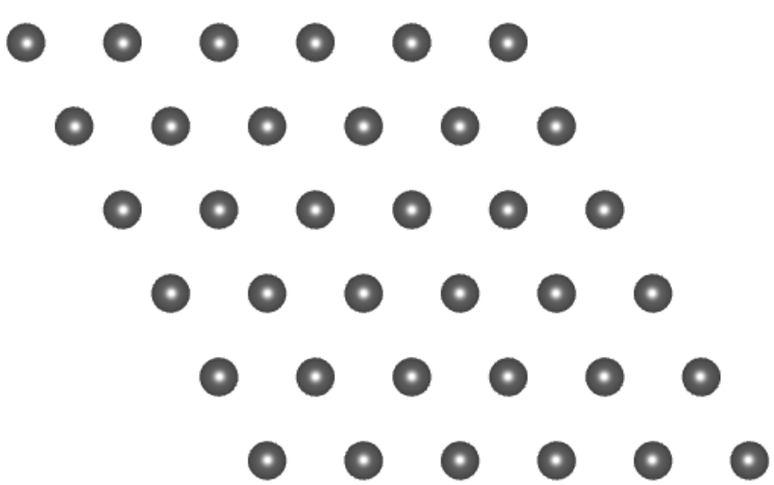
Key: topological bands are not deformable to an atomic limit

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

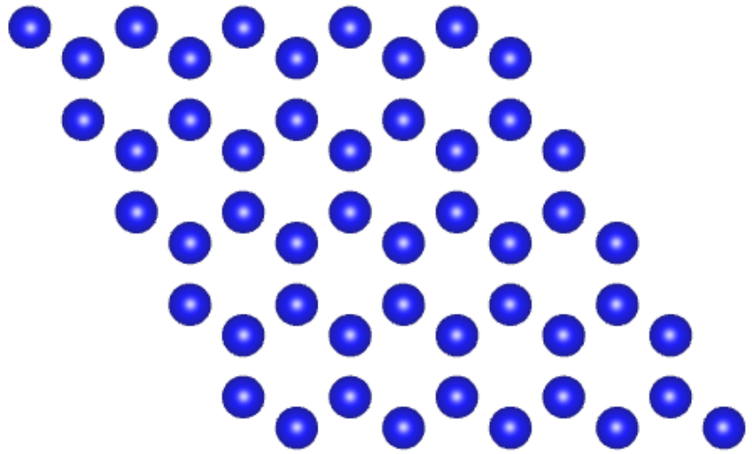
How to identify all atomic limits?

Within one space group, many ways to arrange atoms

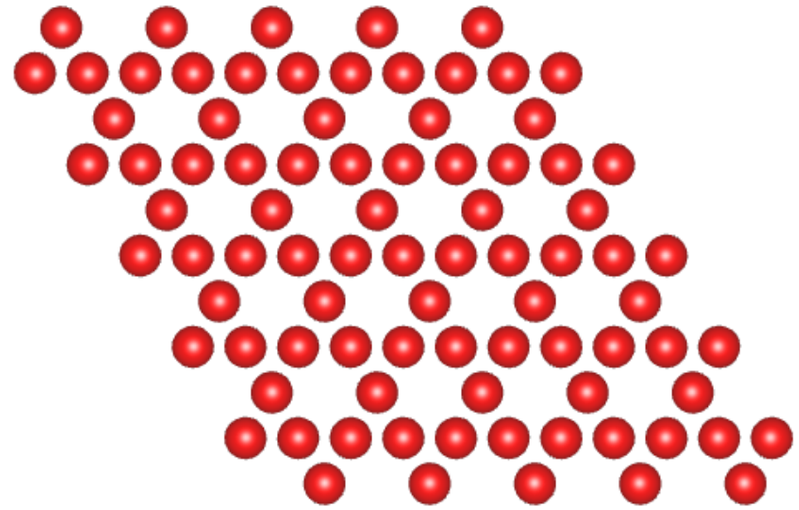
“Wyckoff positions”



1 atom/unit cell
(triangular)



2 atoms/unit cell
(honeycomb)

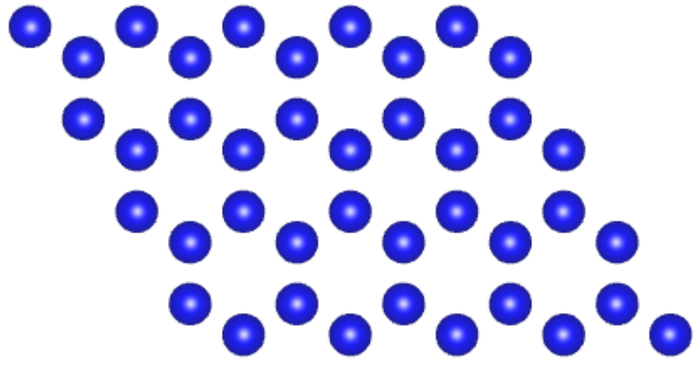


3 atoms/unit cell
(kagome)

All atoms are related by symmetry

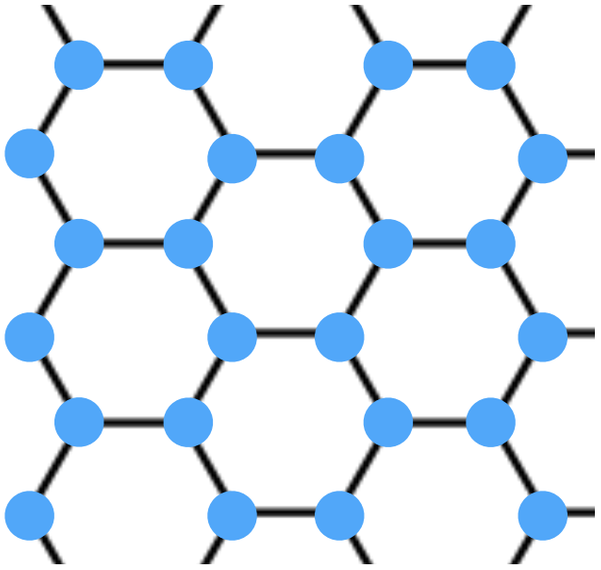
How to identify all atomic limits?

Within one arrangement, many choices of orbitals

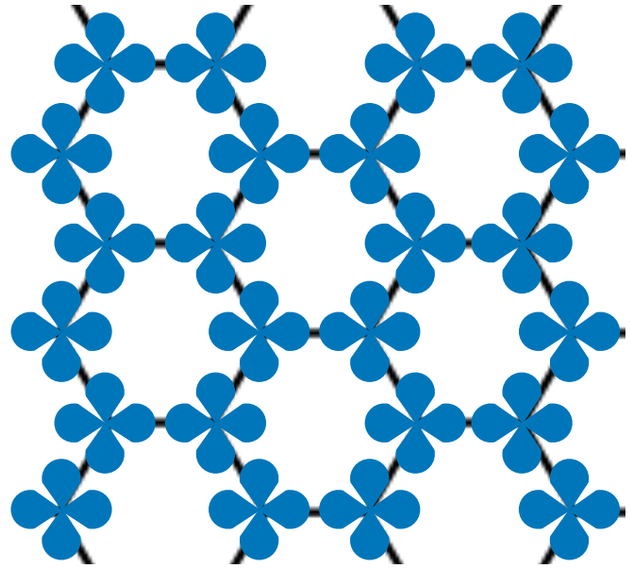


2 atoms/unit cell

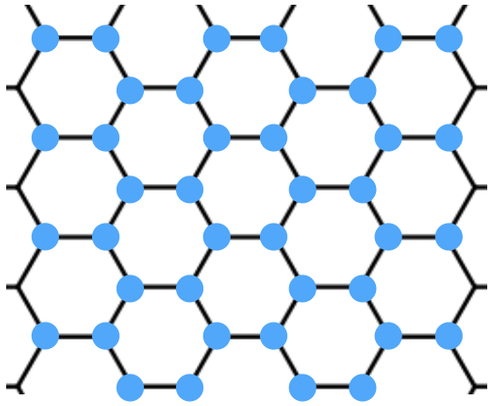
s (or p_z) orbitals



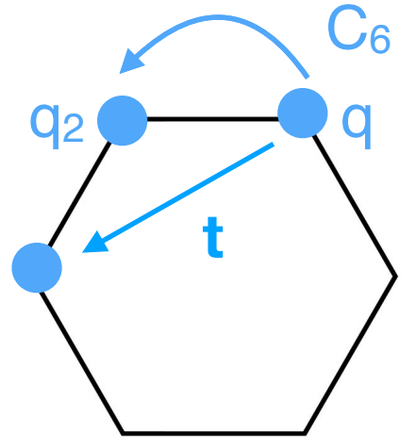
p_x and p_y orbitals



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



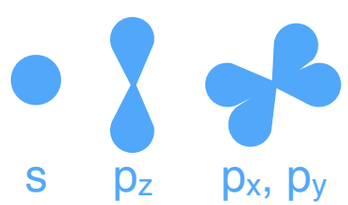
Symmetry of a single site determines symmetry of entire lattice



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

C_3, m_y

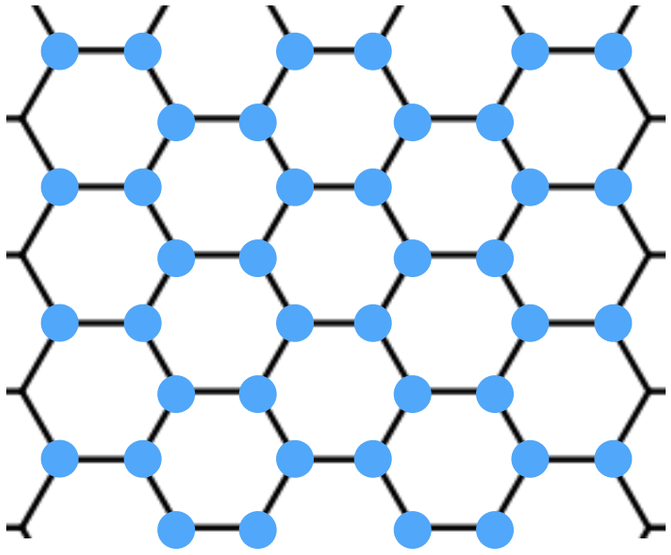
Orbitals at q transform under a rep, $\rho(g)$, of G_q



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

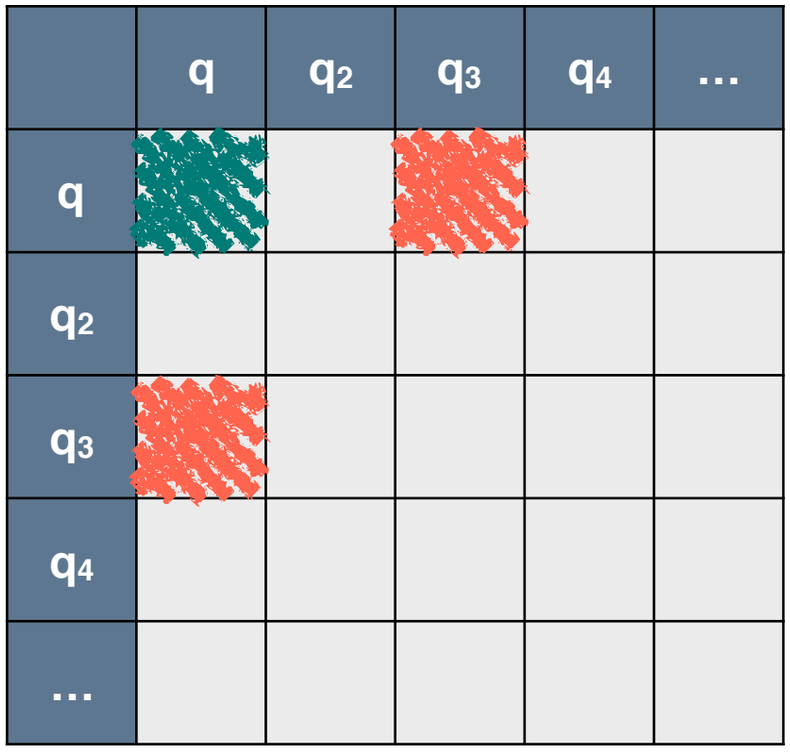
Group theory: induced representation of subgroup uniquely determines representation of group $\mathrm{Ind}_{G_\mathbf{q}}^{G}\rho$

How to construct a band representation:

Each symmetry operation represented by BIG matrix

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

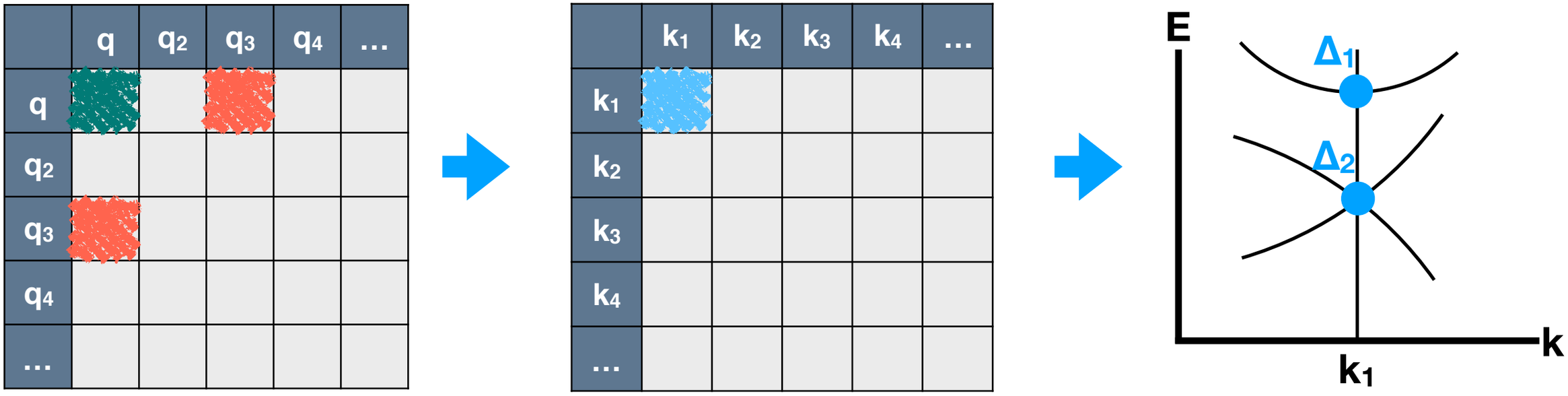
Off-diagonal block if g interchanges sites



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

Zak PRL 1980, PRB 1981, 1982

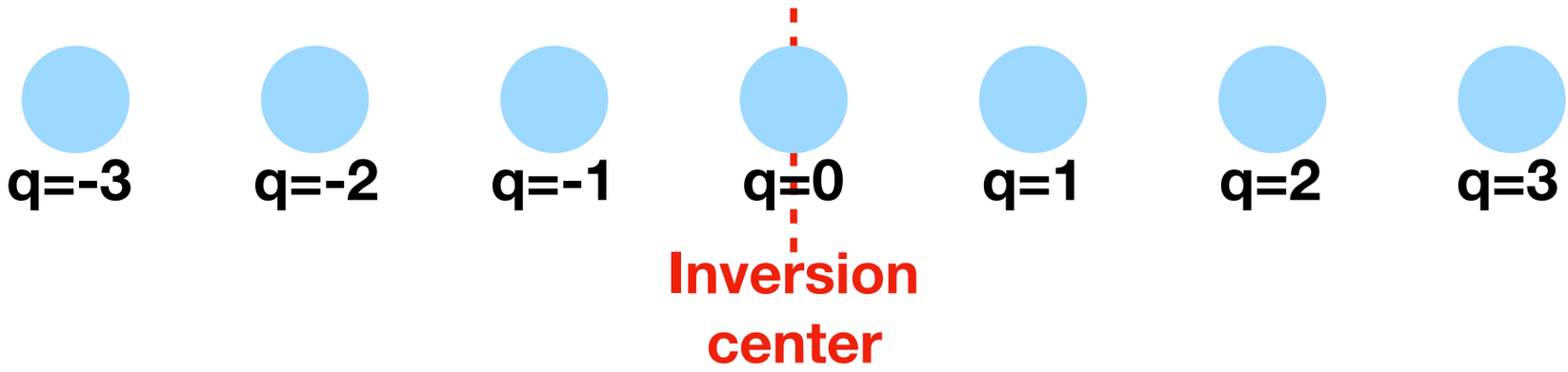
Fourier transforming matrix gives irreps at any k point



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:

Identity

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

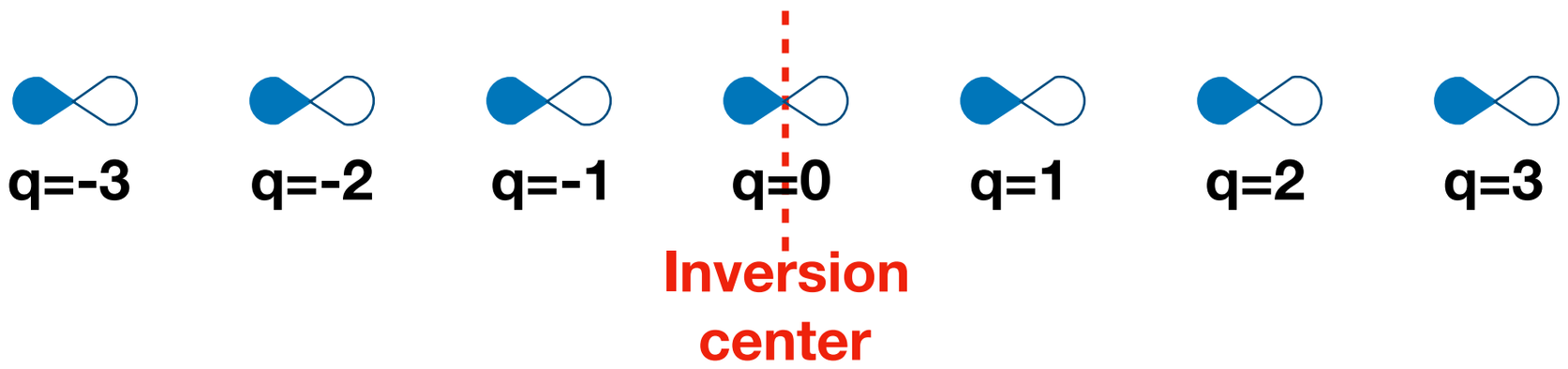
Inversion

…	-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

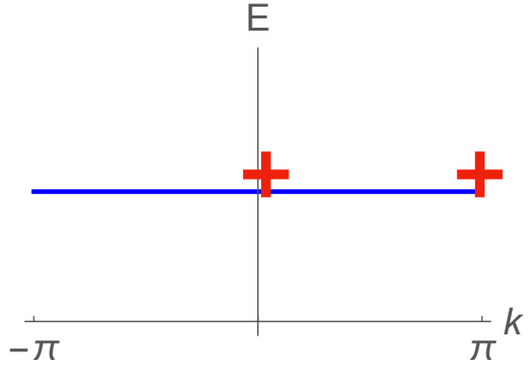
…	-2	-1	0	1	2	…
-2					-1	
-1				-1		
0			-1			
1		-1				
2	-1					
…						

translation by 1

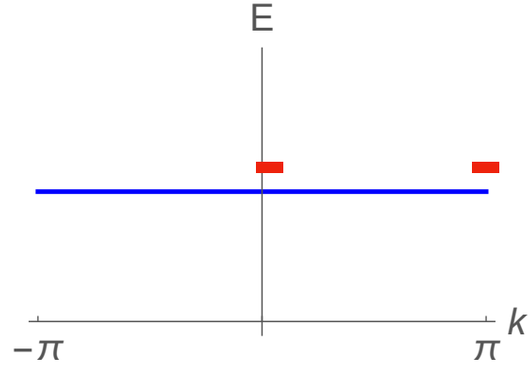
…	-2	-1	0	1	2	…
-2						
-1	1					
0		1				
1			1			
2				1		
…					1	

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

Atomic limit s orbitals:

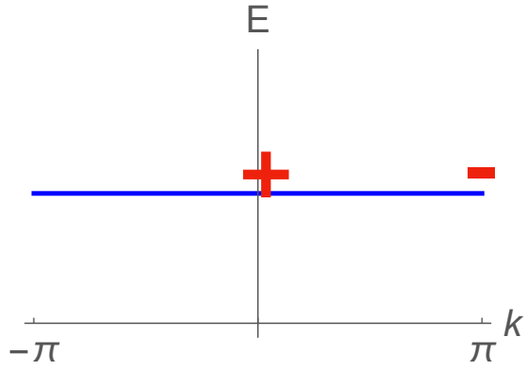


Atomic limit p orbitals:

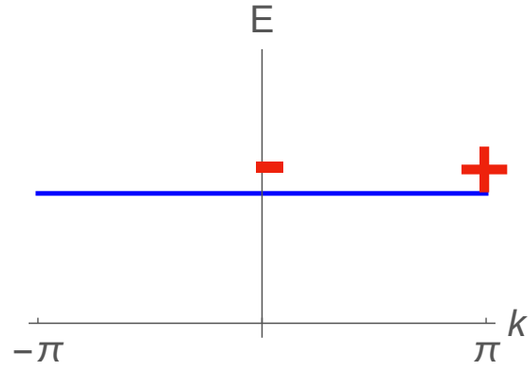


Repeat with atoms shifted by half a unit cell:

Atomic limit s orbitals:



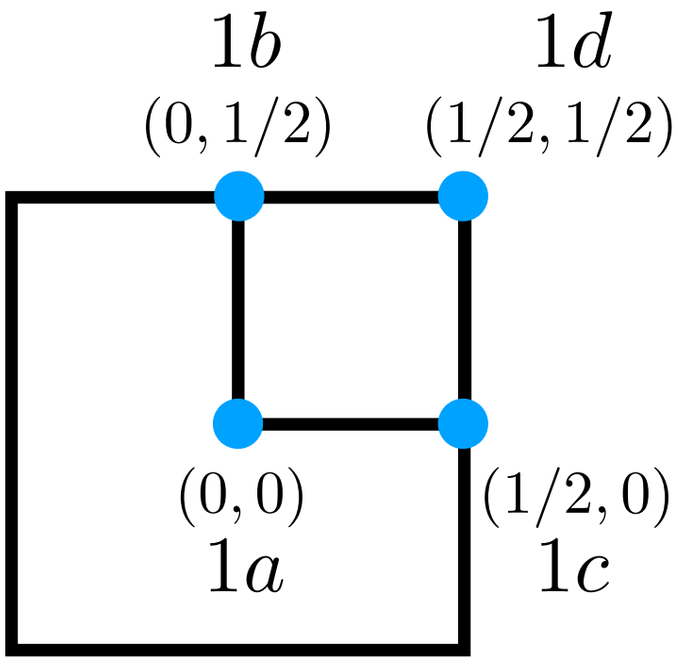
Atomic limit p orbitals:



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:



Negative inversion eigenvalues appear at pairs of TRIMs!

Inversion eigenvalues for *s* orbitals

	(0,0)	(0,π)	(π,0)	(π,π)
1a	+	+	+	+
1b	+	−	+	−
1c	+	+	−	−
1d	+	−	−	+

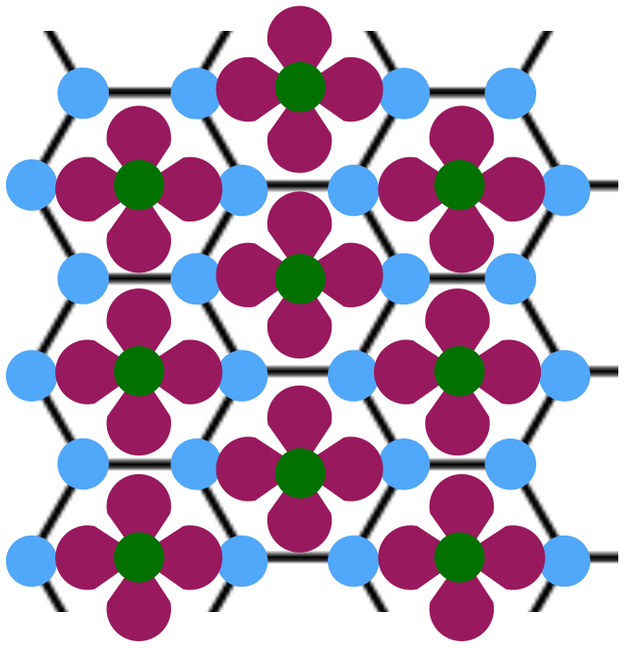
Inversion eigenvalues for *p* orbitals

	(0,0)	(0,π)	(π,0)	(π,π)
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 all atomic limit phases for all space groups

Problem: there are infinitely many atomic limits!



$$\Gamma_1, \Gamma_4, K_3, M_1, M_4\,, \Gamma_6, K_3, M_3, M_4\,, \Gamma_1, K_1, M_1$$

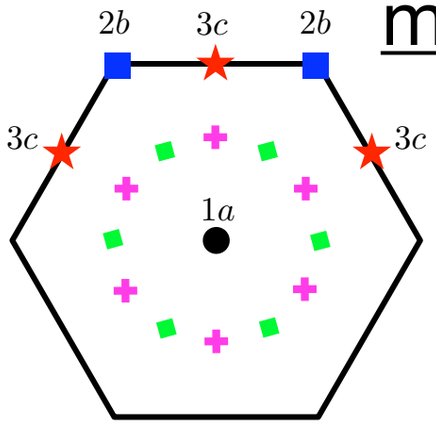
Elementary band representations do not decompose into sum of band representations

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



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

$$K \subset H \subset G$$

⇒ Symmetry labels of atomic limits can be obtained by adding EBRs

⇒ 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

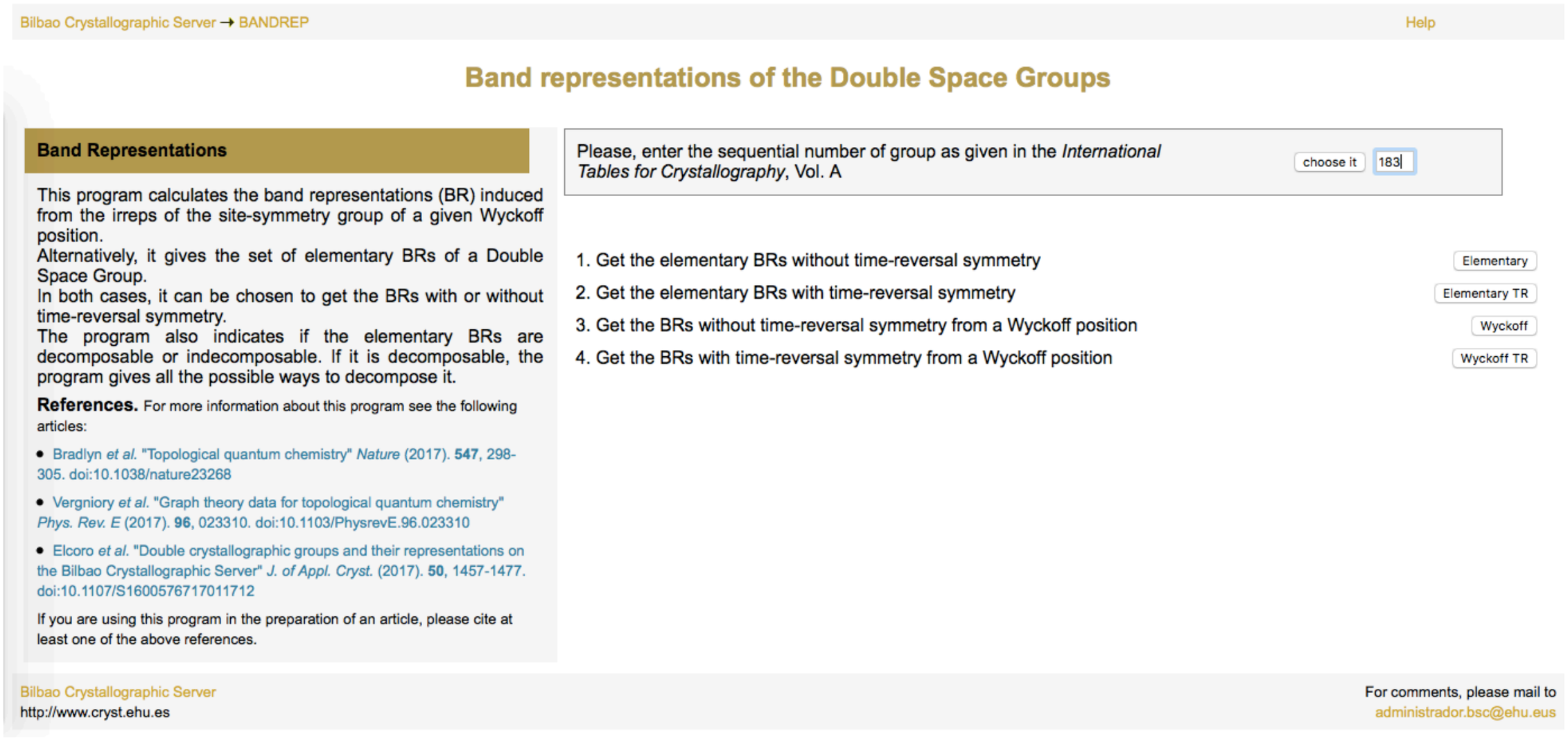
Symmetry labels for all EBRs are enumerated on the Bilbao Crystallographic Server

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

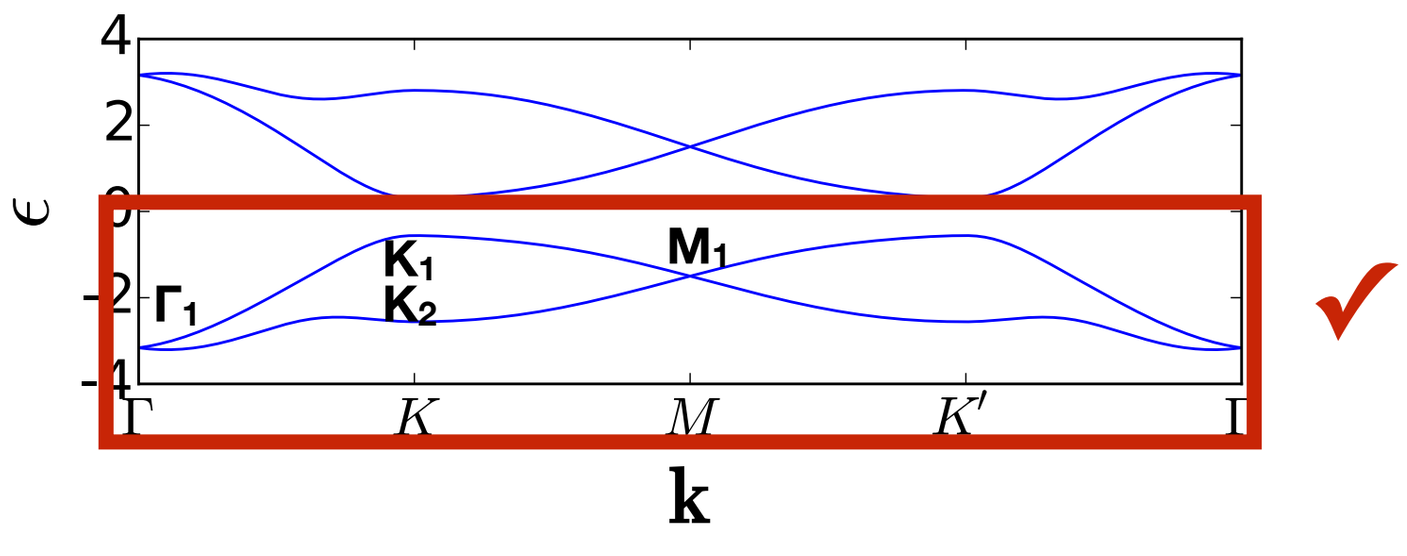
Show all types of k-vectors

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:

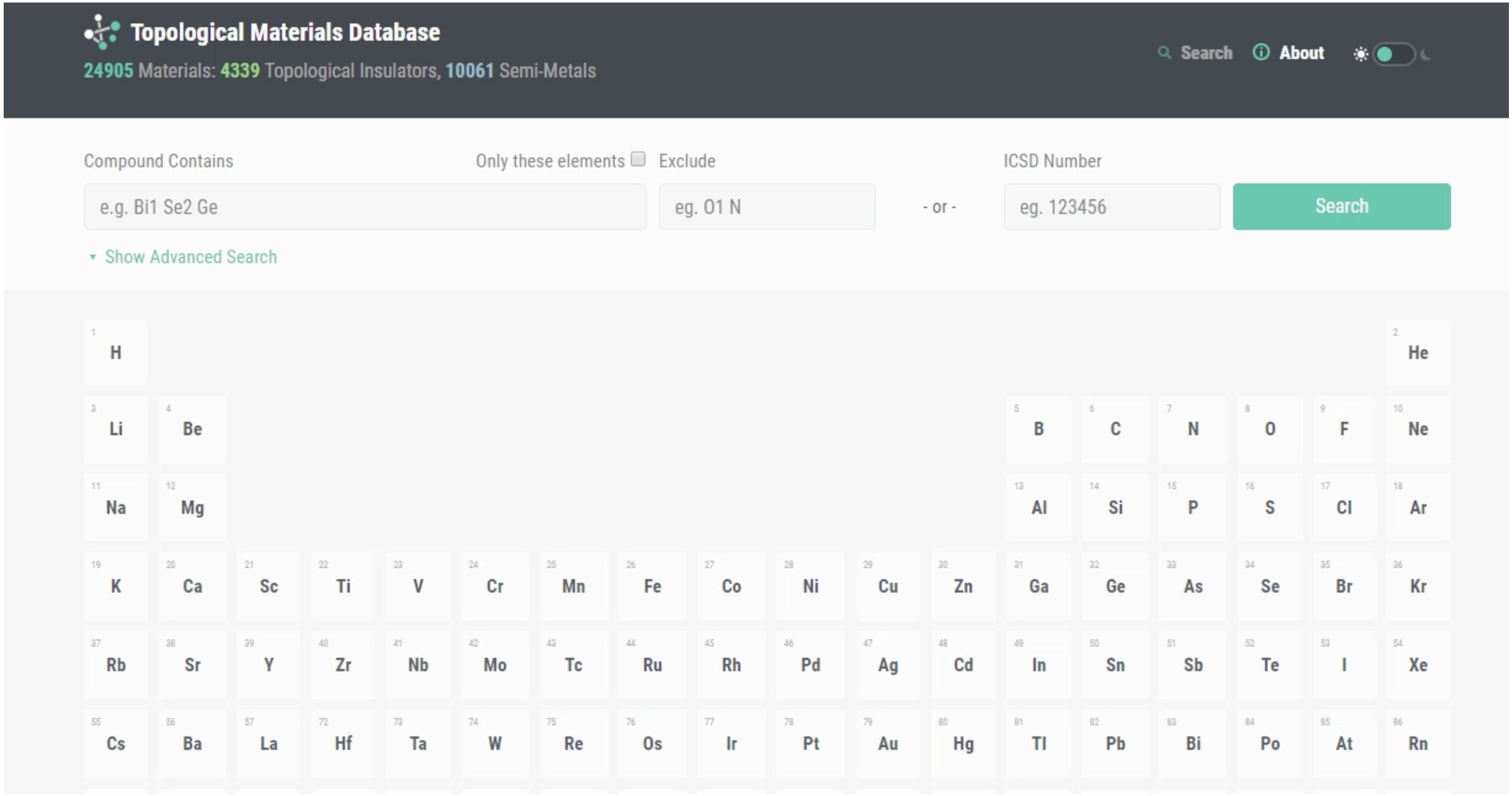
For every known chemical compound:

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

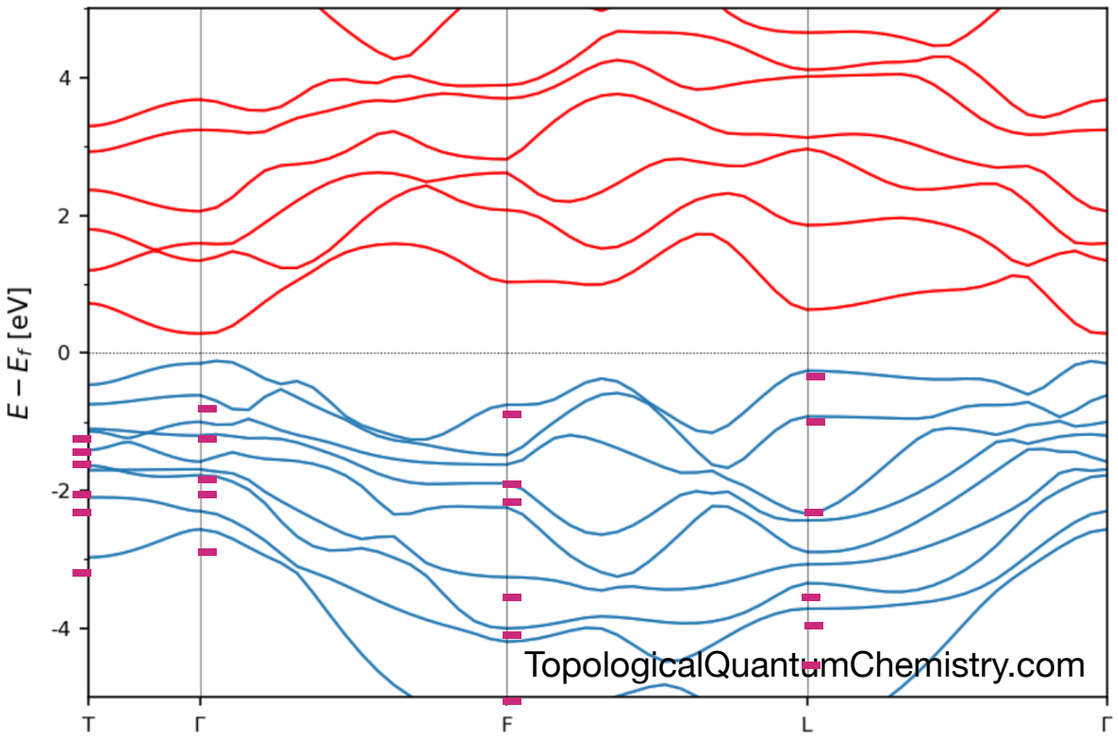
2019: Databases of topological materials

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

Materiae: http://materiae.iphy.ac.cn
(Zhang, Jiang, Song, Huang, He, Fang, Weng, Fang, *Nature* 566, 475 (2019))



Summary



Crystal symmetry can protect and identify topological phases

Exs: mirror Chern, inversion formula, …

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

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