Topological Quantum Chemistry

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Bradlyn et al, *Nature* 547, 298–305 (ArXiv:1703.02050)
Vergniory et al, Phys Rev E 96, 023310 (ArXiv:1706.08529)
Elcoro et al, J. Appl. Cryst. 50, 1457 (ArXiv:1706.09272),
Cano et al (ArXiv:1709.01935),
Bradlyn et al (ArXiv:1709.01937)

ICMT workshop

Collaborators

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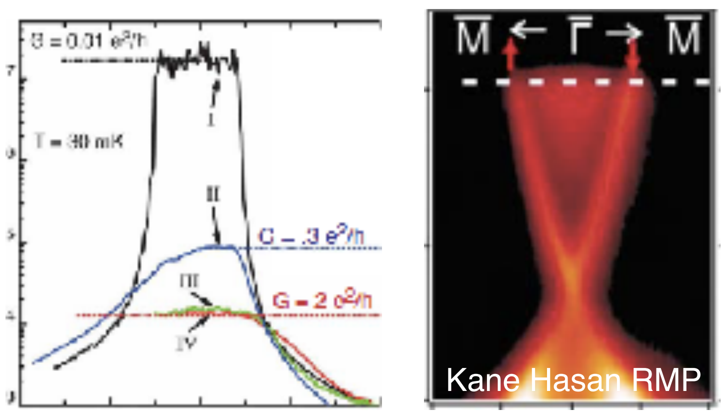
(Max Planck)

Mois Aroyo (EHU)

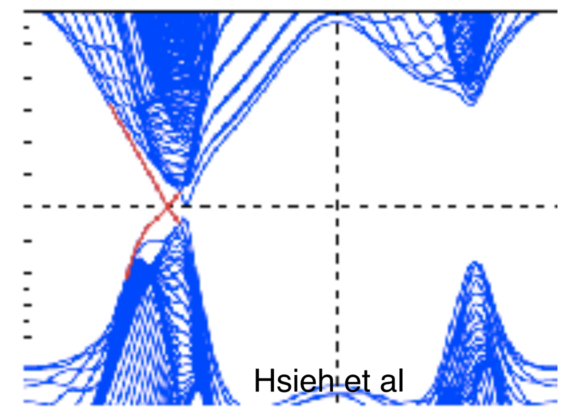
Luis Elcoro (EHU)

Andrei Bernevig
(Princeton)



$\mathbb{Z}_2$

Topological insulators

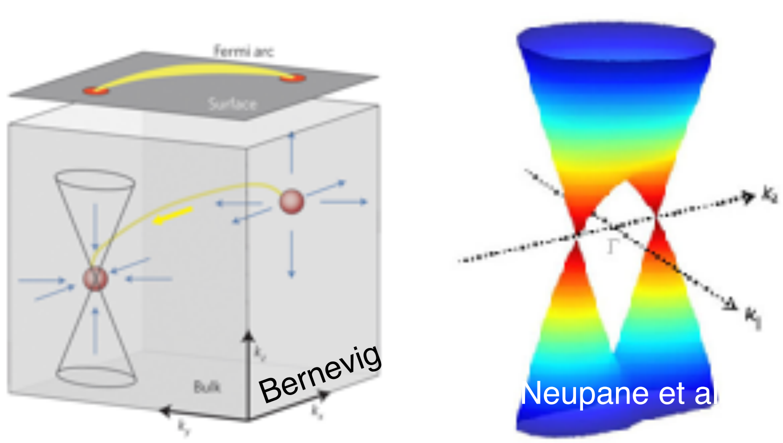


$\mathbb{Z}$

Mirror Chern Insulator

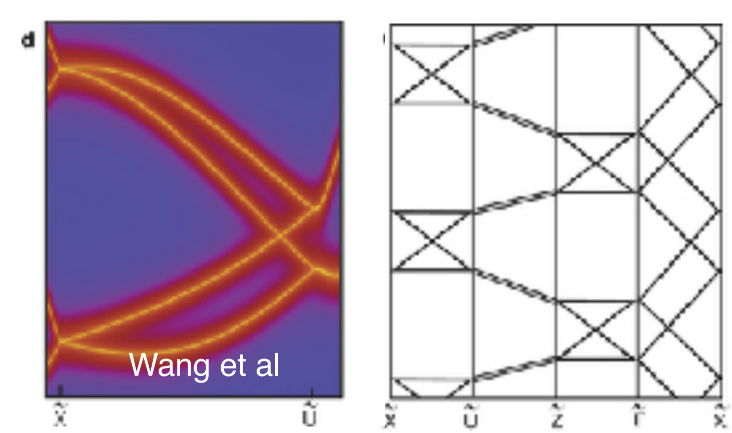
Topological Insulators and Topological Semimetals

$\mathbb{Z}$



$\mathbb{Z}_2$

Weyl and Dirac fermions



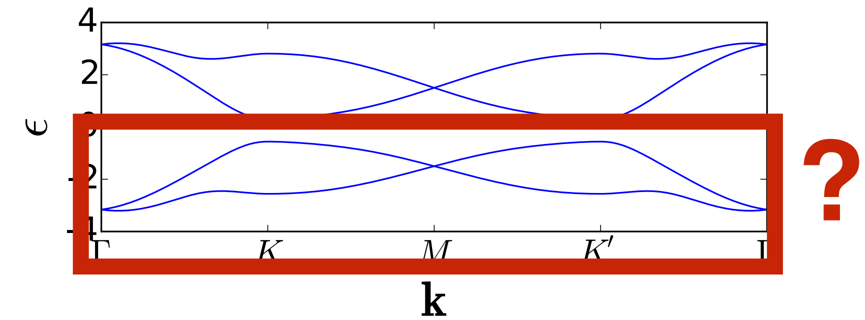
$\mathbb{Z}_4$

Hourglass fermions

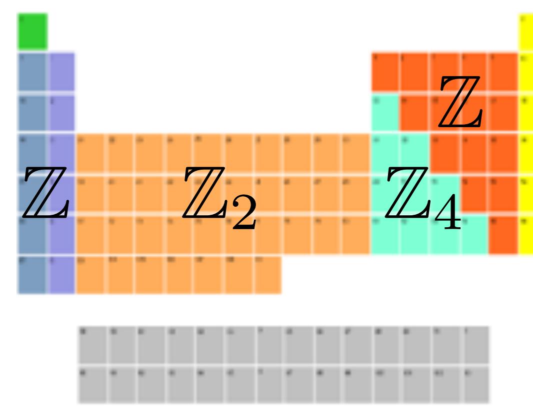
Piecewise classification of topological (crystalline) insulators

Open questions:

How do we know when the classification is complete?



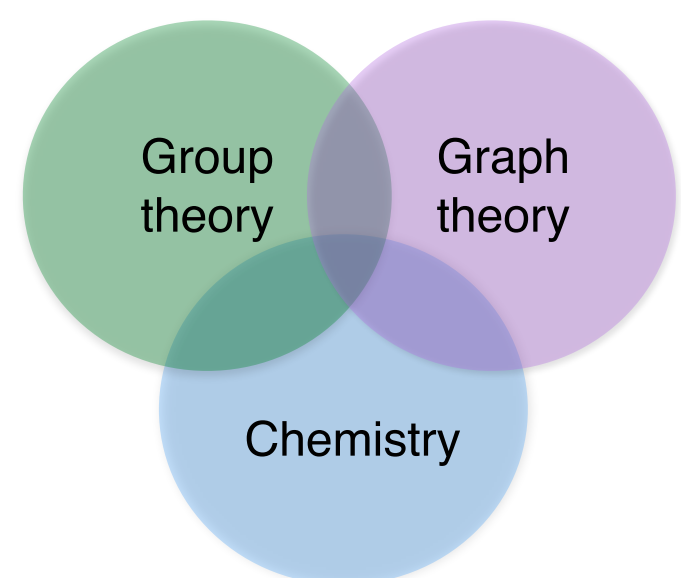
How can we find topological materials?



200000 materials in ICSD database:

100 time reversal topological insulators
10 mirror Chern insulators
15 Weyl semimetals
15 Dirac semimetals
3 Non-Symmorphic topological insulators

Set of measure zero…
Are topological materials that esoteric?



We propose a classification that captures all crystal symmetries and has predictive power

Recall: a space group is a set of symmetries that defines a crystal structure in 3D

Consists of:

- unit lattice translations (Z^3)
- point group operations (rotations, reflections)
- non-symmorphic (screw, glide)

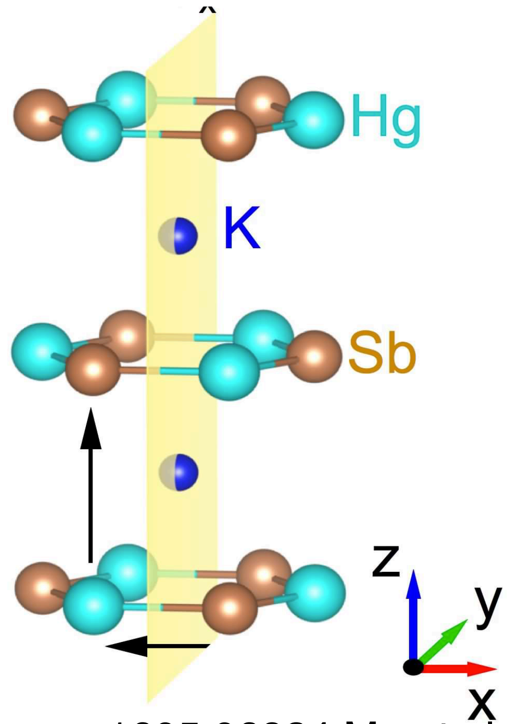
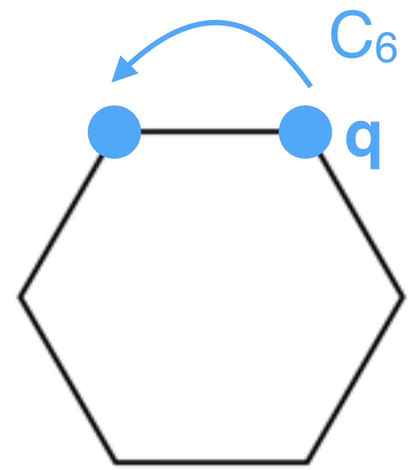


Image: 1605.06824 Ma et al

230 space groups

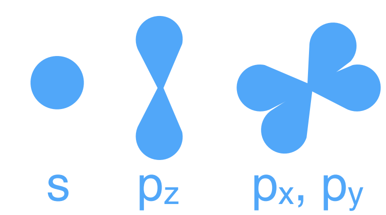
Given a space group, how to define an atomic limit?

Consider one lattice site:



Site-symmetry group: $G_{\mathbf{q}}$, leaves **q** invariant C_3, m_y

Orbitals at **q** transform under a rep, ρ, of $G_{\mathbf{q}}$

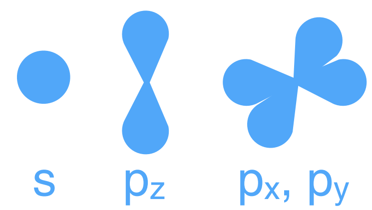


Elements of space group $g \notin G_{\mathbf{q}}$ move sites in an orbit "Wyckoff position" C_6

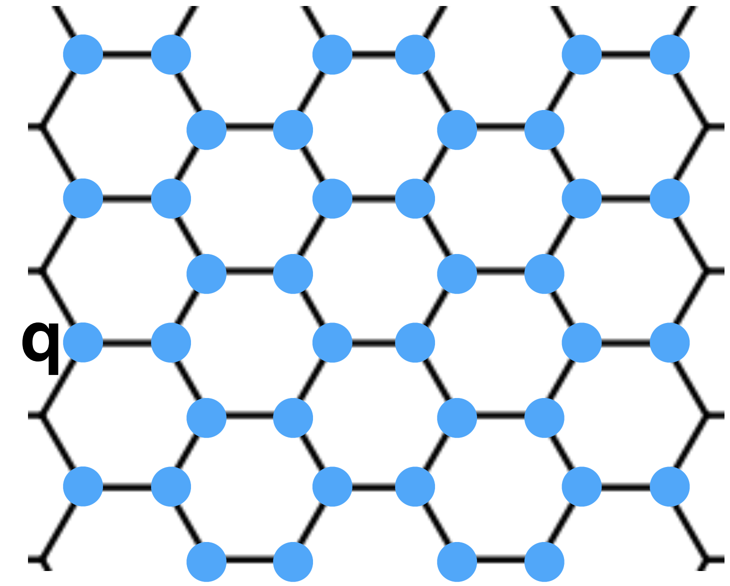
Each Wyckoff position and irrep of $G_{\mathbf{q}}$ define an atomic limit

The orbital symmetry and Wyckoff position determine the irreps that at high-symmetry points in the Brillouin zone

1. Orbitals at **q** described by ρ, a representation of $G_{\mathbf{q}}$



ρ describes an orbital



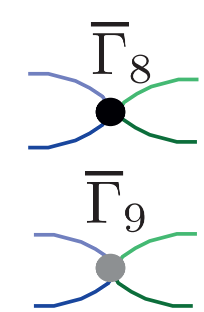
2. ρ induces a rep. of the full space group

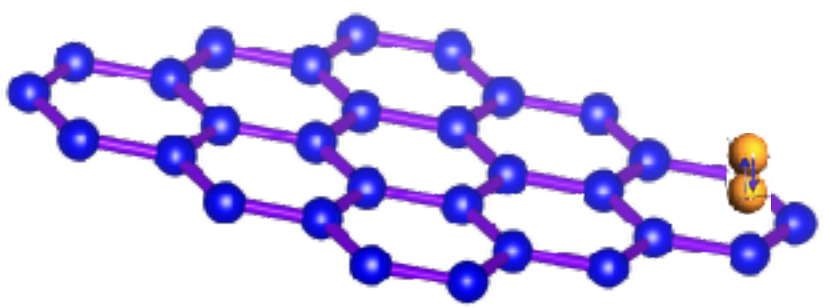
$$\rho \uparrow G$$ "band representation"

determines how orbitals transform into each other under full space group

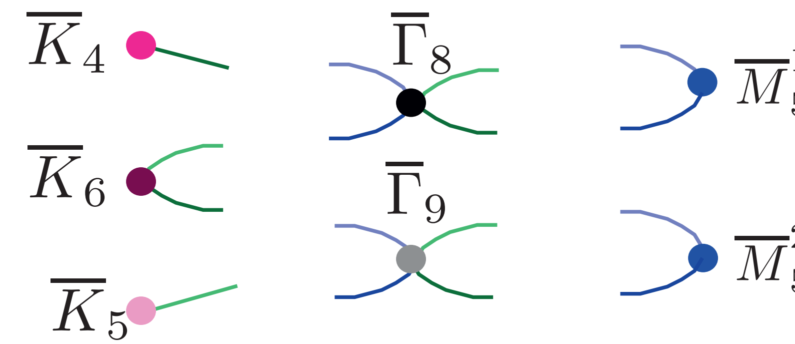
3. Band representation restricts to little group at **k**, $G_{\mathbf{k}}$

$$(\rho \uparrow G) \downarrow G_{\mathbf{k}}$$ determines irreps that appear at **k**





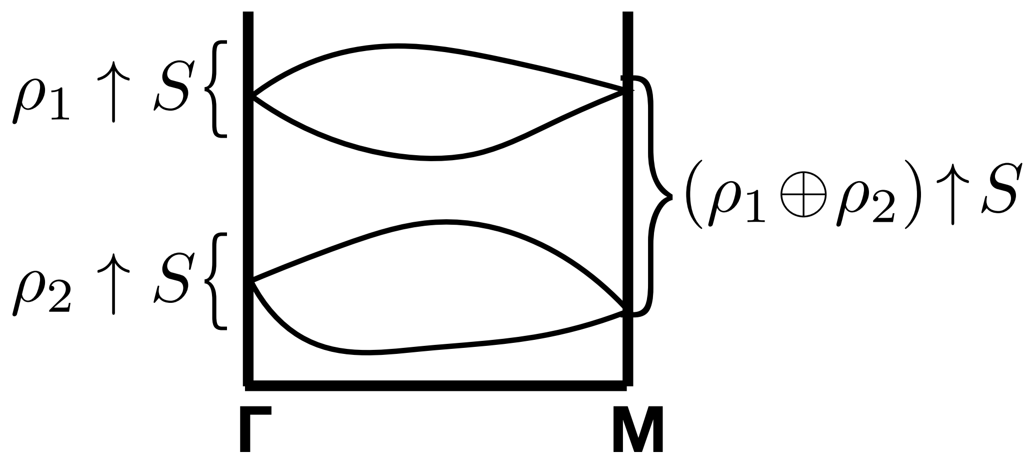
Real space: orbitals and symmetries



Momentum space: k.p
Irreps/degeneracies uniquely determined

Enumerating all atomic limit band structures serves as a classification…..
What does it mean to consider ALL atomic limits?

Band representations can decompose



Distributive:

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

Transitive:

$$(\rho \uparrow H) \uparrow G = \rho \uparrow G, \quad H \subset G$$

Elementary band representations are
those that cannot be decomposed

Zak PRL 1980

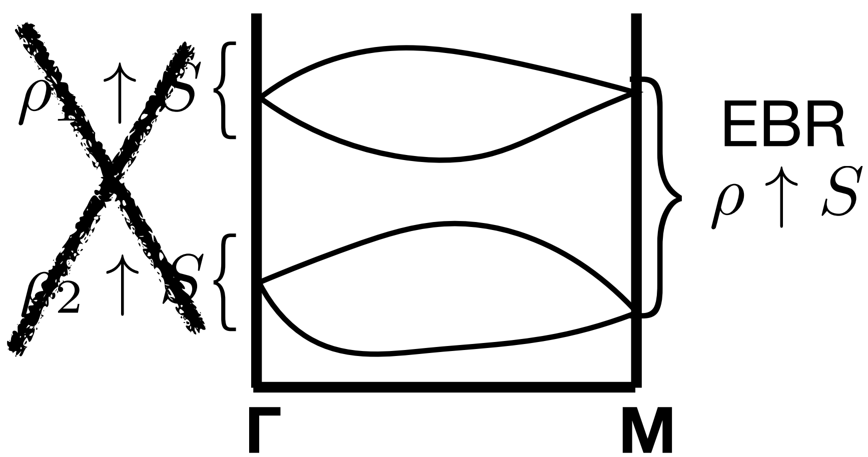
We have enumerated all elementary band
representations and their irreps at high-symmetry points

Bradlyn, **JC**, et al., *Nature* 547, 298–305;
JC et al., ArXiv:1709.01935

Elementary band representations are special

Bands in an elementary band representation might be connected or disconnected

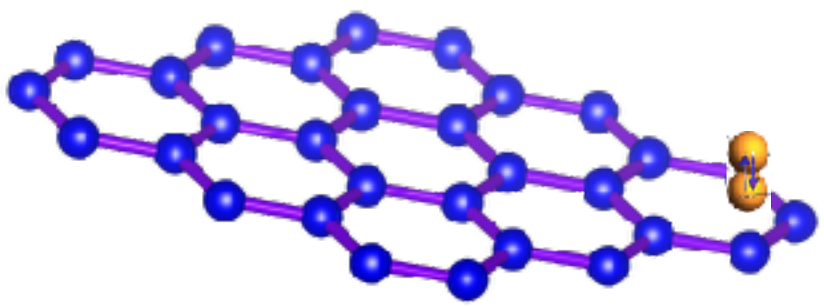
If disconnected, some or all bands are topological



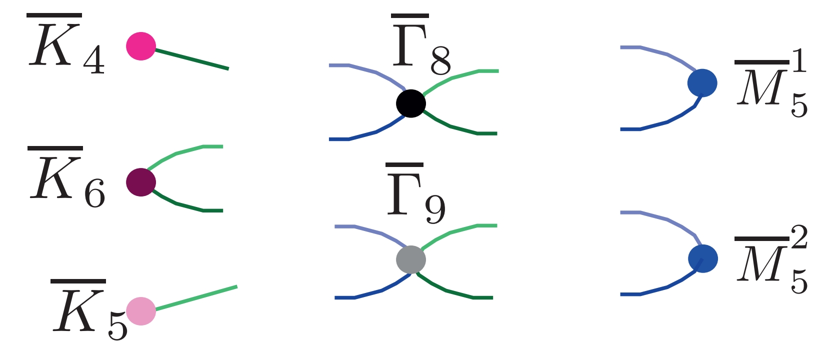
Proof by contradiction:
if they could decompose into atomic limit bands, then would not have been elementary

Bradlyn, **JC** et al., *Nature* 547, 298–305;
JC et al., ArXiv:1709.01935

Completes research program by Zak and Michel from 1999, 2000, 2001



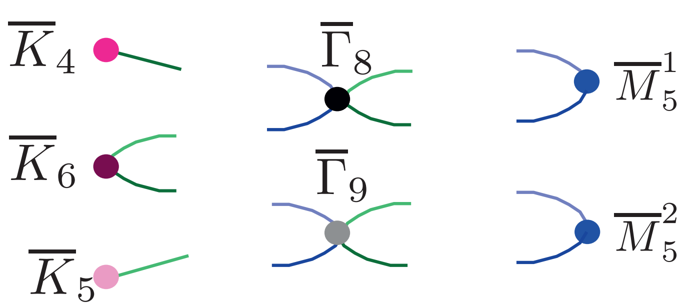
Real space: orbitals and symmetries



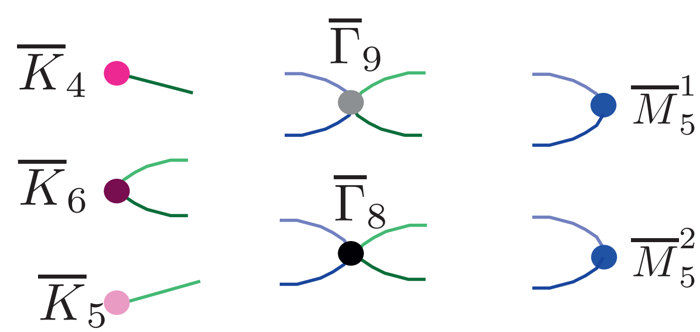
Momentum space: k.p

Irreps/degeneracies uniquely determined

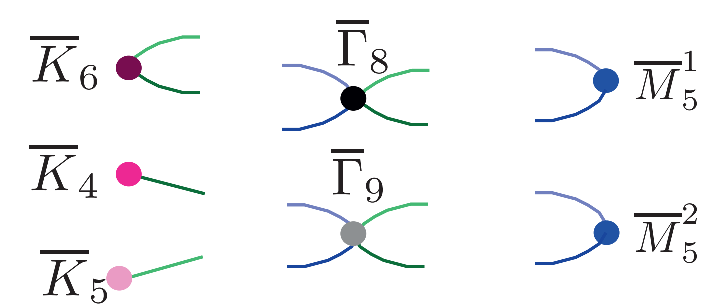
Only based on symmetry — haven't inputted energetics!



or

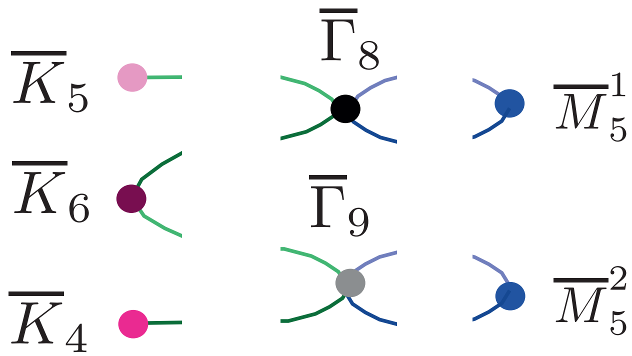


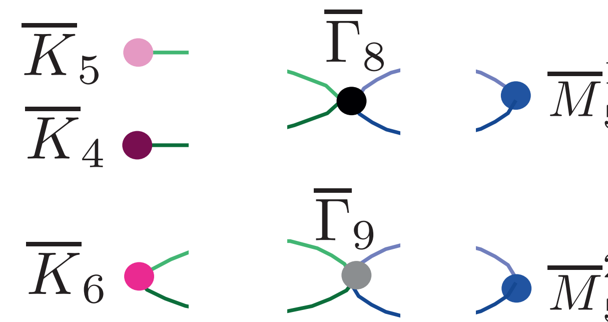
or



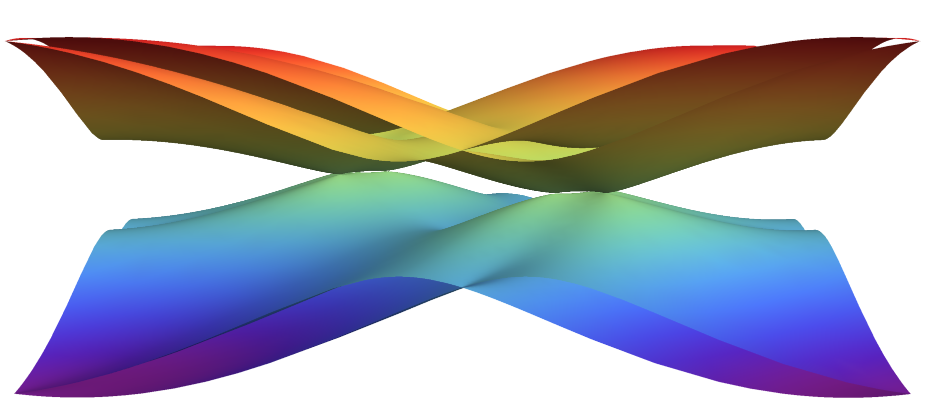
…

So far, we have only used symmetry, not energetics

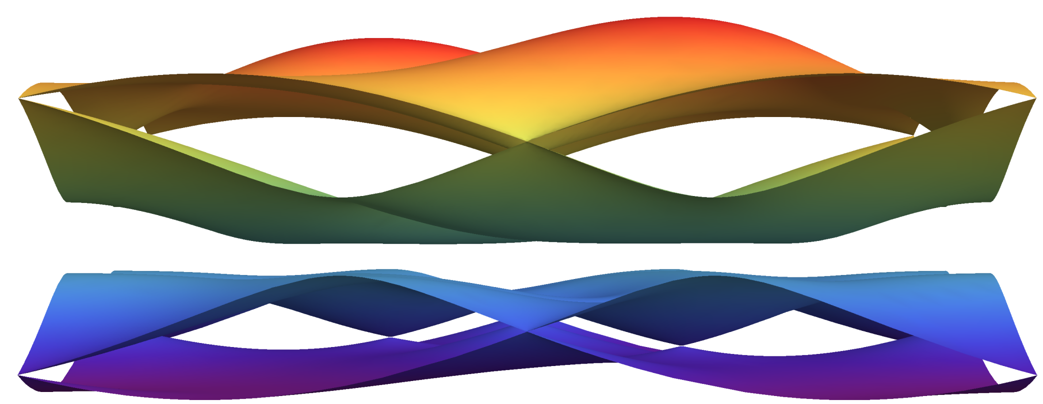




Energy ordering can change band connectivity



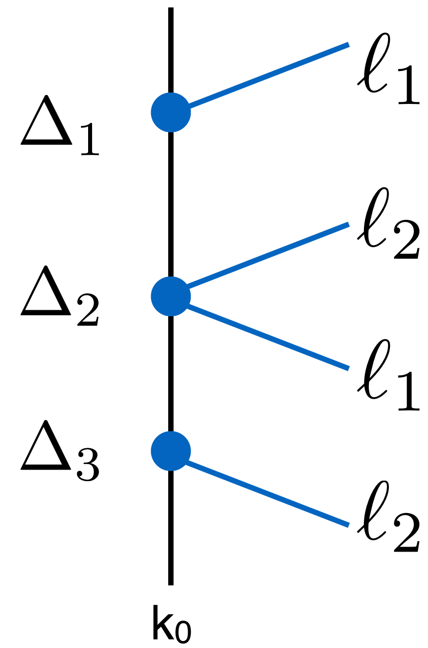
Symmetry enforced semi-metal



Topological insulator

Want to determine **connectivity** for each set of atomic limit bands

"Little group" of k0: $\mathcal{G}\mathbf{k}_0 = \mathbf{k}_0$



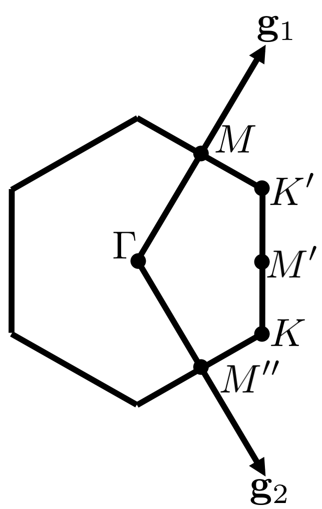
Eigenstates transform under little group irreps

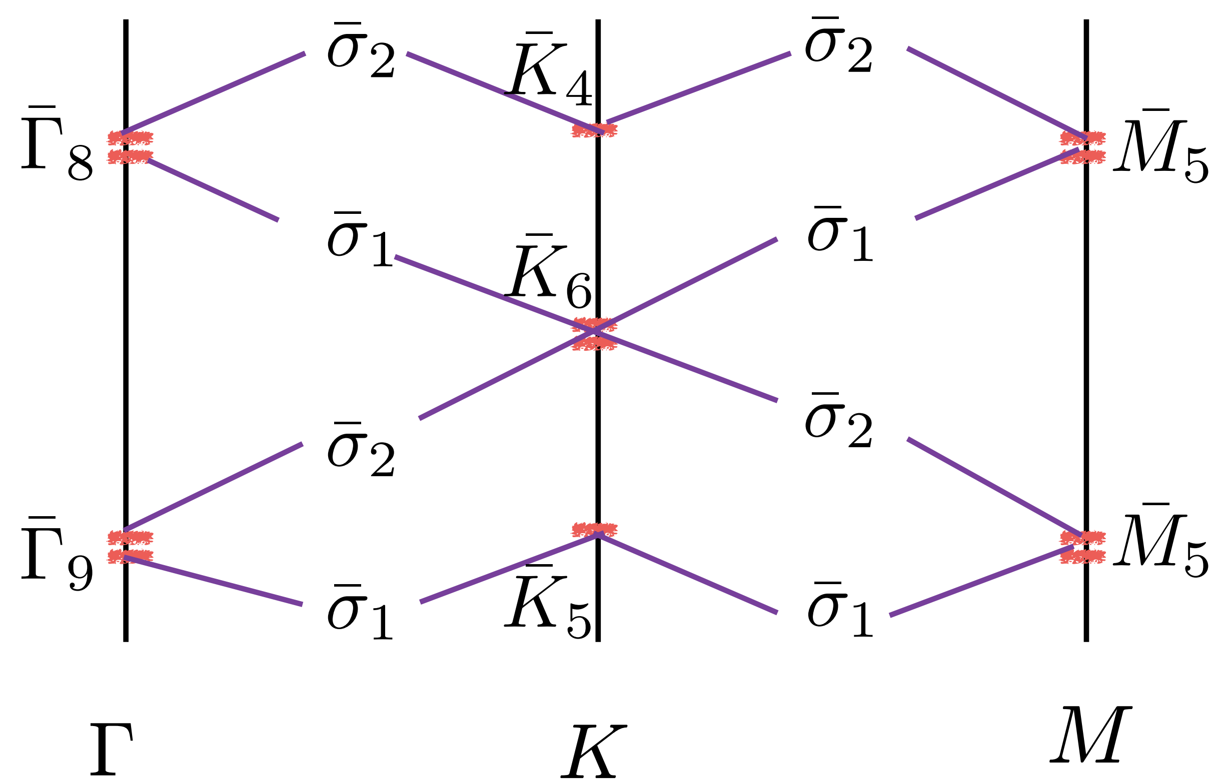
Irreps at k_0 determine irreps along lines emanating from k_0

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

Compatibility relations
between points and lines

Compatibility relations determine connectivity between different k





Allowed band structures:

- Compatibility between points and lines
- One label per line segment

Enumerating all possible band connectivities is a huge problem!

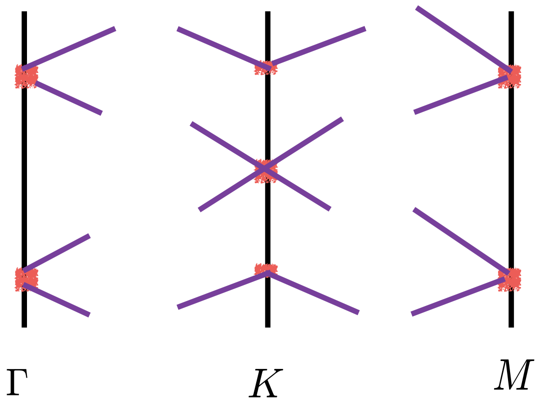
230 space groups

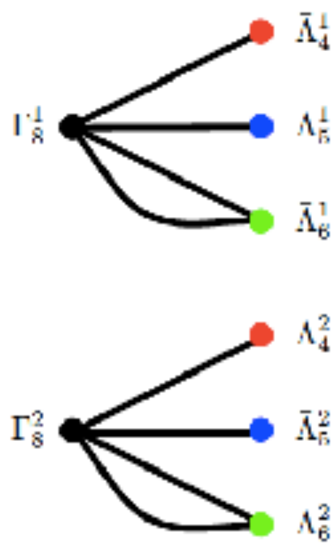
Each space group has several (1 to 4) maximal Wyckoff positions

Symmetry group of each position has several irreps

For each combination: permute irreps at each point and check compatibility

To enumerate all allowed band connectivities: map to graph theory





Input: irreps at high-symmetry points and lines

Map: irreps ⇨ graph nodes

Enumerate allowed graphs

For each matrix, null vectors gives graph connectivity

Map: graph connectivity ⇨ band connectivity

Output: list of distinct band connectivities

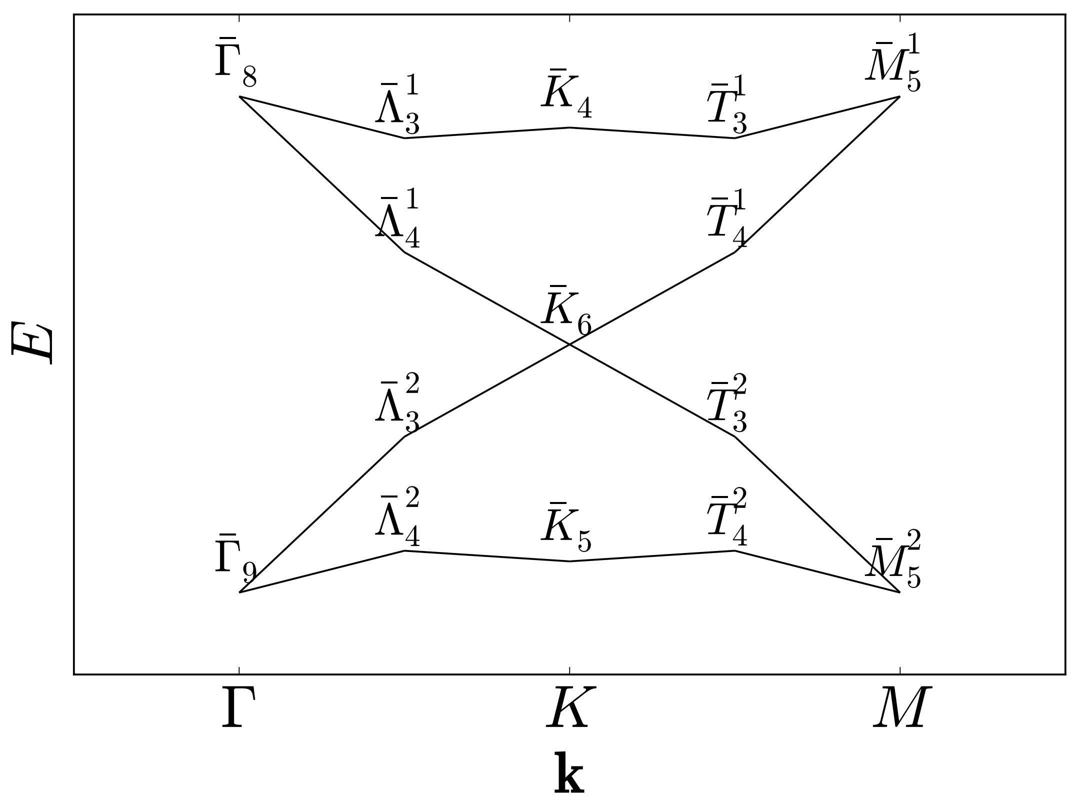
MGV, **JC**, et al., Phys. Rev. E 96, 023310 (2017)
BB, **JC,** arXiv:1709.01937

Graph is represented by a matrix

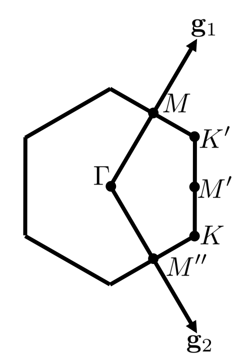
$A_1 =$

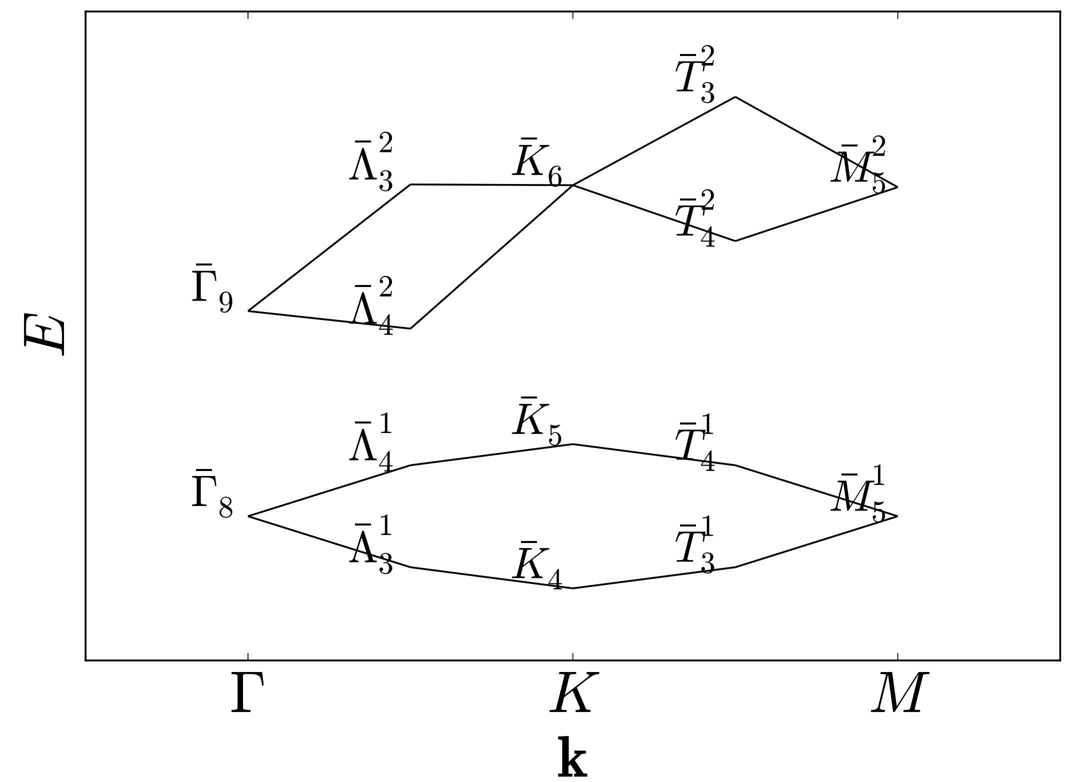
	$\bar{\Gamma}_8$	$\bar{\Gamma}_9$	$\bar{\Sigma}_3^1$	$\bar{\Sigma}_3^2$	$\bar{\Sigma}_4^1$	$\bar{\Sigma}_4^2$	$\bar{\Lambda}_3^1$	$\bar{\Lambda}_3^2$	$\bar{\Lambda}_4^1$	$\bar{\Lambda}_4^2$	$\bar{K}_4$	$\bar{K}_5$	$\bar{K}_6$	$\bar{T}_3^1$	$\bar{T}_3^2$	$\bar{T}_4^1$	$\bar{T}_4^2$	$\bar{M}_5^1$	$\bar{M}_5^2$
$\bar{\Gamma}_8$	0	0	1	0	1	0	1	0	1	0	0	0	0	0	0	0	0	0	0
$\bar{\Gamma}_9$	0	0	0	1	0	1	0	1	0	1	0	0	0	0	0	0	0	0	0
$\bar{\Sigma}_3^1$	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
$\bar{\Sigma}_3^2$	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
$\bar{\Sigma}_4^1$	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
$\bar{\Sigma}_4^2$	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
$\bar{\Lambda}_3^1$	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
$\bar{\Lambda}_3^2$	0	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
$\bar{\Lambda}_4^1$	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
$\bar{\Lambda}_4^2$	0	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
$\bar{K}_4$	0	0	0	0	0	0	1	0	0	0	0	0	0	1	0	0	0	0	0
$\bar{K}_5$	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	1	0	0
$\bar{K}_6$	0	0	0	0	0	0	0	1	1	0	0	0	0	0	1	1	0	0	0
$\bar{T}_3^1$	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	1	0
$\bar{T}_3^2$	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1
$\bar{T}_4^1$	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0
$\bar{T}_4^2$	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	1
$\bar{M}_5^1$	0	0	1	0	1	0	0	0	0	0	0	0	0	1	0	1	0	0	0
$\bar{M}_5^2$	0	0	0	1	0	1	0	0	0	0	0	0	0	0	1	0	1	0	0

Example output: graphene



Semi-metallic phase





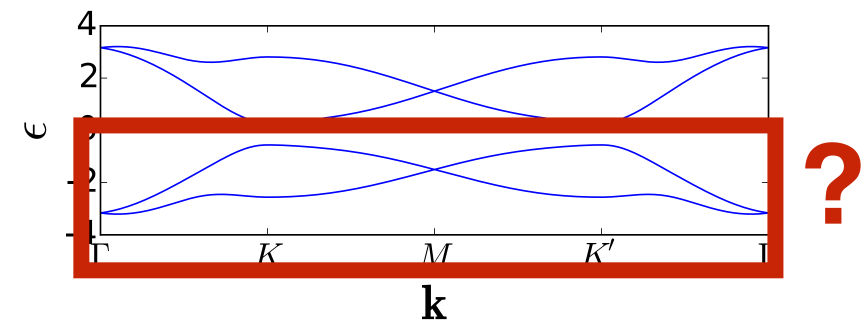
Topological phase

Algorithm enumerates topological insulators and symmetry-protected semi-metals

We computed connectivity for all 10,000 elementary band representations

How to use this information?

1. List of ~~topological~~ trivial invariants for each space group

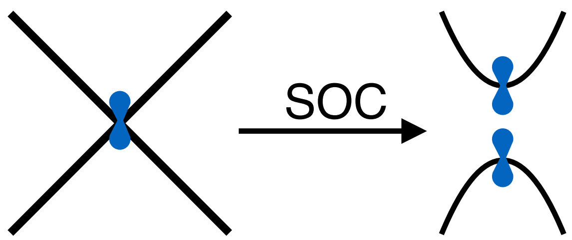


2. List of space groups/orbitals that are necessarily topological when insulating at partial filling

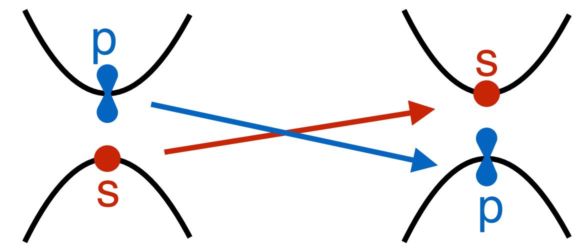
Theory of band reps is both a classification and a predictive scheme

Finding new topological materials

EBR theory classifies all known topological insulators



Disconnected elementary band representations



Composite band representations with band inversion

Finite (long!) list; cross-reference ICSD

Expedite search by:

1. orbitals at E_F
2. electron counting

Symmetry-protected semi-metals: search within connected EBRs

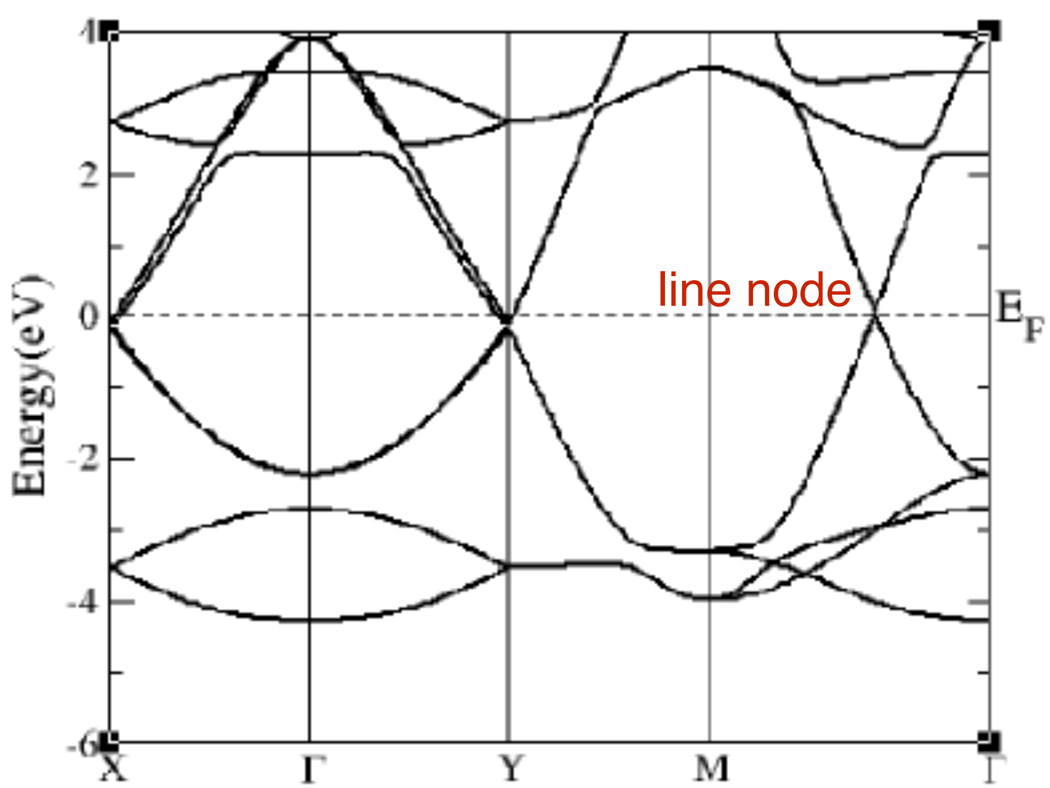
Layered square nets:

ABX_2: A=rare earth; B=Cu, Ag; X=Bi, As, Sb, P

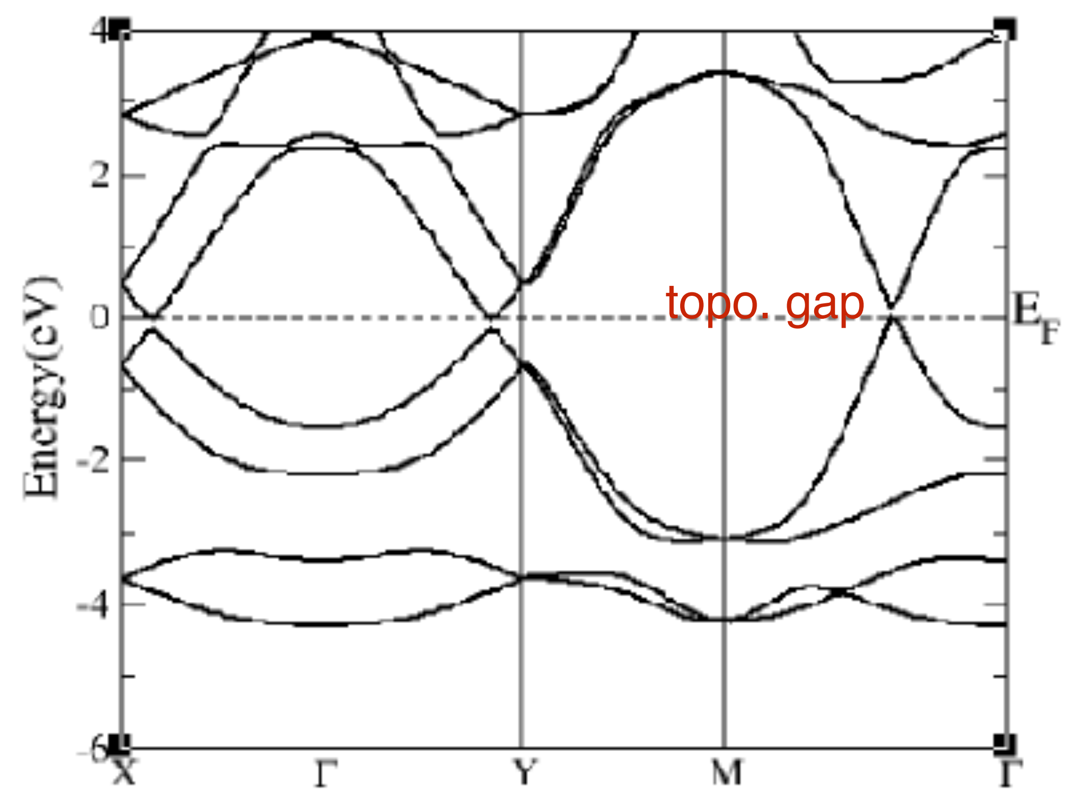
ABX: A=rare earth; B=Si, Ge, Sn, Pb; X=Os, S, Se, Te

~ 50 candidate materials

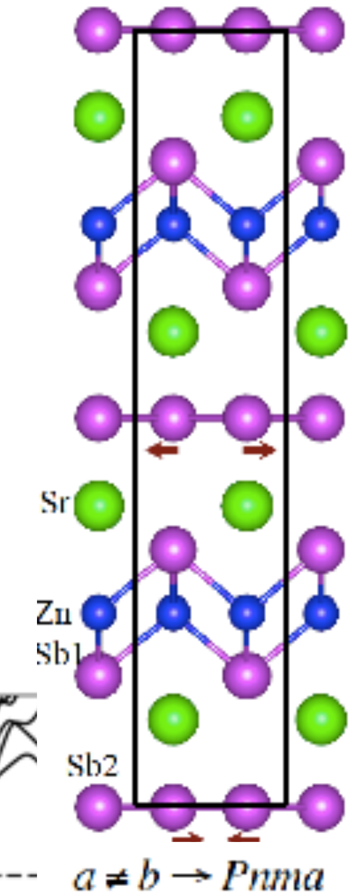
~ 250 candidate materials

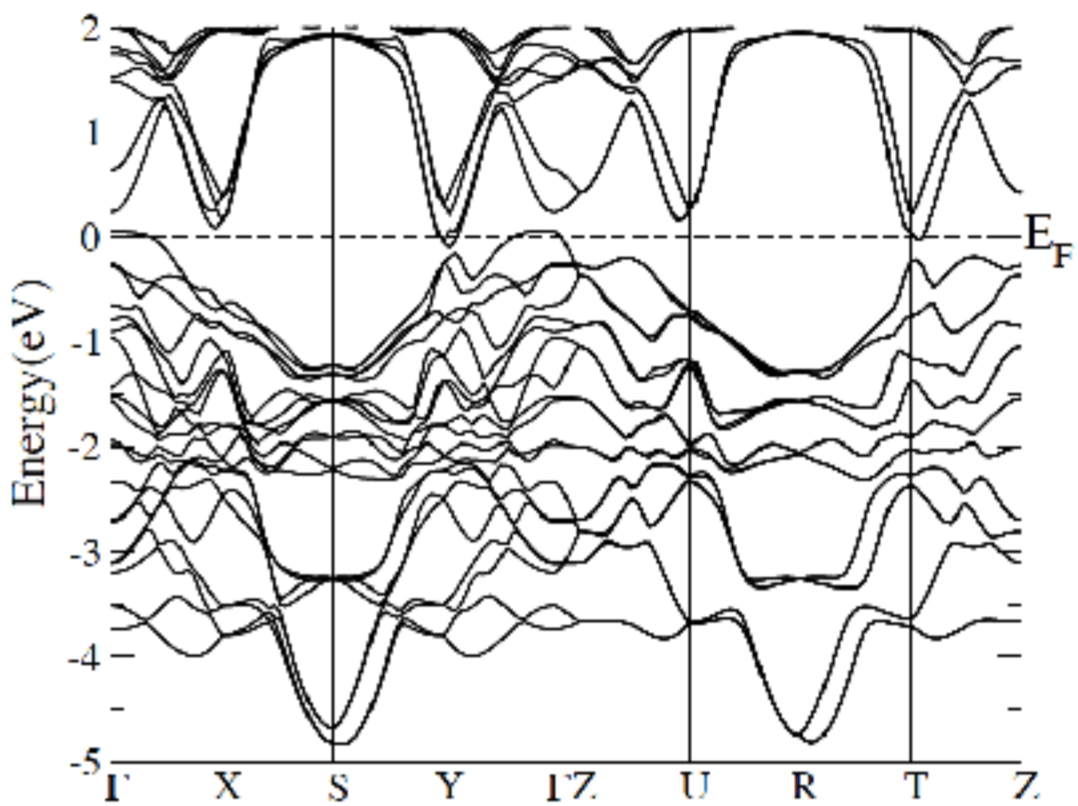


SOC →

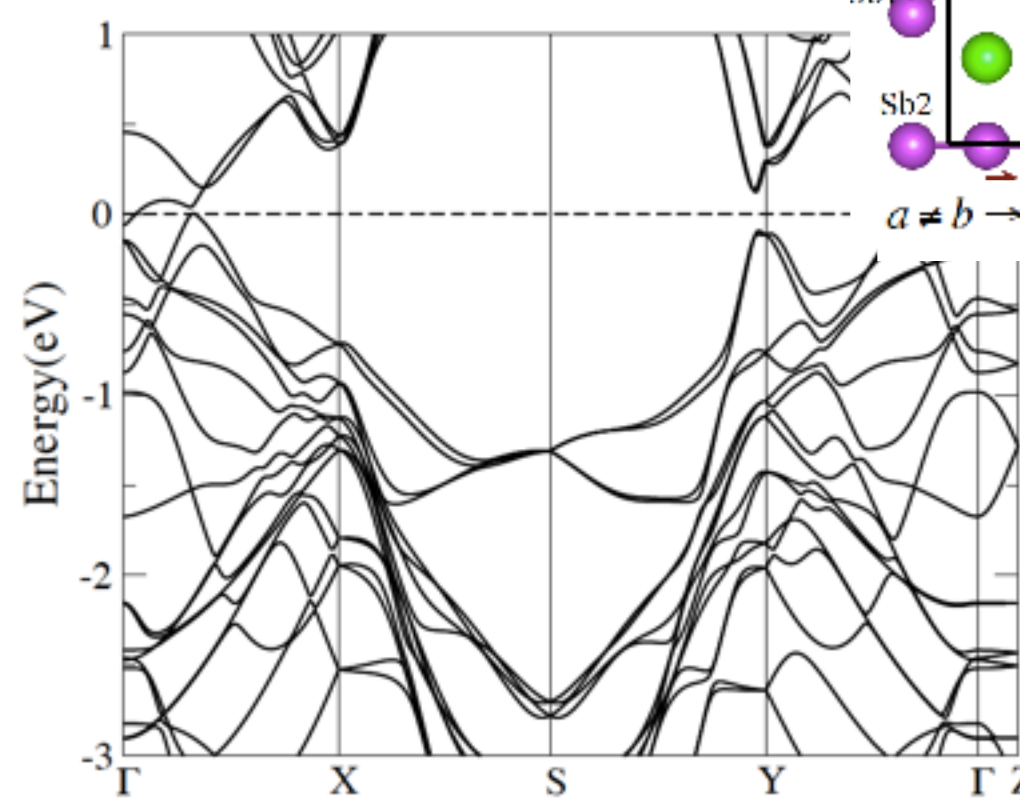


Layered distorted square nets: LaSbTe, $SrZnSb_2$, $AAgX_2$, A=RE, X=P, As, Sb, Bi



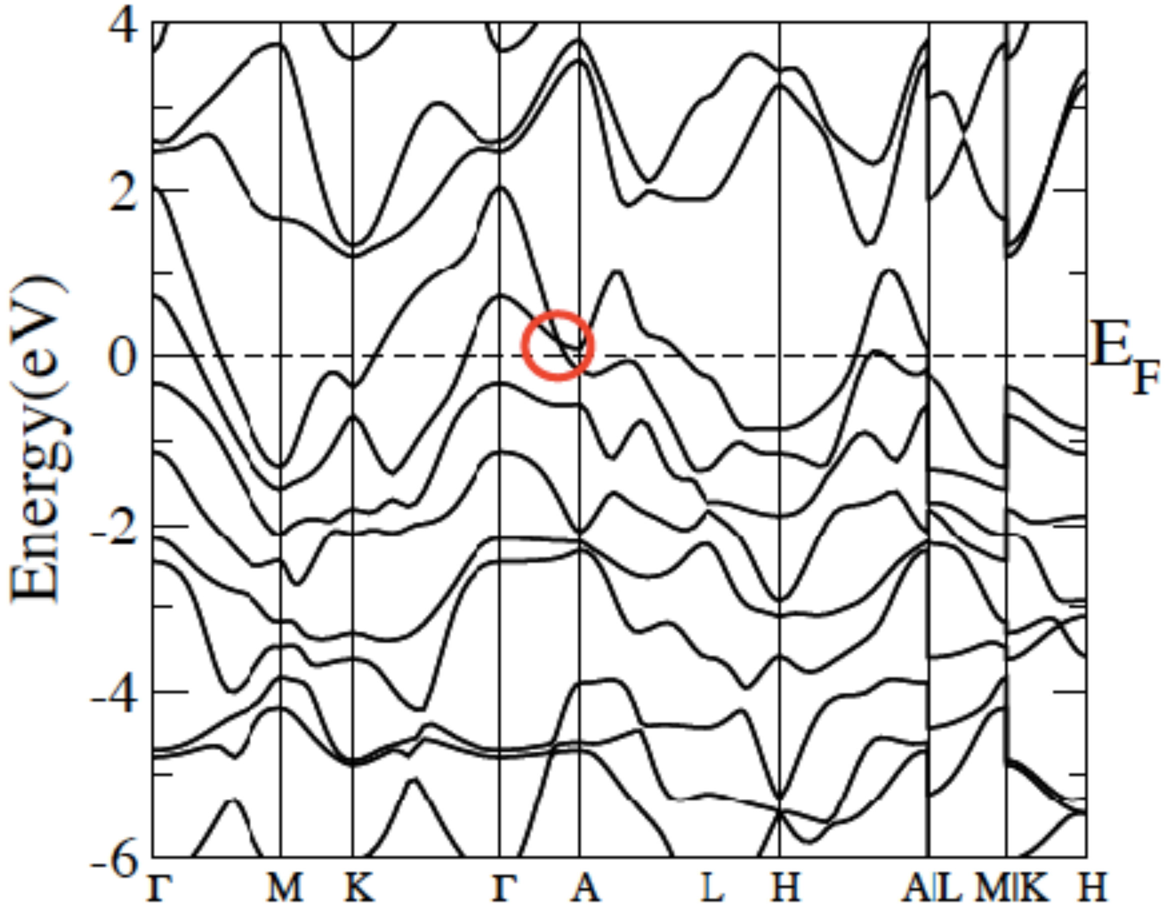


Weak TI: LaSbTe

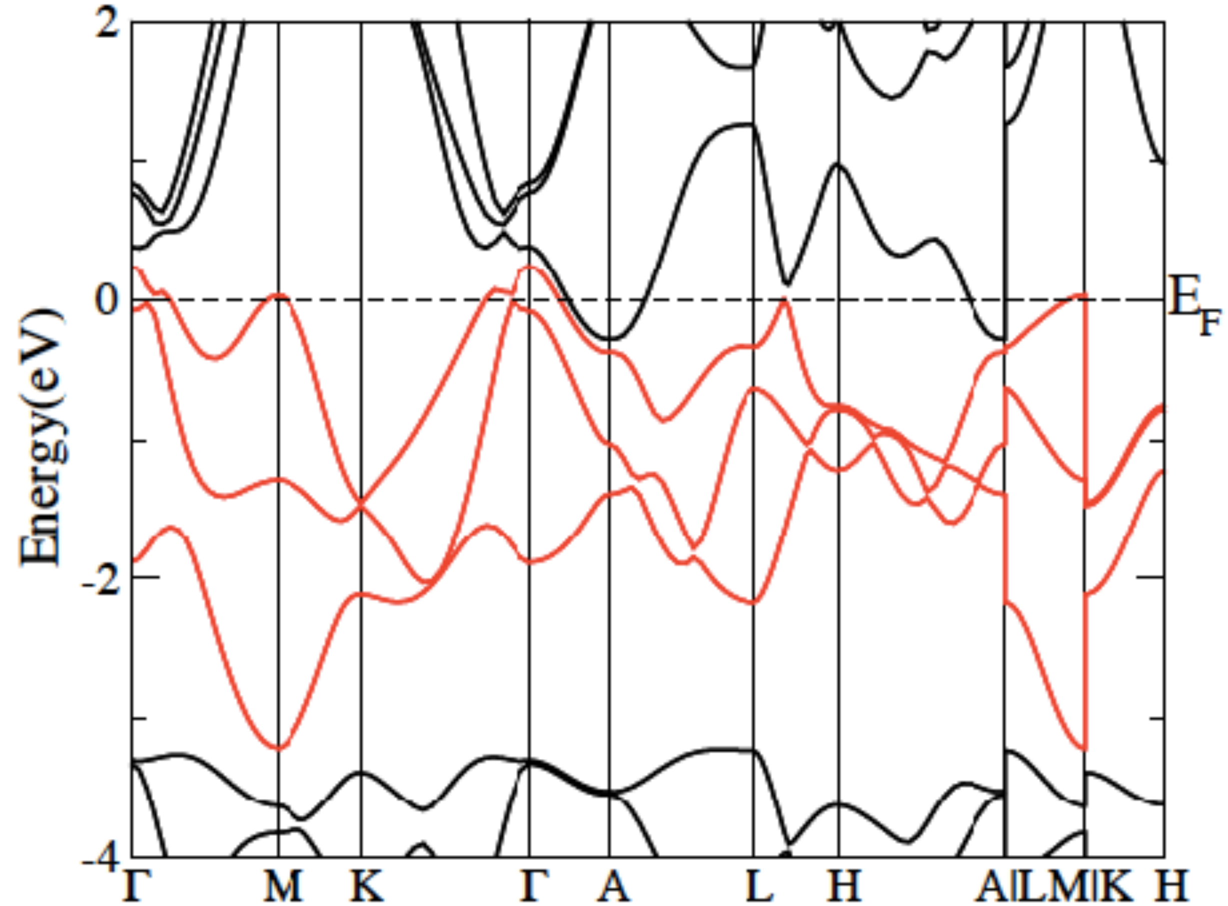


Weak TI: SrZnSb2

Topological insulators and semi-metals in SG 64
(buckled honeycomb layers)

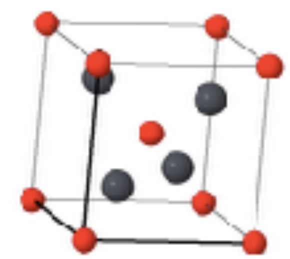


$IrTe_2$ (Type II Weyl)

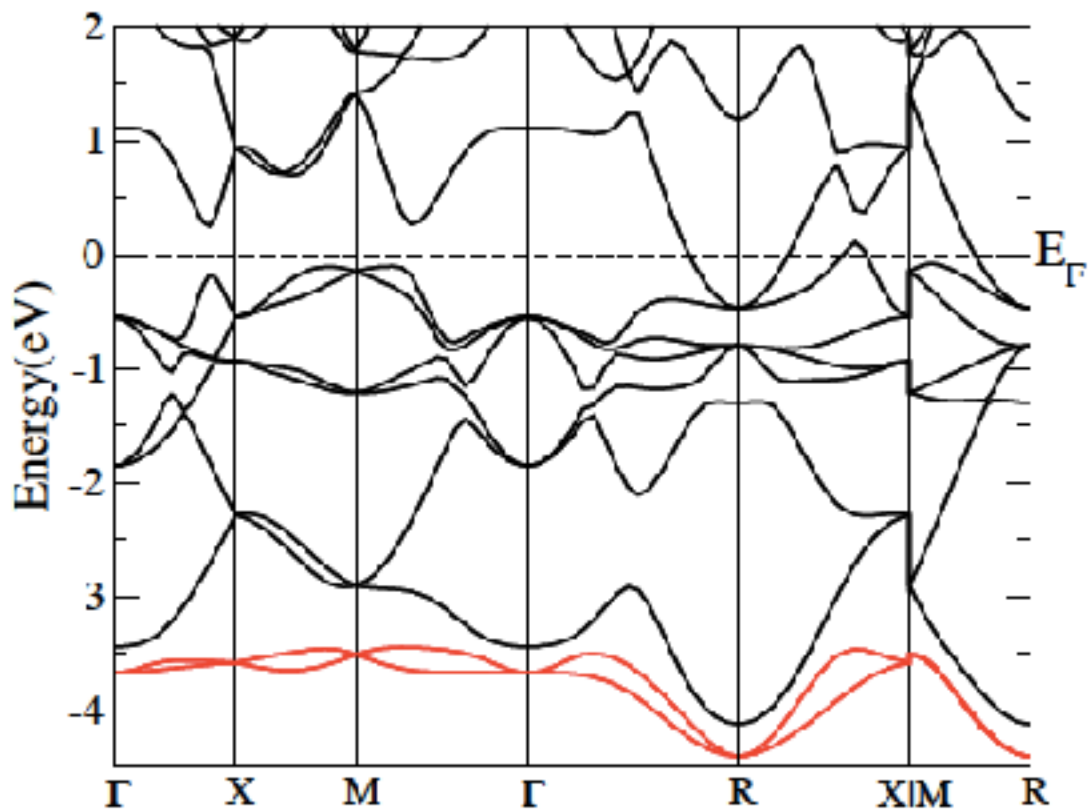


CNb_2 (Small gap, weak TI)

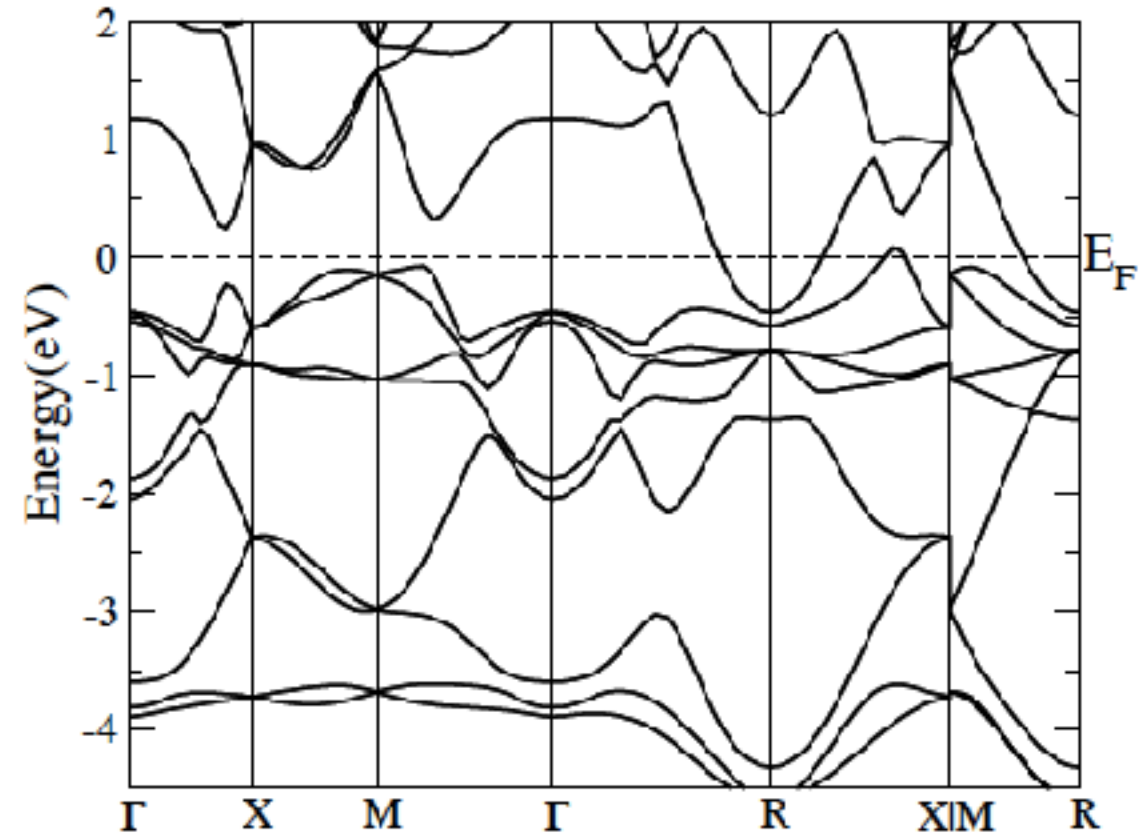
Strained PbO_2



(pic: ICSD)



Strain →

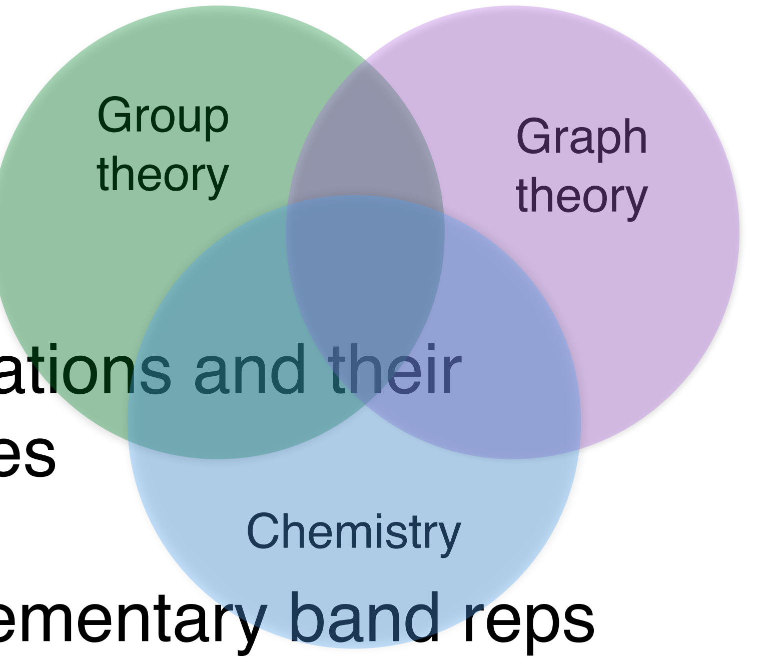


Semi-metal; topological bands -3.5eV

Uniaxial strain opens topological gap near E_F

ArXiv:1703.02050, 1706.08529,
1706.09272, 1709.01935,
1709.01937

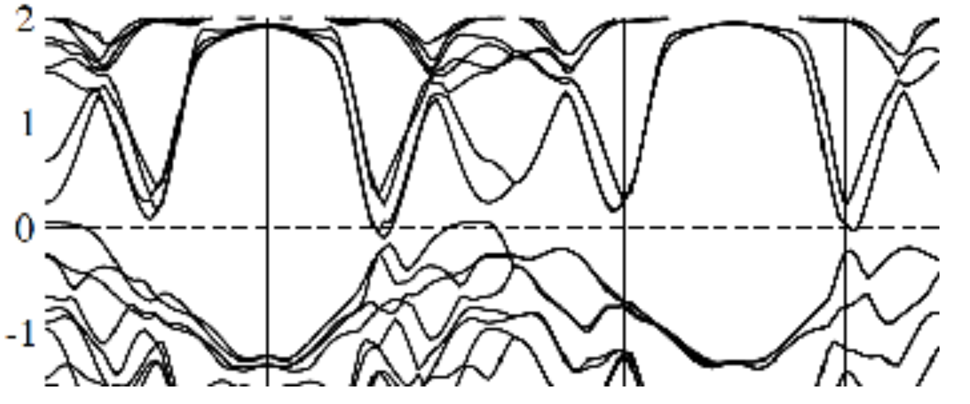
Summary



We computed all elementary (trivial) band representations and their connectivities ➡ classifies all TCI phases

Cross-referencing the list of disconnected(connected) elementary band reps against material databases yields topological insulators(semimetals)

Future directions



How to detect topological phases that do not have surface states?

Can we apply to many-body systems?
How does the classification change with interactions?