Topological Quantum Chemistry

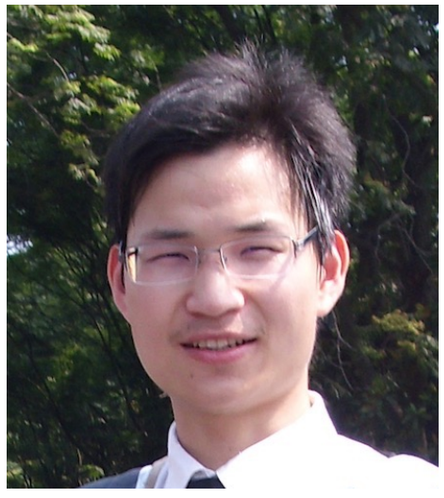
Jennifer Cano

Stony Brook University

FLATIRON INSTITUTE

Collaborators

Barry Bradlyn
(UIUC)



Zhijun Wang
(Princeton)

Maia Garcia Vergniory
(DIPC, EHU)

Claudia Felser
(Max Planck)

Mois Aroyo (EHU)

Luis Elcoro (EHU)

Andrei Bernevig
(Princeton)

Last time: classification of topological insulators with 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

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	$2\mathbb{Z}$	$\cdots$

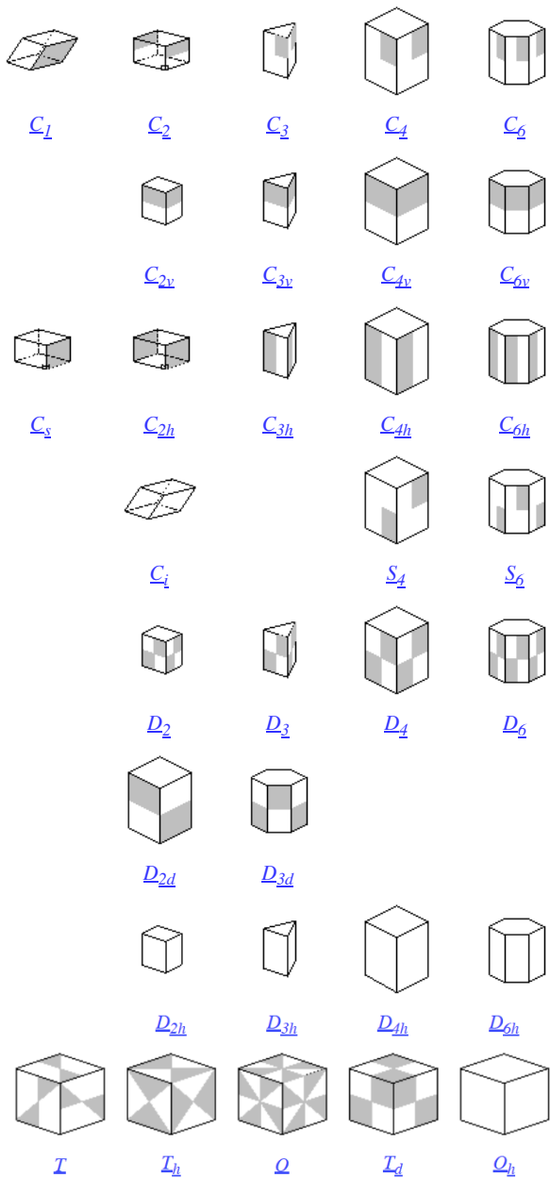
fermions w/ time-reversal →

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

Review of crystal symmetry

32 crystallographic point groups + 14 Bravais lattices = 230 space groups

Contain rotations, mirror planes, and rotoinversions



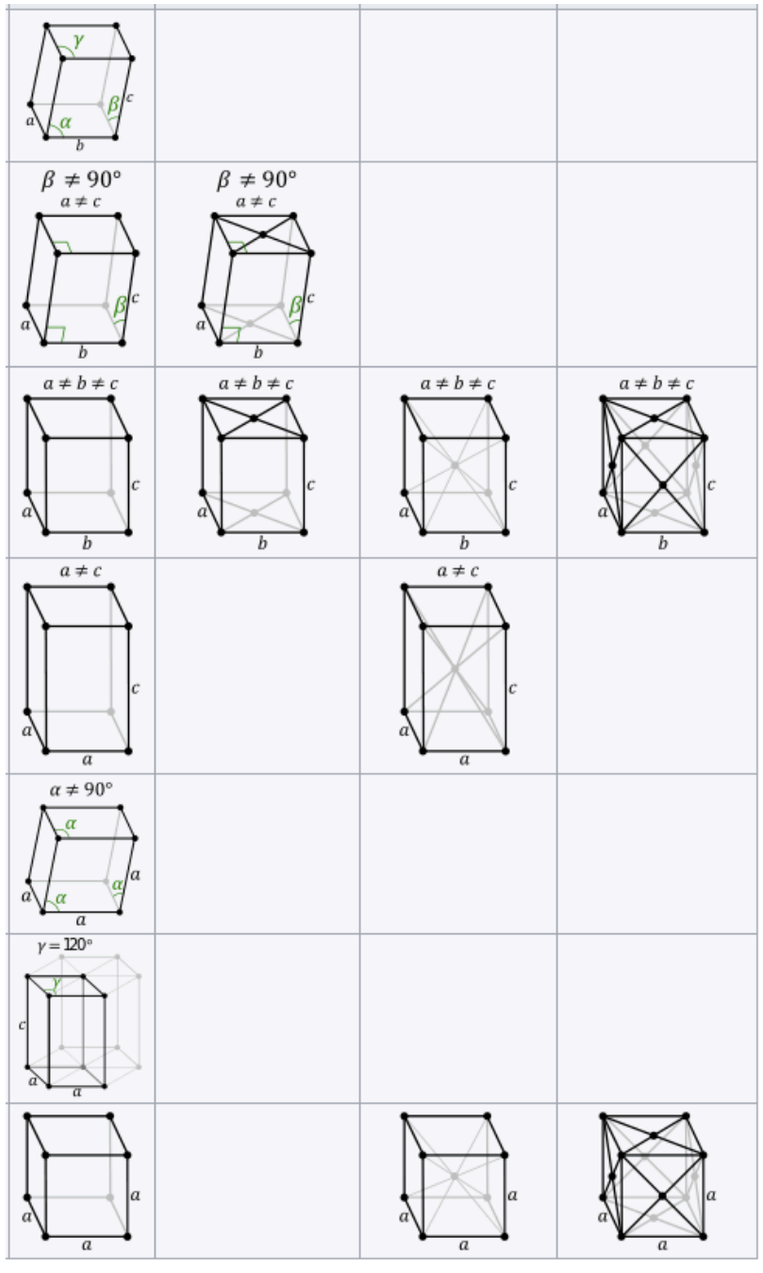


Image: JP Goss http://newton.ex.ac.uk/research/qsystems/people/goss/symmetry/Solids.html

Topological crystalline insulator

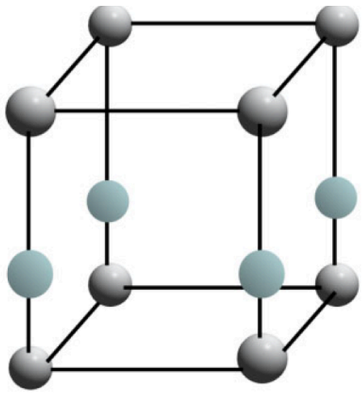
Fu PRL 106, 106802 (2011)

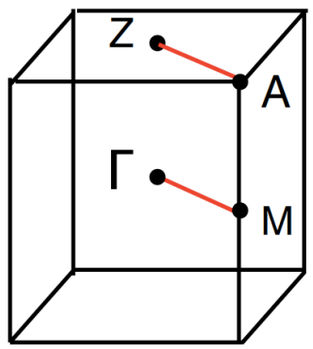
Crystal symmetries can protect topological phase

Surface states are robust if crystal symmetry is preserved

C_4 symmetry

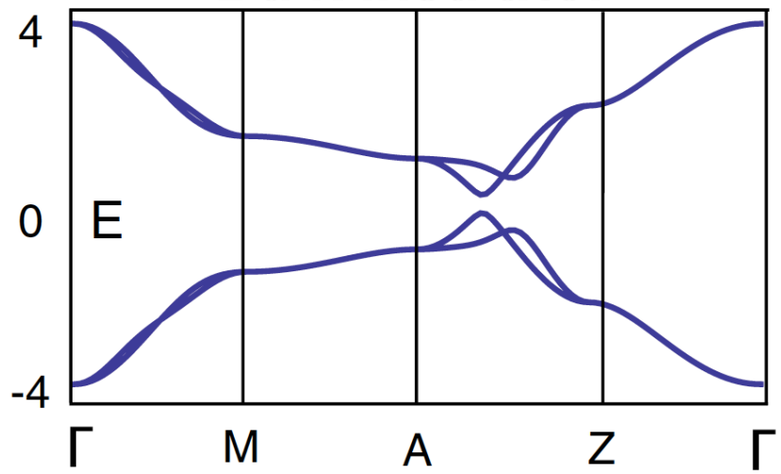
(x,y,z) → (-y,x,z)



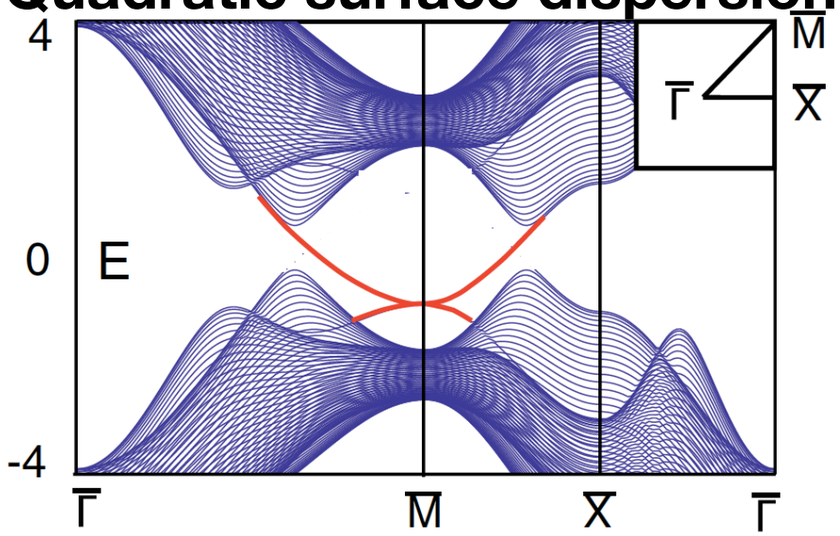


Z_2 Topological invariant

Bulk insulator

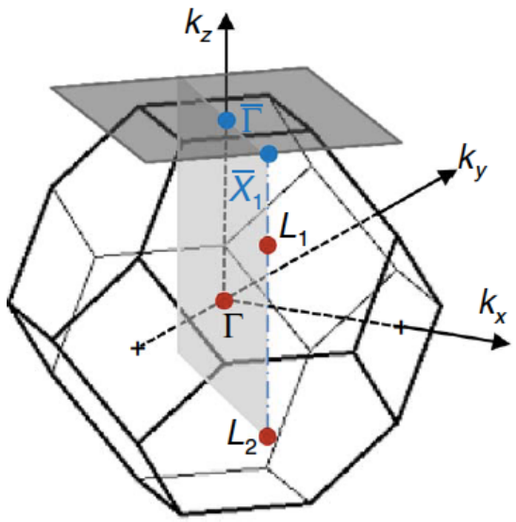


Quadratic surface dispersion



Mirror Chern insulator

Teo, Fu, Kane PRB 045426 (2008)



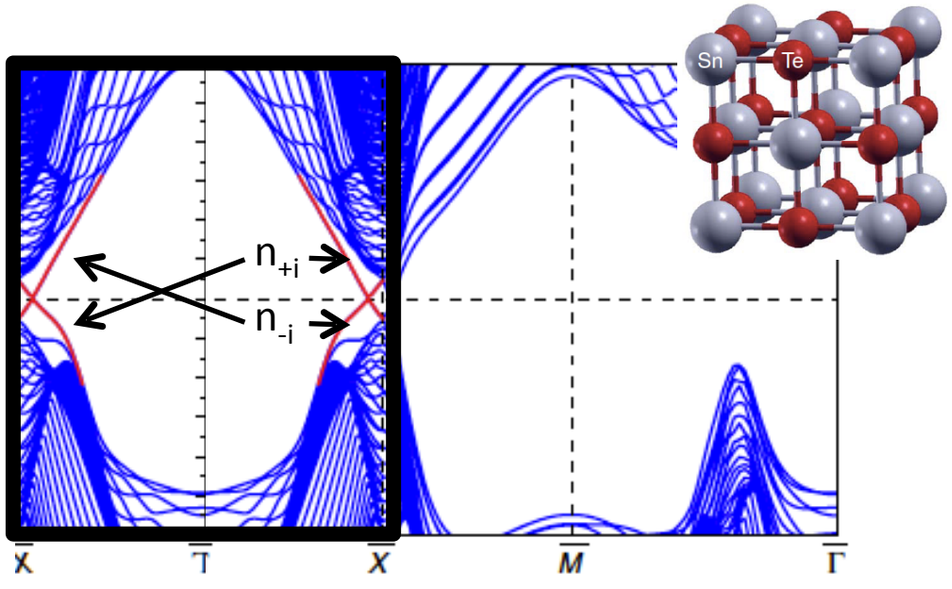
Mirror symmetry: (x,y,z) → (-x,y,z)

Two invariant mirror planes: $k_x = 0$ and $k_x = \pi$

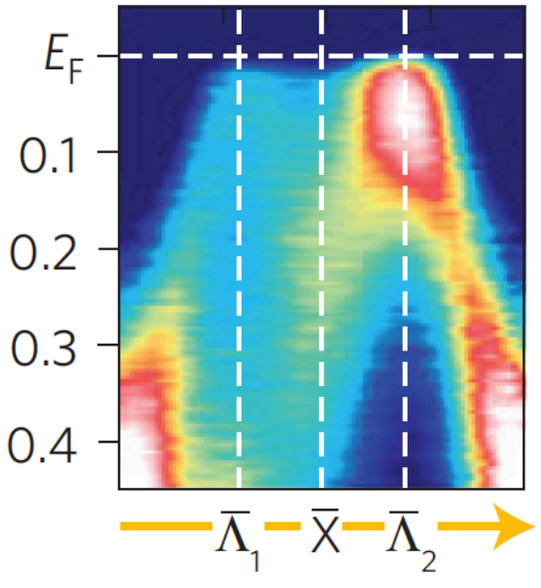
In a mirror plane, each mirror eigenvalue sector can have Chern number

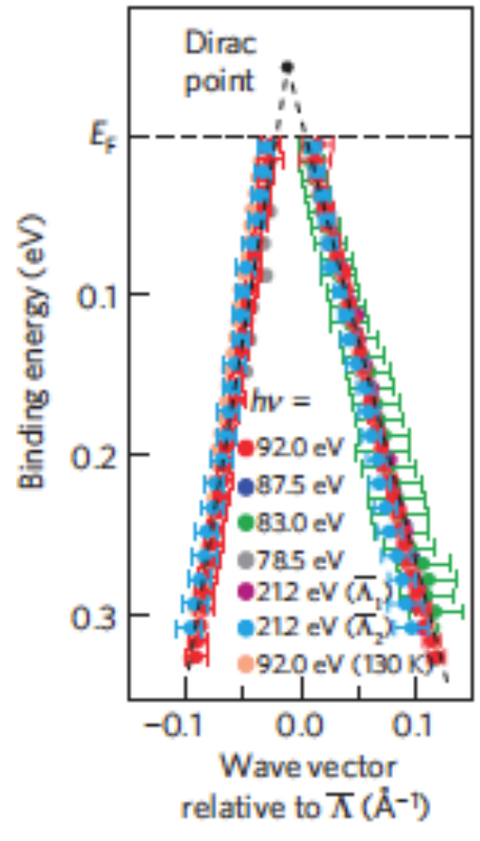
Z invariant

Observation in SnTe by Ando group: Tanaka, et al, Nat. Phys. (2012)



Theory: Hsieh, et al, Nat. Comm. (2012)





“Non-symmorphic symmetries”: screws and glides

Glide symmetry:
mirror followed by 1/2 lattice translation
Ex: (x,y,z) → (x+½,y,-z)

Screw symmetry:
rotation followed by fractional lattice translation

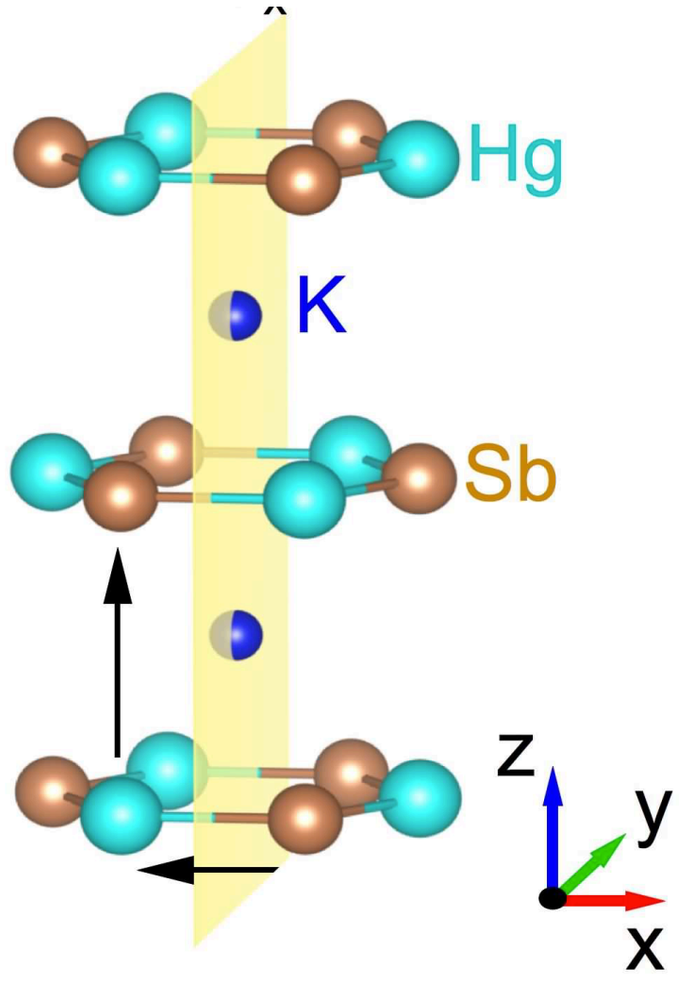
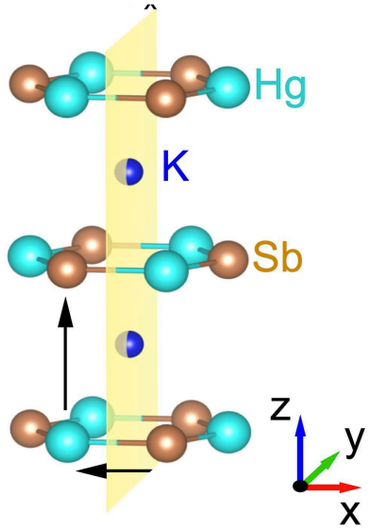


Image: Ma, et al, Sci. Adv. 3, e1602415 (2017)

“Hourglass fermion”

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

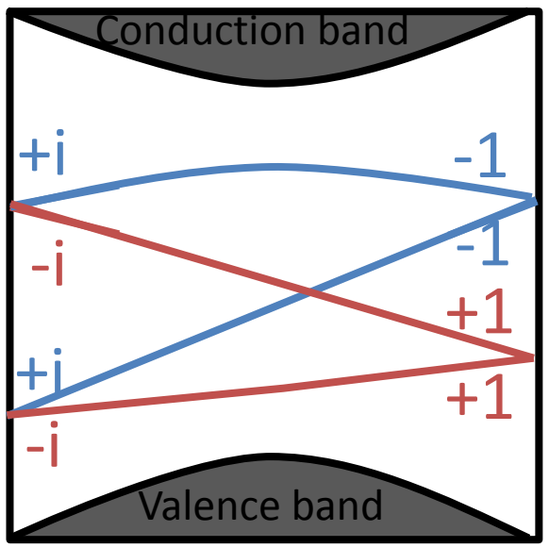


$$g_x^2 = -e^{ik_z}$$

$$\mathcal{T}^2 = -1$$

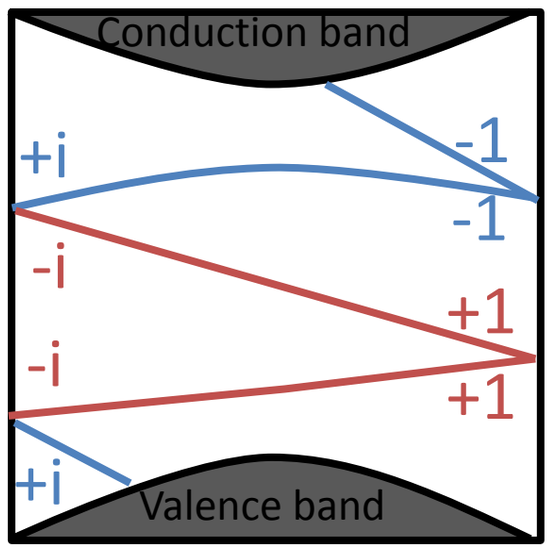
y-normal surface: preserves glide
Label bands by g_x eigenvalue $\pm e^{ikz/2}$

Two possible surface states along k_x=0 or π



(k_x=0,k_z=0) (k_x=0,k_z=π)

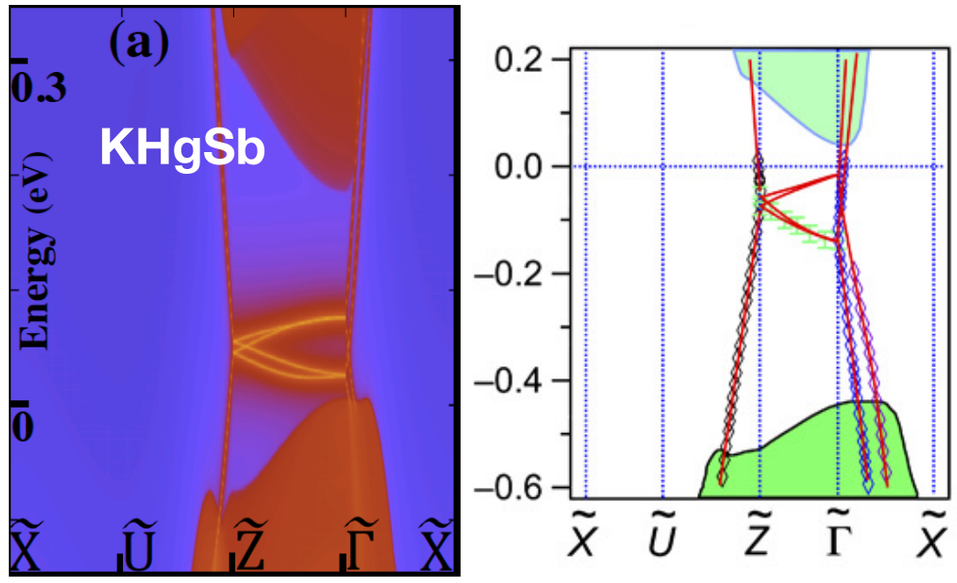
Hourglass fermion



(k_x=0,k_z=0) (k_x=0,k_z=π)

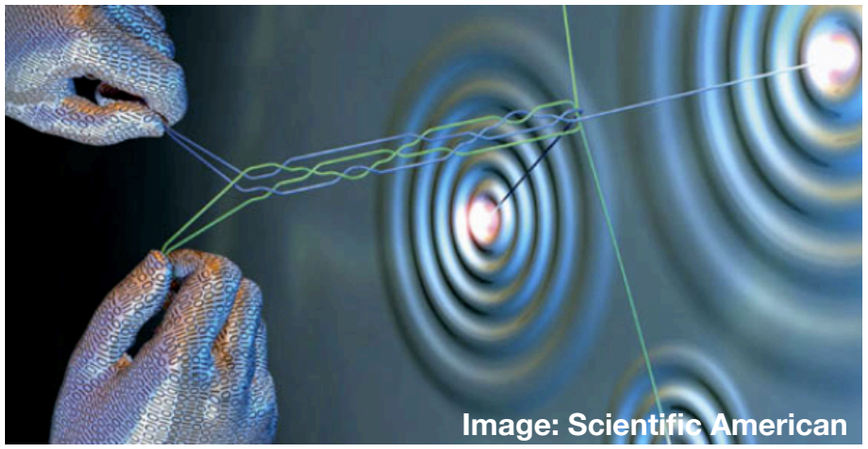
Glide spin Hall

Observation in KHgSb

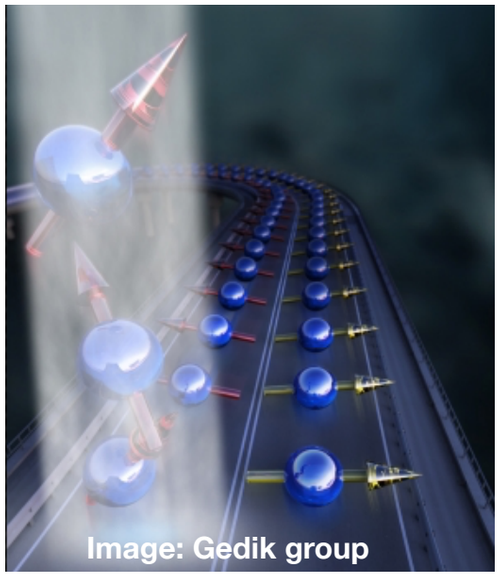


Ding group: Ma, et al, Sci. Adv. (2017)

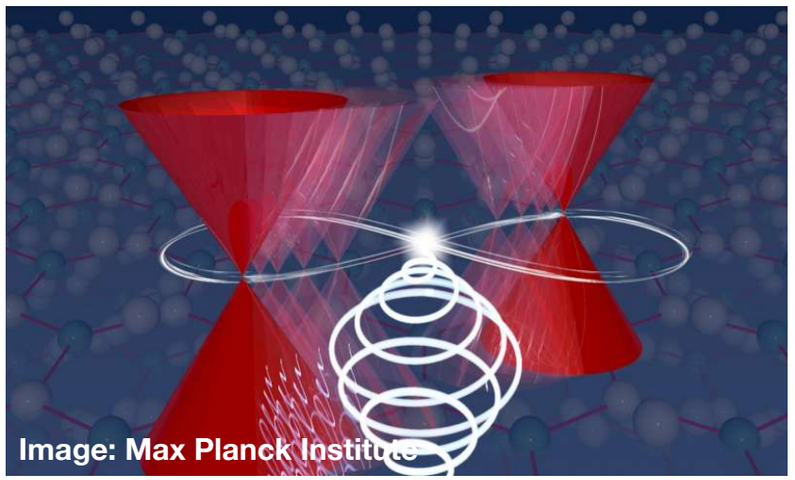
Topological phases can be used for technological applications



Quantum computing



Spintronics



Ultra-fast switches

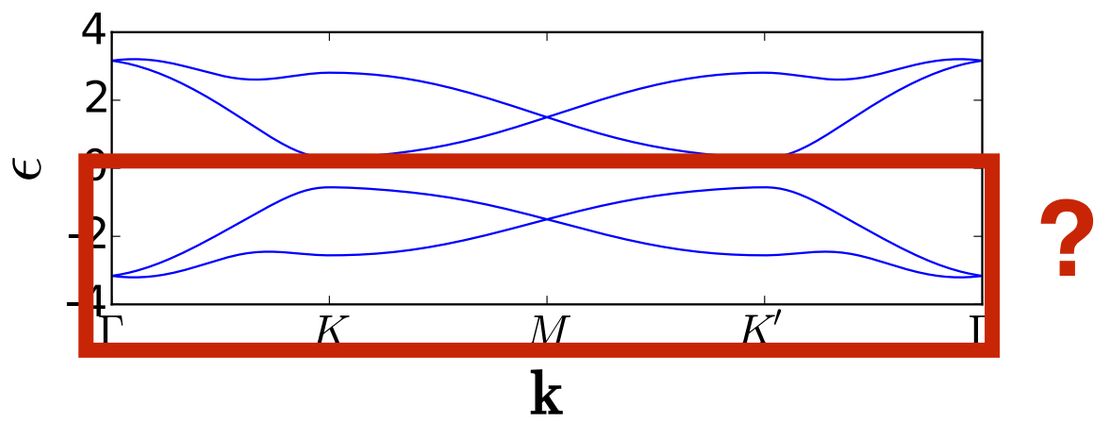
Problem: how to find materials to realize topological phases??

Challenges to finding topological materials

1. Piecewise approach to classification

Mirror, C_4, C_6, glide, time reversal, ….

What about crystals with combinations of symmetries?

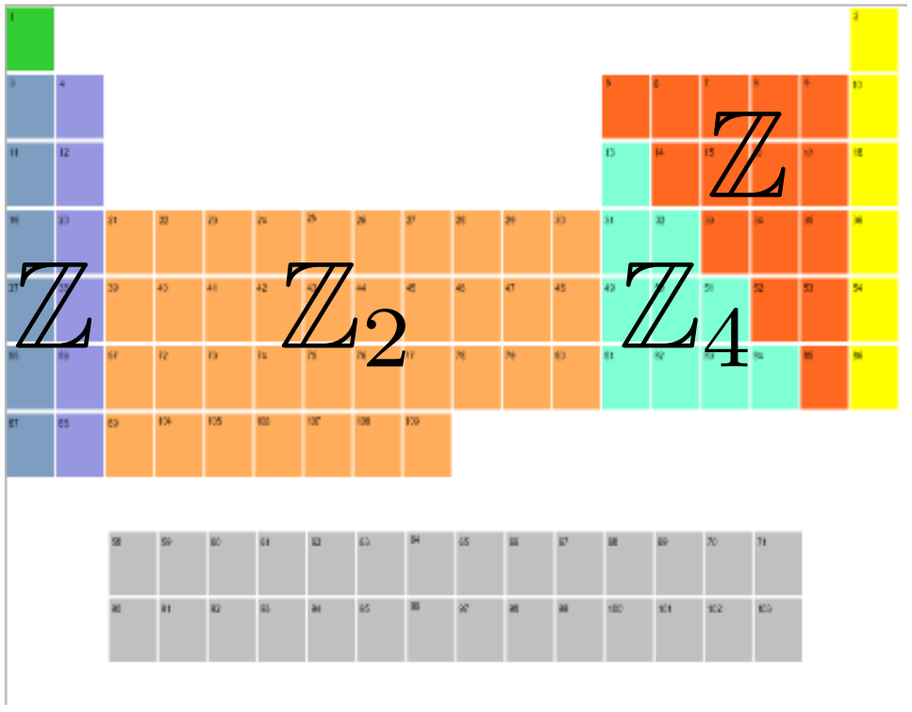


If we don’t know all the topological phases, then how can we identify all topological materials?

Challenges to finding topological materials

2. Emphasis on abstract topological invariant

Z, Z_2, Z_4, Z_2 x Z_4, …



What chemical compounds will yield a Z_n topological invariant?!?!

Topological quantum chemistry can diagnose and predict topological materials

JC et al., ArXiv:1709.01935 (PRB 2018); BB, **JC**, et al., *Nature* 547, 298–305 (2017)

Key: topological bands are not deformable to an atomic limit

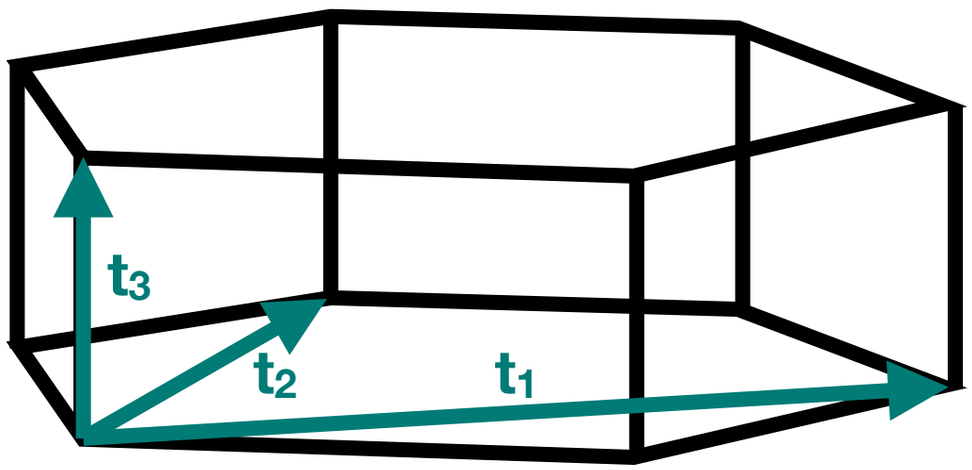
1. Identify atomic limit band structures with symmetry
2. Systematic search for topological bands
3. New topological materials

Space groups describe 3D crystals

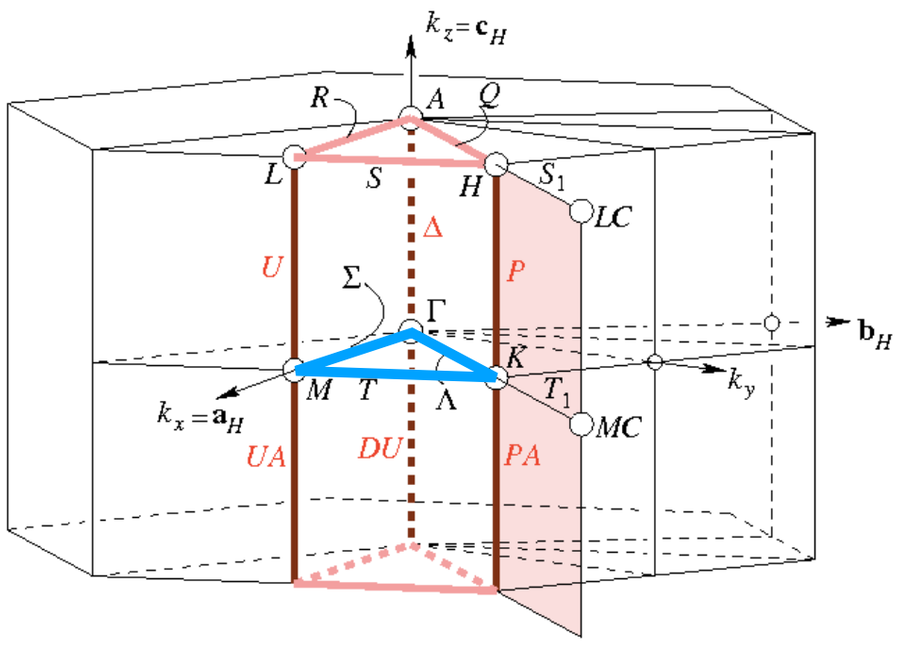
Ex: P6mm, (#183)

C_{6z}, m_x, lattice translations

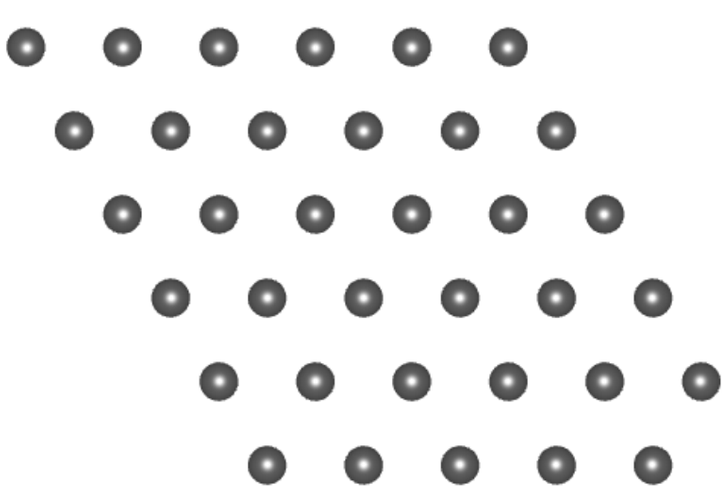
Real space



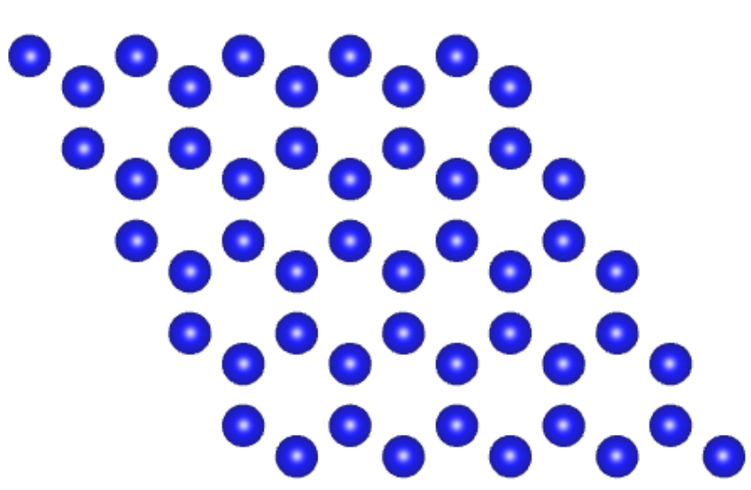
Brillouin zone



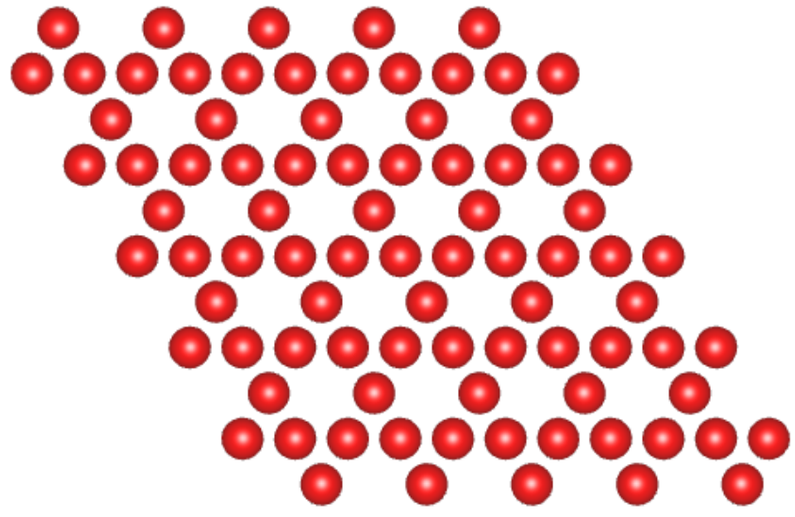
Within one space group, many ways to arrange atoms



1 atom/unit cell
(triangular)



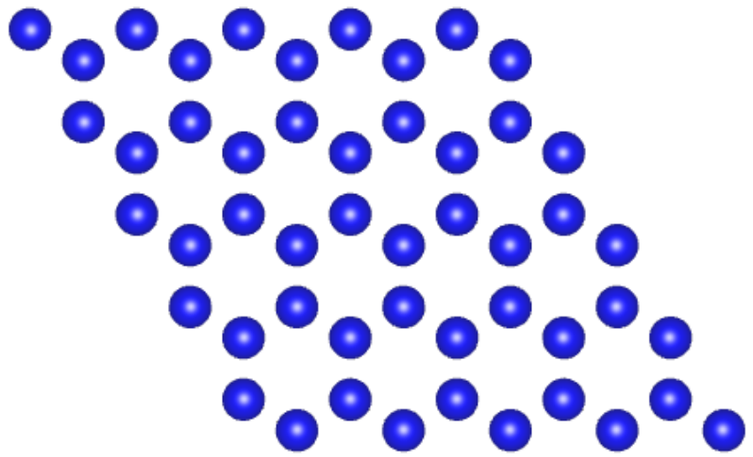
2 atoms/unit cell
(honeycomb)



3 atoms/unit cell
(kagome)

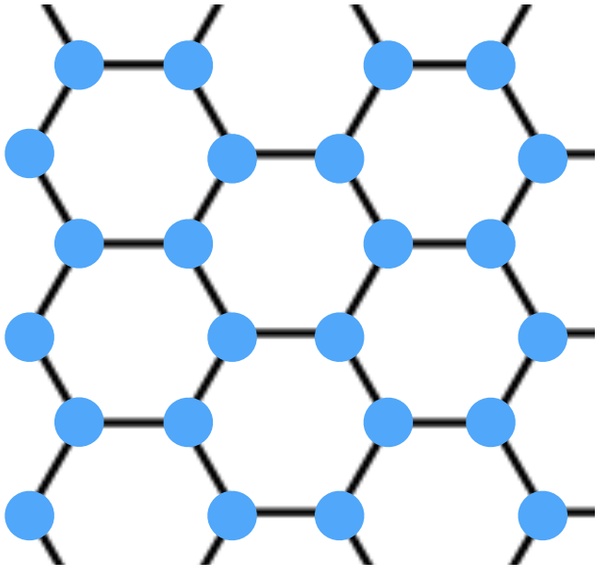
All atoms are related by symmetry

Within one arrangement, many choices of orbitals

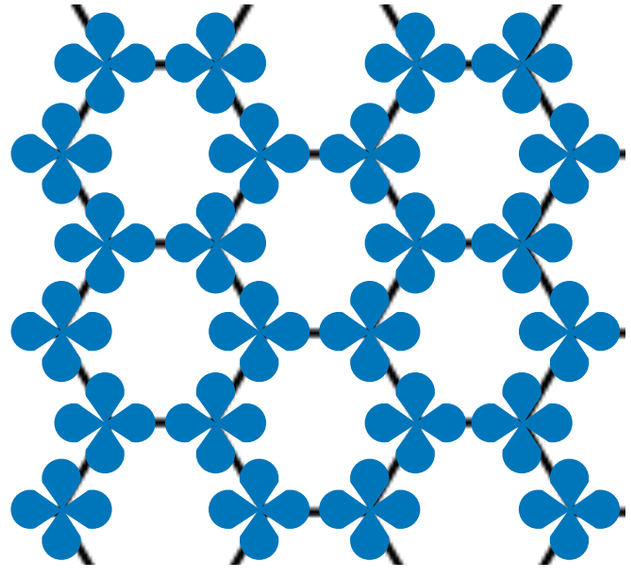


2 atoms/unit cell

s (or p_z) orbitals

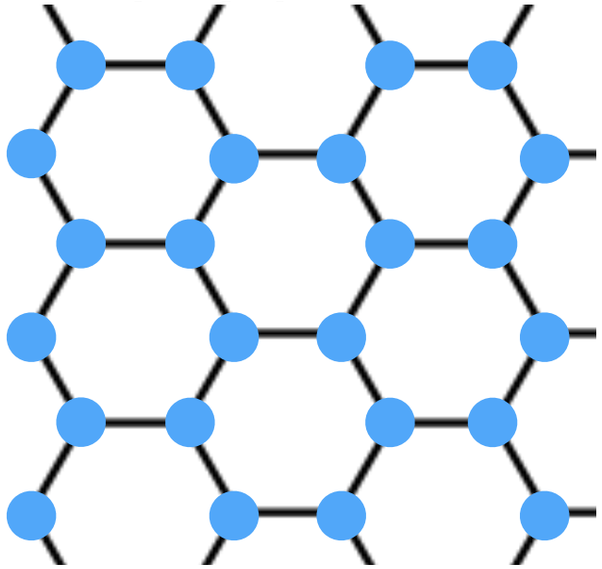


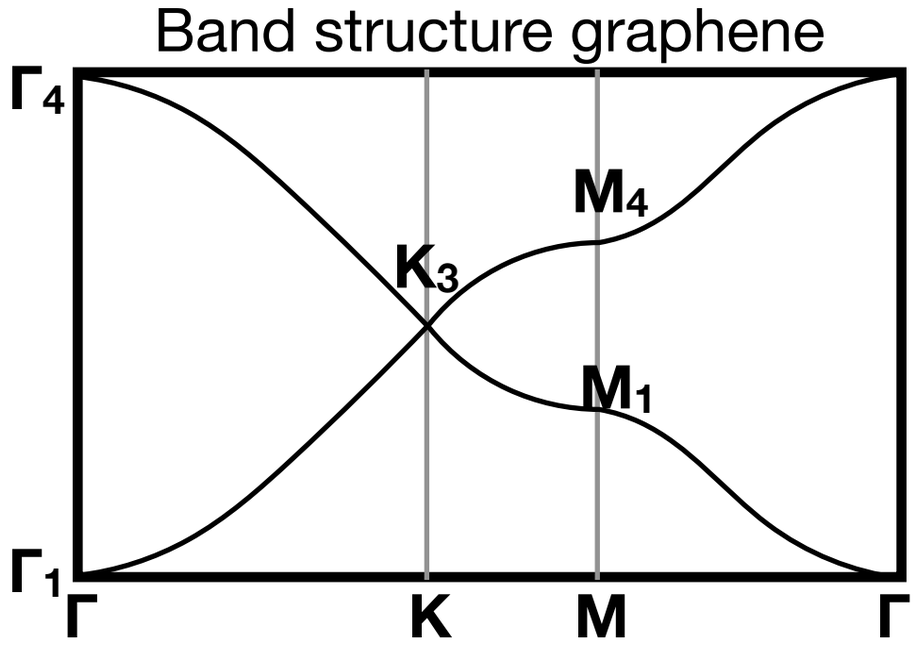
p_x and p_y orbitals



Each arrangement/orbital determines symmetry representations in Brillouin zone

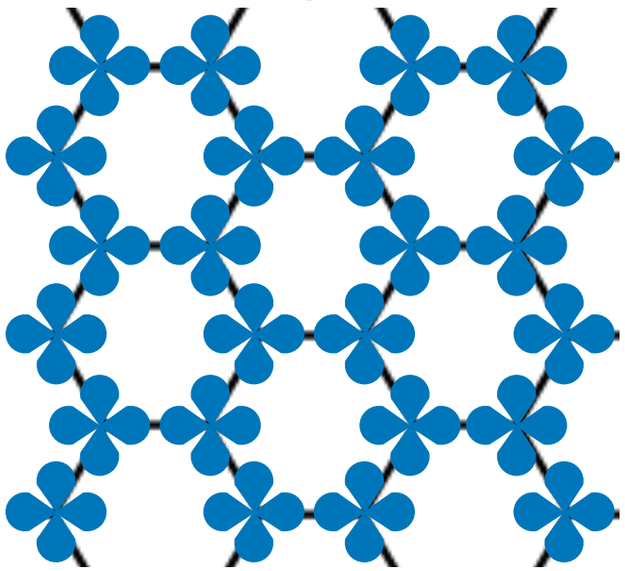
s (or p_z) orbitals

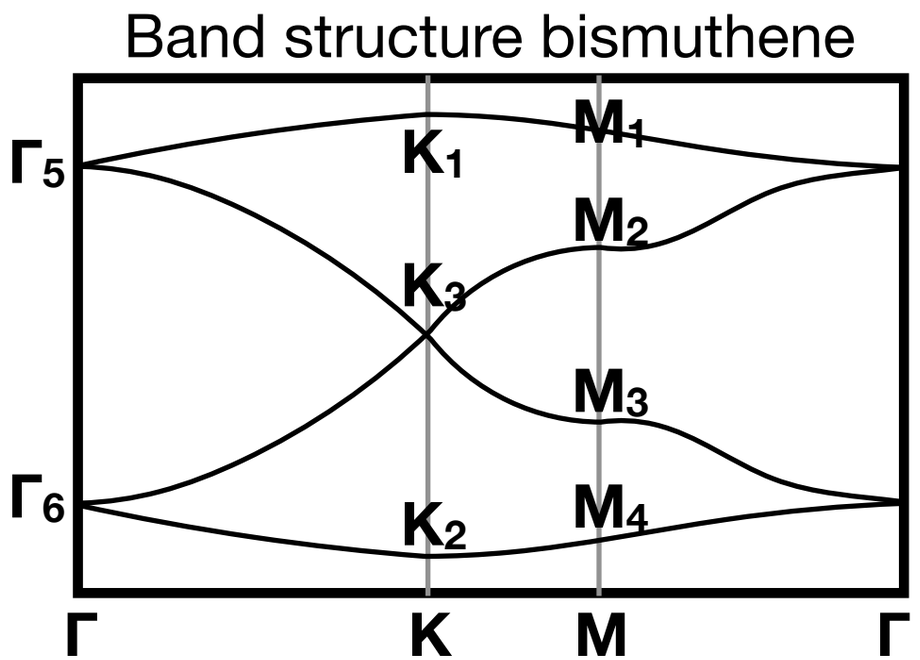




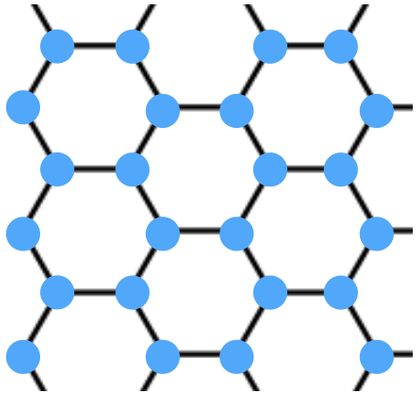
Real space vs momentum space

p_x and p_y orbitals

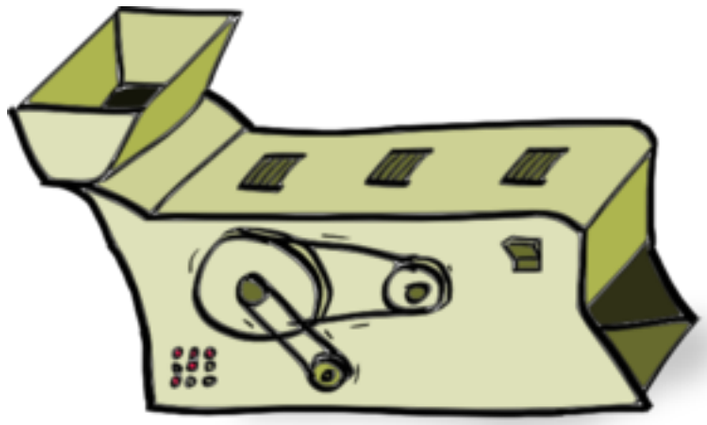




Input real space symmetry



1. space group
2. atom positions
3. orbitals



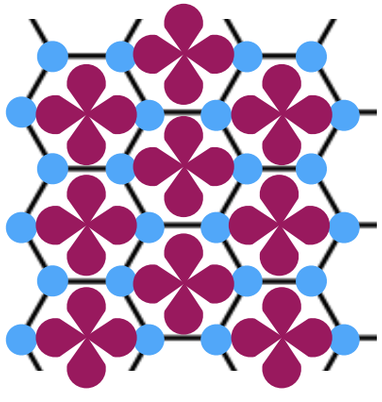
Band representation: atomic limit and its symmetry

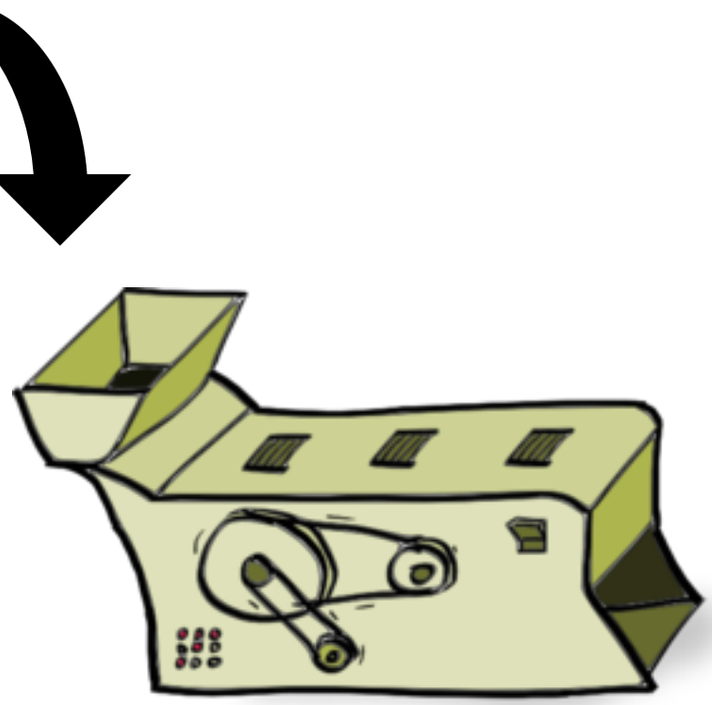
Zak PRL 1980, PRB 1981, 1982

Brillouin zone symmetry

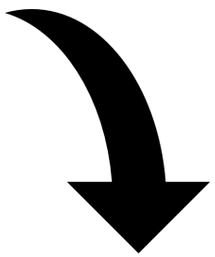
Γ_1 Γ_4 K_3 M_1 M_4

Band representations can describe multiple orbitals in different positions





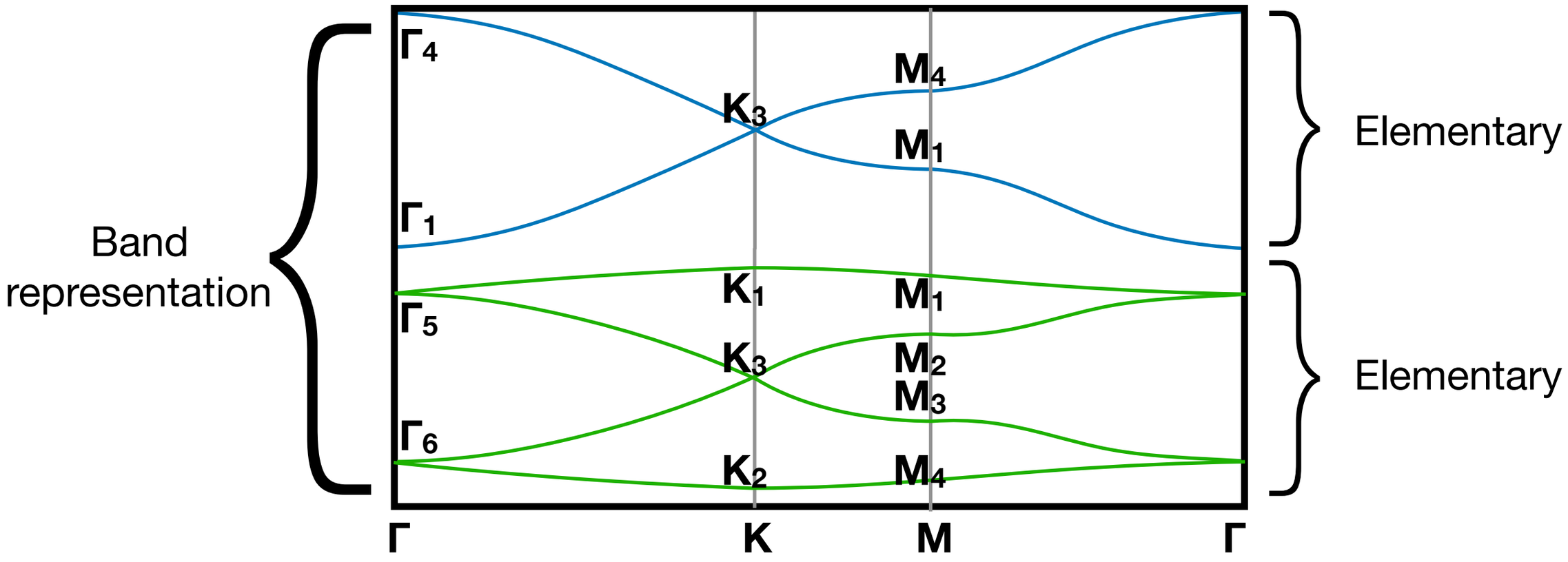
Infinitely many!



Γ_1 Γ_4 Γ_5 Γ_6 K_3 K_3 K_3 M_1 M_1 M_2 M_3 M_4 M_4

Elementary band reps are the building blocks

Zak PRL 1980, PRB 1981, 1982
JC, et al, PRB 2018



Identify elementary band reps from their real space symmetry

10,000 elementary band reps (with and without TR, SOC)

Compute symmetry labels for each elementary band representation

bilbao crystallographic server

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

Mois Aroyo Luis Elcoro
Univ. Basque Country

Elcoro, …, **JC**, et al, J. Appl. Cryst. 50, 1457-1477 (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 [183]

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

Bilbao Crystallographic Server
http://www.cryst.ehu.es

For comments, please mail to
administrador.bsc@ehu.eus

Each column is elementary band representation

Bilbao Crystallographic Server → BANDREP Help

Elementary band-representations without time-reversal symmetry of the Double Space Group *P*6*mm* (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.

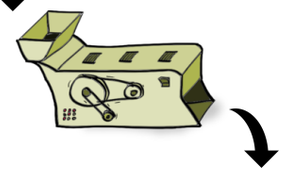
Minimal set of paths and compatibility relations to analyse the connectivity

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

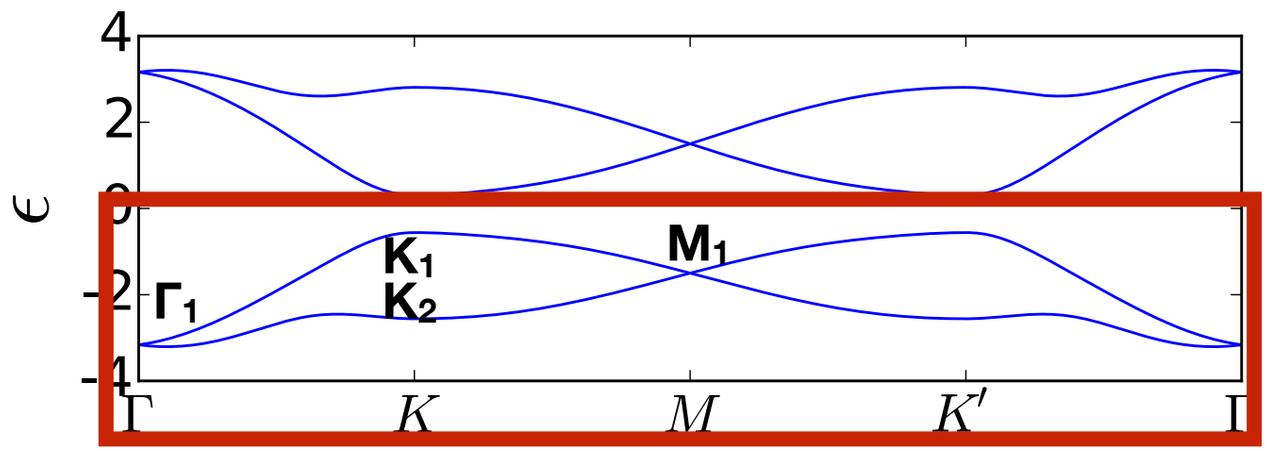
Orbital



High-symmetry points

We can now identify topological bands

JC et al., ArXiv:1709.01935 (PRB 2018), BB, **JC**, et al., *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 (inefficient) materials search:

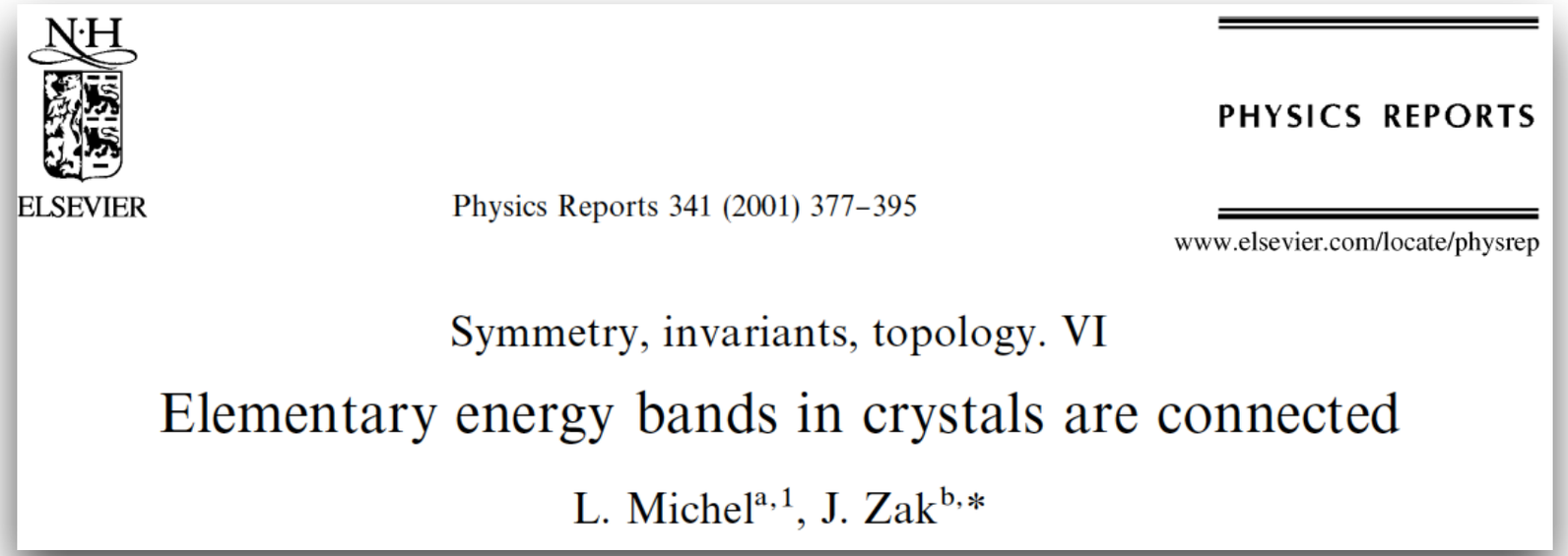
For every known chemical compound:

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

I will describe a more efficient search

Other search algorithms: BB, **JC**, et al., *Nature* 547, 298–305

Michel and Zak believed elementary bands could not be gapped



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Physics Reports 341 (2001) 377–395

PHYSICS REPORTS

www.elsevier.com/locate/physrep

Symmetry, invariants, topology. VI

Elementary energy bands in crystals are connected

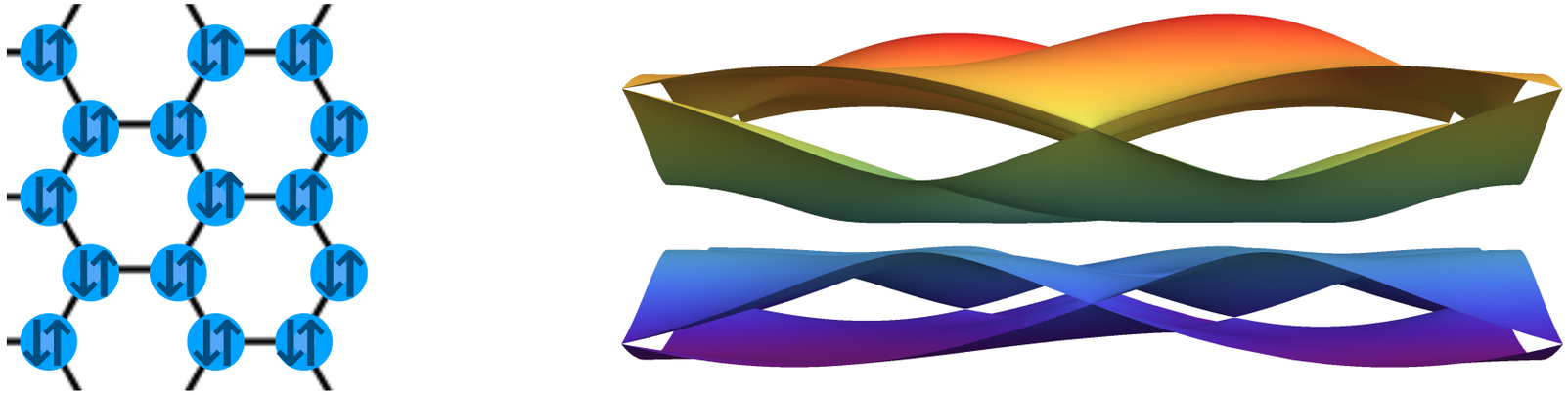
L. Michel[a,1], J. Zak[b,*]

“we present the topologically global concepts necessary for the proof”

Disconnected elementary bands are topological

JC et al., ArXiv:1709.01935 (PRB 2018), BB, **JC**, et al., *Nature* 547, 298–305 (2017)

Ex: p_z orbitals on honeycomb with SOC (Kane-Mele model)



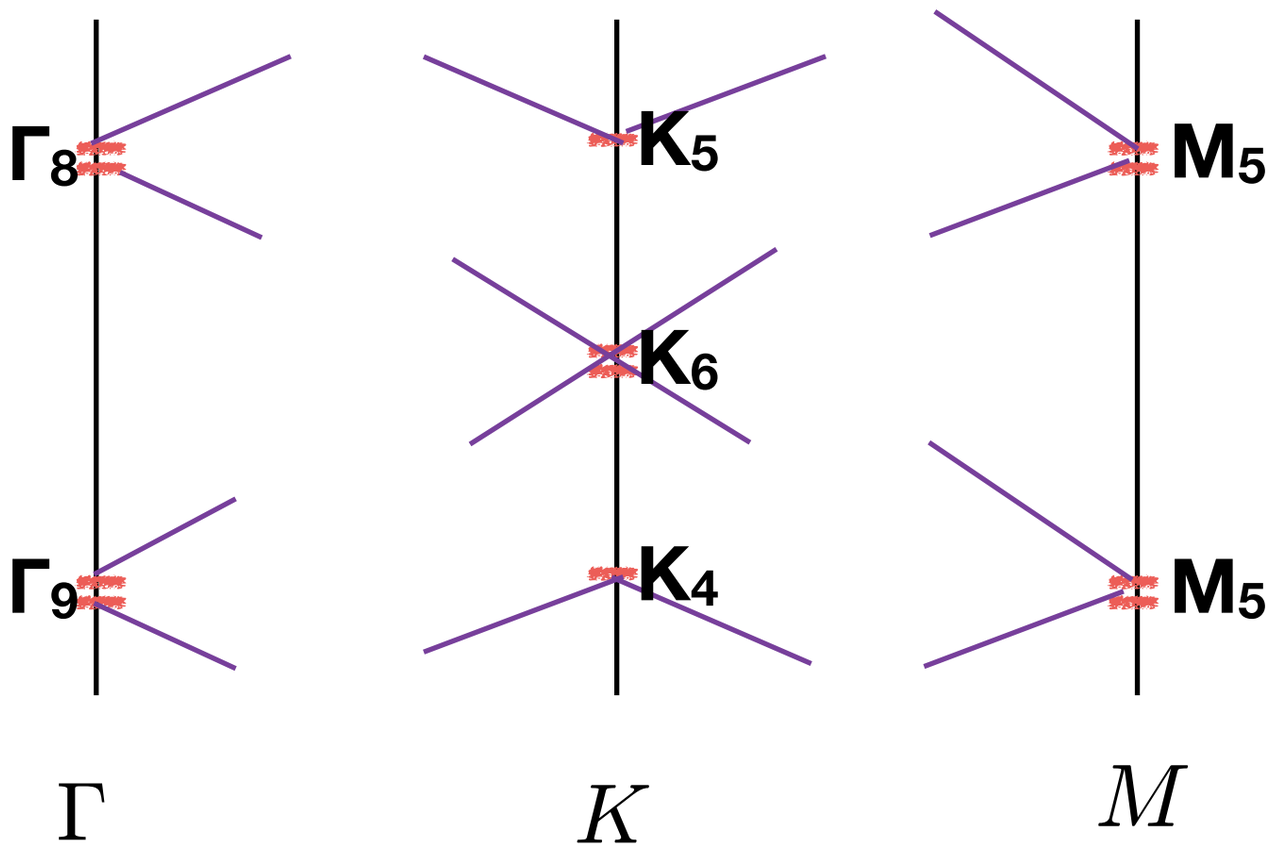
TR requires 4 sites per unit cell on honeycomb lattice

4n+2 valence bands must be topological!

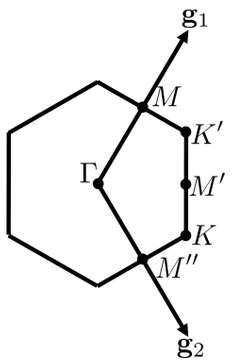
See also: Po, Watanabe, Zalatel, Vishwanath, Sci. Adv. 2(4), (2016)

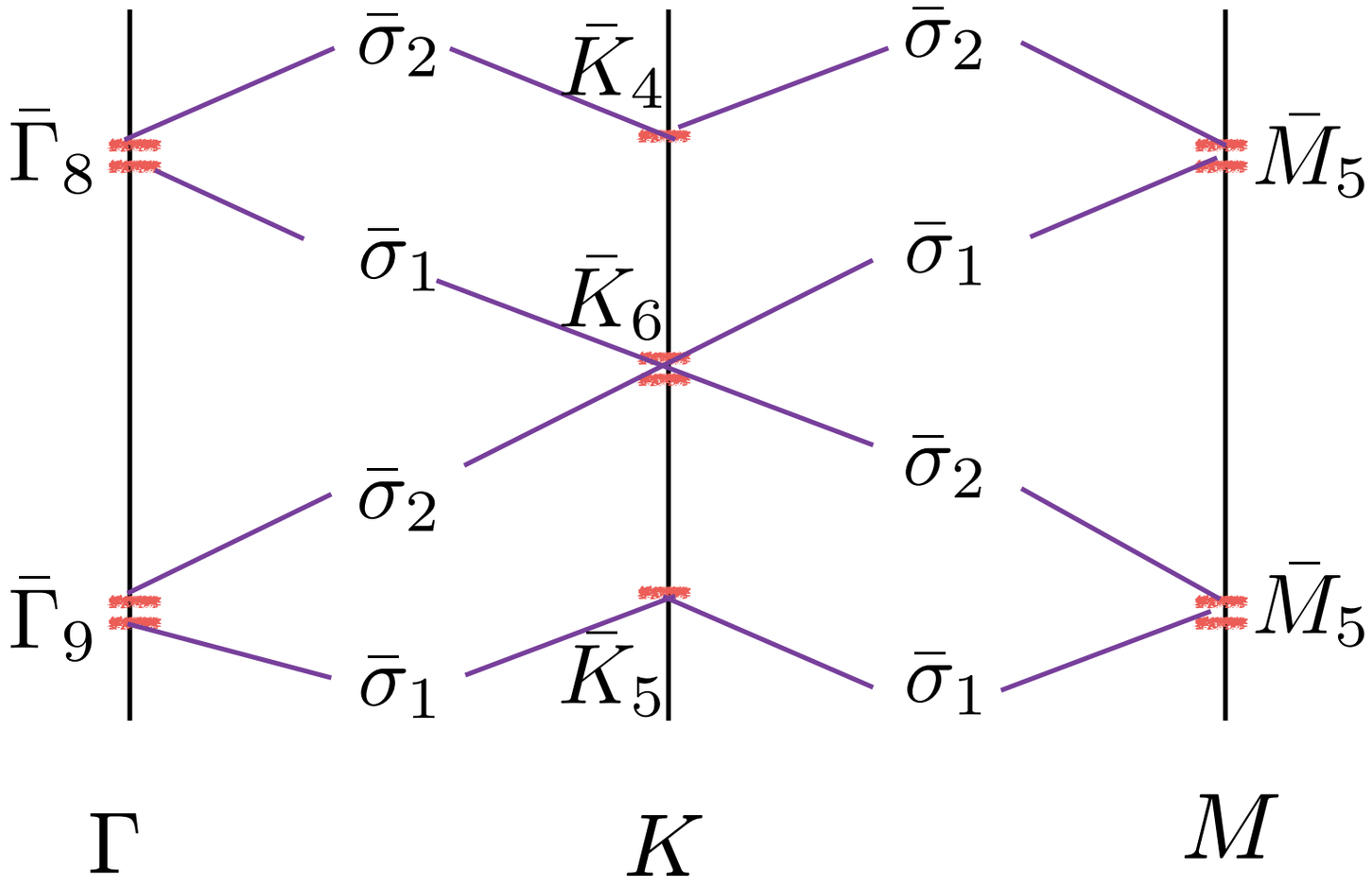
Strategy for finding topological materials

1. enumerate elementary bands ✓
2. determine whether bands can be gapped



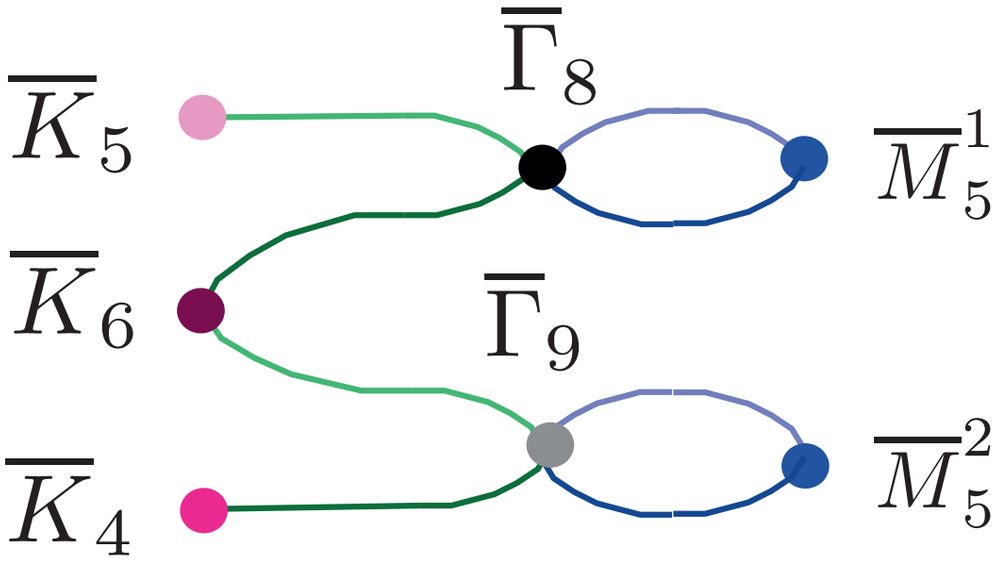
Compatibility relations determine connectivity

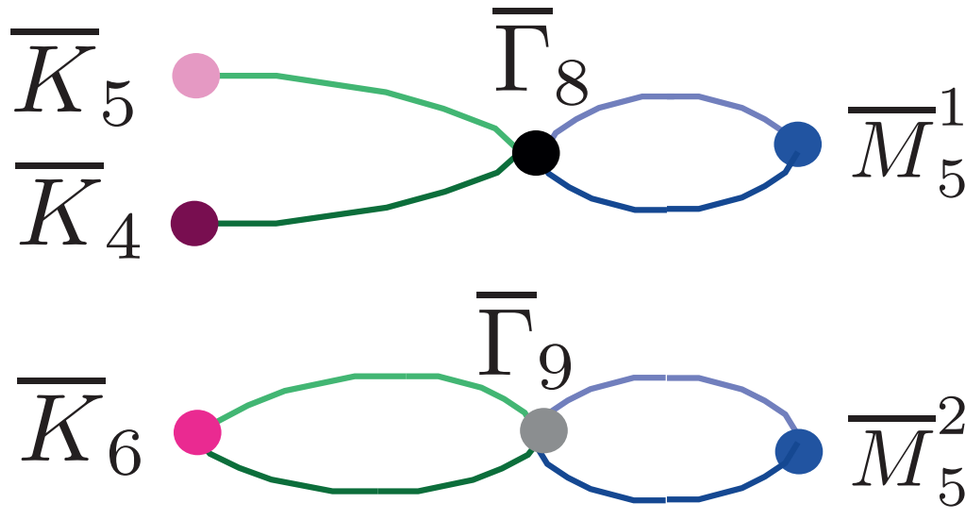




- Compatibility between points and lines
- One label per line segment
- Lines with same symmetry label gap

Symmetry does not uniquely determine connectivity

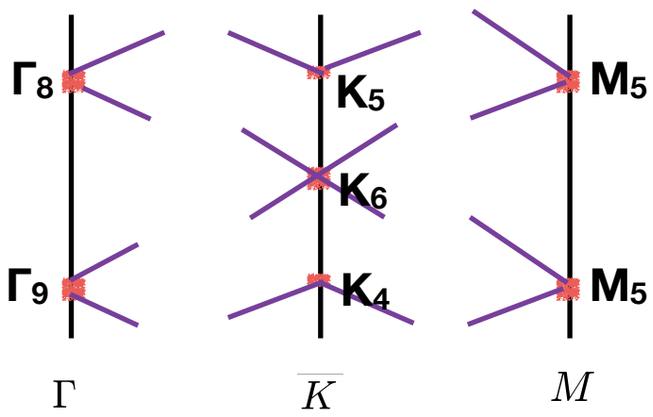


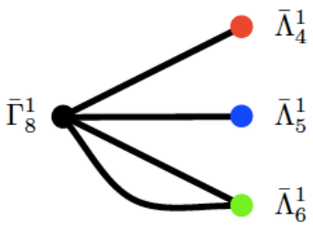


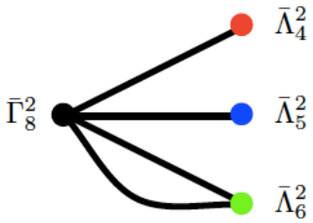
Computing connectivity is harder than symmetry irreps

Map to graph theory

MGV, .., **JC**, et al., PRE 96, 023310 (2017);
BB, .., **JC,** et al, PRB 97, 035138 (2018))







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: distinct band connectivities

$A_1 =$

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

http://www.cryst.ehu.es/ **bilbao crystallographic server**

Band-representations with time-reversal symmetry of the Double Space Group *P6mm* (No. 183)

and Wyckoff position 2b:(1/3,2/3,z)

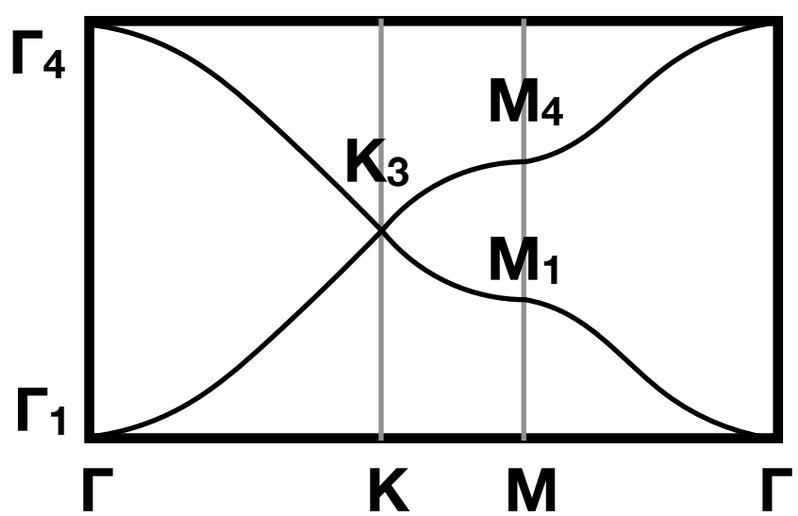
spinless s, p_z

Orbital →

Can it gap? →

Band-Rep.	$A_1\uparrow G(2)$	$A_2\uparrow G(2)$	$E\uparrow G(4)$	${}^1\bar{E}{}^2\bar{E}\uparrow G(4)$	$E_1\uparrow G(4)$
Band-type	Elementary	Elementary	Elementary	Elementary	Elementary
Decomposable\ Indecomposable	Indecomposable	Indecomposable	Decomposable	Decomposable	Decomposable
Γ:(0,0,0)	$\Gamma_1(1) \oplus \Gamma_4(1)$	$\Gamma_2(1) \oplus \Gamma_3(1)$	$\Gamma_5(2) \oplus \Gamma_6(2)$	$2\,\Gamma_7(2)$	$\Gamma_8(2) \oplus \Gamma_9(2)$
A:(0,0,1/2)	$A_1(1) \oplus A_4(1)$	$A_2(1) \oplus A_3(1)$	$A_5(2) \oplus A_6(2)$	$2\,\bar{A}_7(2)$	$\bar{A}_8(2) \oplus \bar{A}_9(2)$
K:(1/3,1/3,0)	$K_3(2)$	$K_3(2)$	$K_1(1) \oplus K_2(1) \oplus K_3(2)$	$2\,\bar{K}_6(2)$	$\bar{K}_4(1) \oplus \bar{K}_5(1) \oplus \bar{K}_6(2)$
H:(1/3,1/3,1/2)	$H_3(2)$	$H_3(2)$	$H_1(1) \oplus H_2(1) \oplus H_3(2)$	$2\,\bar{H}_6(2)$	$\bar{H}_4(1) \oplus \bar{H}_5(1) \oplus \bar{H}_6(2)$
M:(1/2,0,0)	$M_1(1) \oplus M_4(1)$	$M_2(1) \oplus M_3(1)$	$M_1(1) \oplus M_2(1) \oplus M_3(1) \oplus M_4(1)$	$2\,\bar{M}_5(2)$	$2\,\bar{M}_5(2)$
L:(1/2,0,1/2)	$L_1(1) \oplus L_4(1)$	$L_2(1) \oplus L_3(1)$	$L_1(1) \oplus L_2(1) \oplus L_3(1) \oplus L_4(1)$	$2\,\bar{L}_5(2)$	$2\,\bar{L}_5(2)$

Graphene without SOC has a Dirac point



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Band-representations with time-reversal symmetry of the Double Space Group *P6mm* (No. 183)

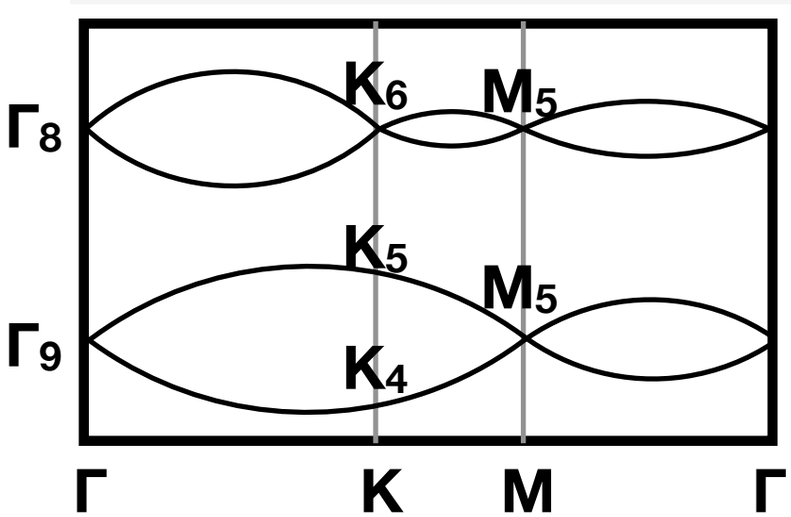
and Wyckoff position 2b:(1/3,2/3,z)

spinful s, p_z

Orbital →

Can it gap? →

Band-Rep.	$A_1\uparrow G(2)$	$A_2\uparrow G(2)$	$E\uparrow G(4)$	$^1\bar{E}^2\bar{E}\uparrow G(4)$	$E_1\uparrow G(4)$
Band-type	Elementary	Elementary	Elementary	Elementary	Elementary
Decomposable\ Indecomposable	Indecomposable	Indecomposable	Decomposable	Decomposable	Decomposable
Γ:(0,0,0)	$\Gamma_1(1) \oplus \Gamma_4(1)$	$\Gamma_2(1) \oplus \Gamma_3(1)$	$\Gamma_5(2) \oplus \Gamma_6(2)$	$2\,\Gamma_7(2)$	$\Gamma_8(2) \oplus \Gamma_9(2)$
A:(0,0,1/2)	$A_1(1) \oplus A_4(1)$	$A_2(1) \oplus A_3(1)$	$A_5(2) \oplus A_6(2)$	$2\,\bar{A}_7(2)$	$\bar{A}_8(2) \oplus \bar{A}_9(2)$
K:(1/3,1/3,0)	$K_3(2)$	$K_3(2)$	$K_1(1) \oplus K_2(1) \oplus K_3(2)$	$2\,\bar{K}_6(2)$	$\bar{K}_4(1) \oplus \bar{K}_5(1) \oplus \bar{K}_6(2)$
H:(1/3,1/3,1/2)	$H_3(2)$	$H_3(2)$	$H_1(1) \oplus H_2(1) \oplus H_3(2)$	$2\,\bar{H}_6(2)$	$\bar{H}_4(1) \oplus \bar{H}_5(1) \oplus \bar{H}_6(2)$
M:(1/2,0,0)	$M_1(1) \oplus M_4(1)$	$M_2(1) \oplus M_3(1)$	$M_1(1) \oplus M_2(1) \oplus M_3(1) \oplus M_4(1)$	$2\,\bar{M}_5(2)$	$2\,\bar{M}_5(2)$
L:(1/2,0,1/2)	$L_1(1) \oplus L_4(1)$	$L_2(1) \oplus L_3(1)$	$L_1(1) \oplus L_2(1) \oplus L_3(1) \oplus L_4(1)$	$2\,\bar{L}_5(2)$	$2\,\bar{L}_5(2)$



Graphene w SOC can be topological insulator
(Kane Mele PRL 2005)

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

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Band-representations with time-reversal symmetry of the Double Space Group *P6mm* (No. 183)

and Wyckoff position 2b:(1/3,2/3,z)

spinful $p_{x,y}$

Orbital →

Can it gap? →

Band-Rep.	$A_1\uparrow G(2)$	$A_2\uparrow G(2)$	$E\uparrow G(4)$	$^1\bar{E}^2\bar{E}\uparrow G(4)$	$E_1\uparrow G(4)$
Band-type	Elementary	Elementary	Elementary	Elementary	Elementary
Decomposable\ Indecomposable	Indecomposable	Indecomposable	Decomposable	Decomposable	Decomposable
Γ:(0,0,0)	$\Gamma_1(1) \oplus \Gamma_4(1)$	$\Gamma_2(1) \oplus \Gamma_3(1)$	$\Gamma_5(2) \oplus \Gamma_6(2)$	$2\,\Gamma_7(2)$	$\Gamma_8(2) \oplus \Gamma_9(2)$
A:(0,0,1/2)	$A_1(1) \oplus A_4(1)$	$A_2(1) \oplus A_3(1)$	$A_5(2) \oplus A_6(2)$	$2\,\bar{A}_7(2)$	$\bar{A}_8(2) \oplus \bar{A}_9(2)$
K:(1/3,1/3,0)	$K_3(2)$	$K_3(2)$	$K_1(1) \oplus K_2(1) \oplus K_3(2)$	$2\,\bar{K}_6(2)$	$\bar{K}_4(1) \oplus \bar{K}_5(1) \oplus \bar{K}_6(2)$
H:(1/3,1/3,1/2)	$H_3(2)$	$H_3(2)$	$H_1(1) \oplus H_2(1) \oplus H_3(2)$	$2\,\bar{H}_6(2)$	$\bar{H}_4(1) \oplus \bar{H}_5(1) \oplus \bar{H}_6(2)$
			$M_1(1) \oplus M_2(1) \oplus M_3(1) \oplus M_4(1)$	$2\,\bar{M}_5(2)$	$2\,\bar{M}_5(2)$
			$L_1(1) \oplus L_2(1) \oplus L_3(1) \oplus L_4(1)$	$2\,\bar{L}_5(2)$	$2\,\bar{L}_5(2)$

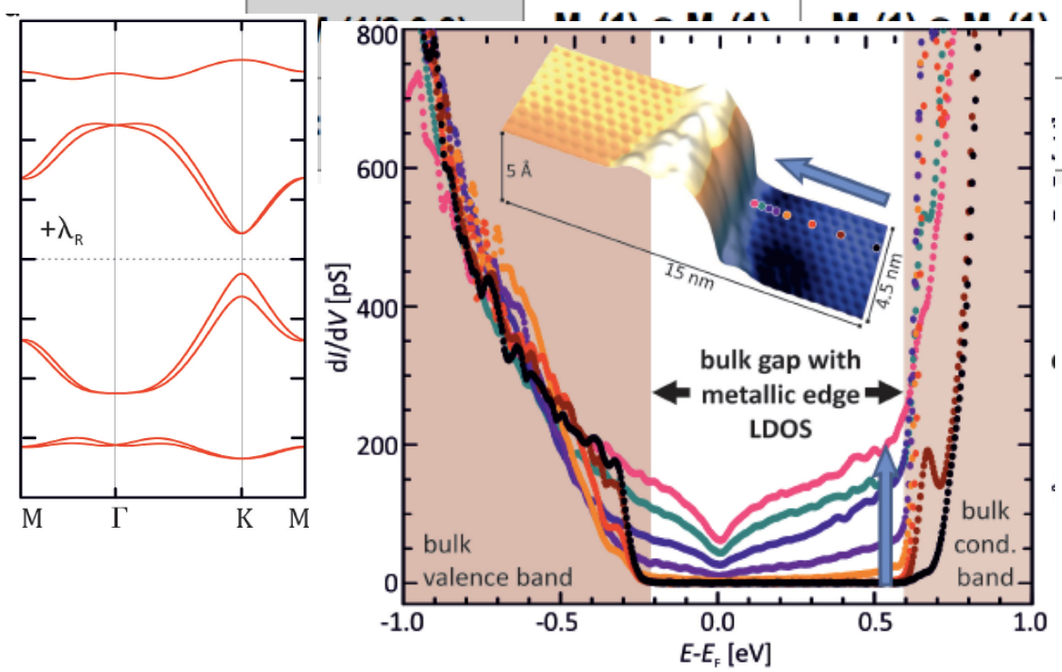

Figure 4 Spectroscopy of the Edge State

Science

Bismuthene on a SiC substrate: A candidate for a high-temperature quantum spin Hall material

F. Reis,[1]* G. Li,[2,3]* L. Dudy,[1] M. Bauernfeind,[1] S. Glass,[1] W. Hanke,[3] R. Thomale,[3] J. Schäfer,[1]† R. Claessen[1]

Group theory and phase diagram:
JC, et al, PRL 120, 266401 (2018)

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

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Band-representations with time-reversal symmetry of the Double Space Group *P6mm* (No. 183)

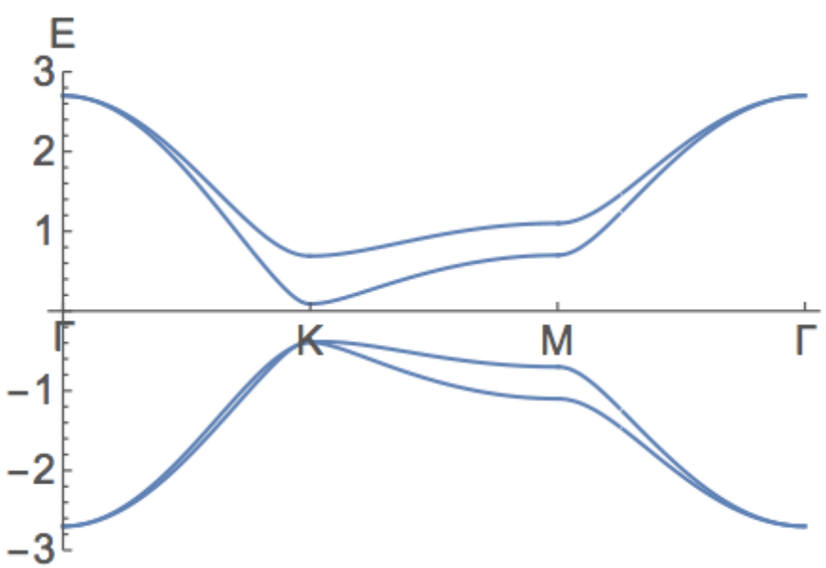
and Wyckoff position 2b:(1/3,2/3,z)

spinless $p_{x,y}$

Orbital →

Can it gap? →

Band-Rep.	$A_1\uparrow G(2)$	$A_2\uparrow G(2)$	$E\uparrow G(4)$	${}^1\bar{E}^2\bar{E}\uparrow G(4)$	$E_1\uparrow G(4)$
Band-type	Elementary	Elementary	Elementary	Elementary	Elementary
Decomposable\ Indecomposable	Indecomposable	Indecomposable	Decomposable	Decomposable	Decomposable
Γ:(0,0,0)	$\Gamma_1(1) \oplus \Gamma_4(1)$	$\Gamma_2(1) \oplus \Gamma_3(1)$	$\Gamma_5(2) \oplus \Gamma_6(2)$	$2\,\Gamma_7(2)$	$\Gamma_8(2) \oplus \Gamma_9(2)$
A:(0,0,1/2)	$A_1(1) \oplus A_4(1)$	$A_2(1) \oplus A_3(1)$	$A_5(2) \oplus A_6(2)$	$2\,\bar{A}_7(2)$	$\bar{A}_8(2) \oplus \bar{A}_9(2)$
K:(1/3,1/3,0)	$K_3(2)$	$K_3(2)$	$K_1(1) \oplus K_2(1) \oplus K_3(2)$	$2\,\bar{K}_6(2)$	$\bar{K}_4(1) \oplus \bar{K}_5(1) \oplus \bar{K}_6(2)$
H:(1/3,1/3,1/2)	$H_3(2)$	$H_3(2)$	$H_1(1) \oplus H_2(1) \oplus H_3(2)$	$2\,\bar{H}_6(2)$	$\bar{H}_4(1) \oplus \bar{H}_5(1) \oplus \bar{H}_6(2)$
M:(1/2,0,0)	$M_1(1) \oplus M_4(1)$	$M_2(1) \oplus M_3(1)$	$M_1(1) \oplus M_2(1) \oplus M_3(1) \oplus M_4(1)$	$2\,\bar{M}_5(2)$	$2\,\bar{M}_5(2)$
			$L_1(1) \oplus L_2(1) \oplus L_3(1) \oplus L_4(1)$	$2\,\bar{L}_5(2)$	$2\,\bar{L}_5(2)$



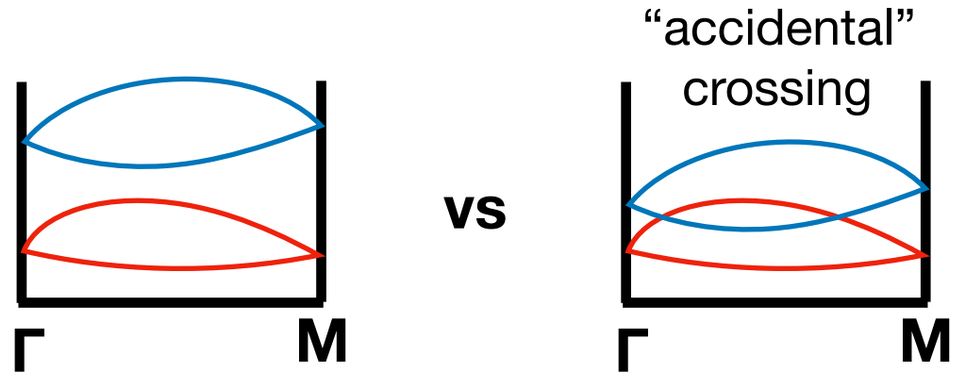
Spinless topological phase protected by C_{2z}:
JC, et al, PRL 120, 266401 (2018)

Now we are ready to find some materials!

Challenges….

Real materials have many orbitals (although usually <3 relevant near Fermi level)

Symmetry can permit a gapped phase, but can't require it

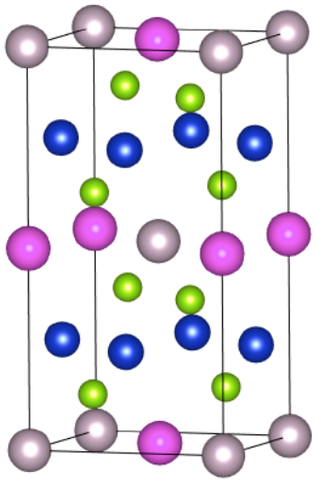


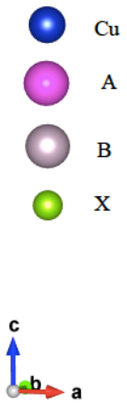
Small band gaps

Claudia Felser
(Max Planck)

Zhijun Wang
(Princeton)

Maia Garcia Vergniory
(DIPC, EHU)





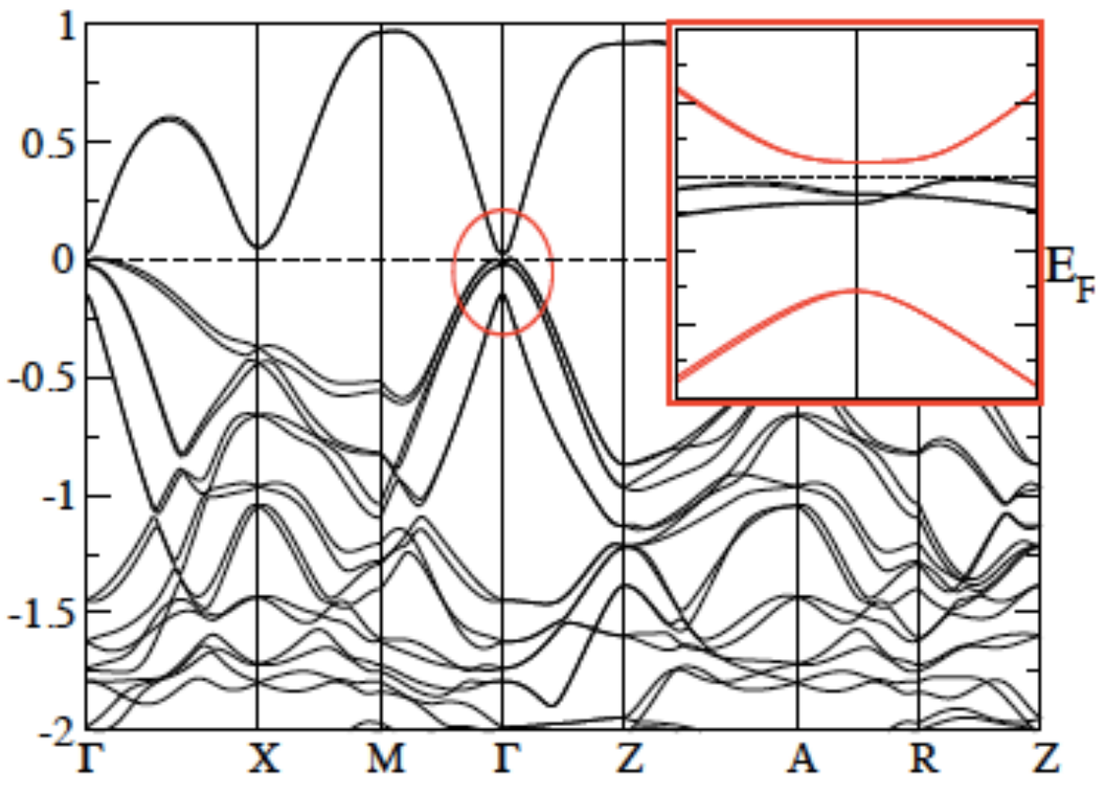
SG $I\bar{4}2m$

New topological materials: Cu_3ABX_4 class

Non-centrosymmetric

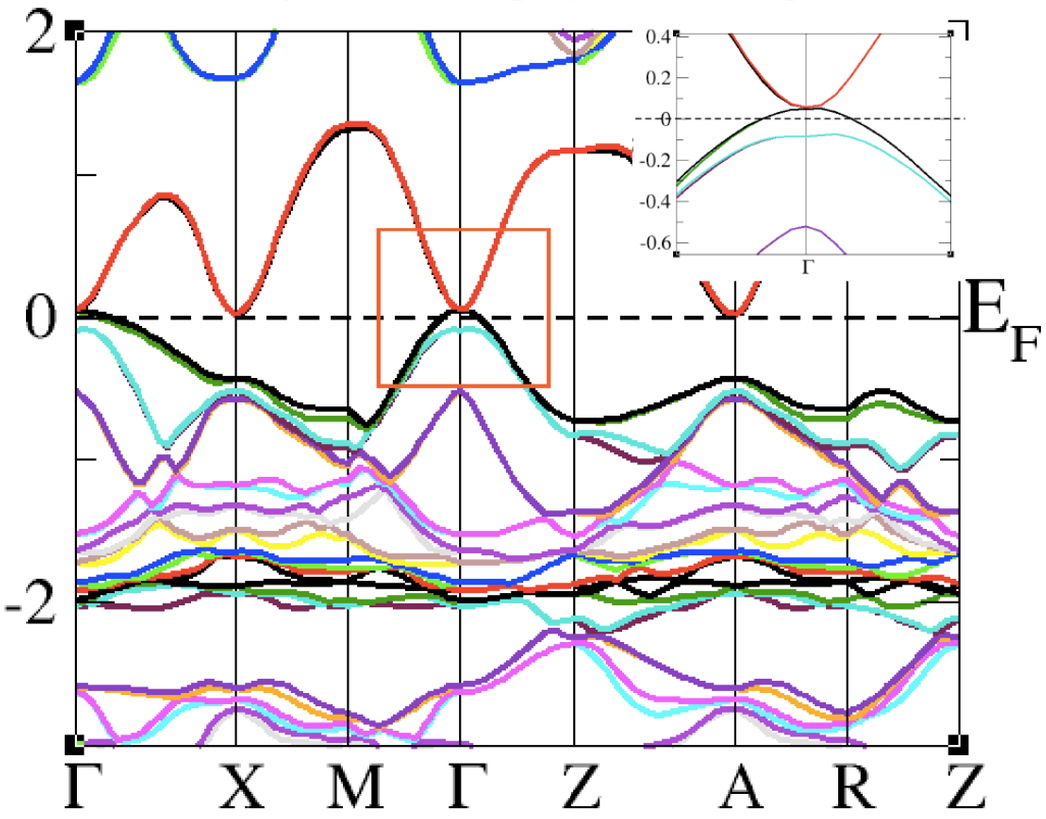
Cu_2SbCuS_4

Upper bands topological



$Cu_2SnHgSe_4$

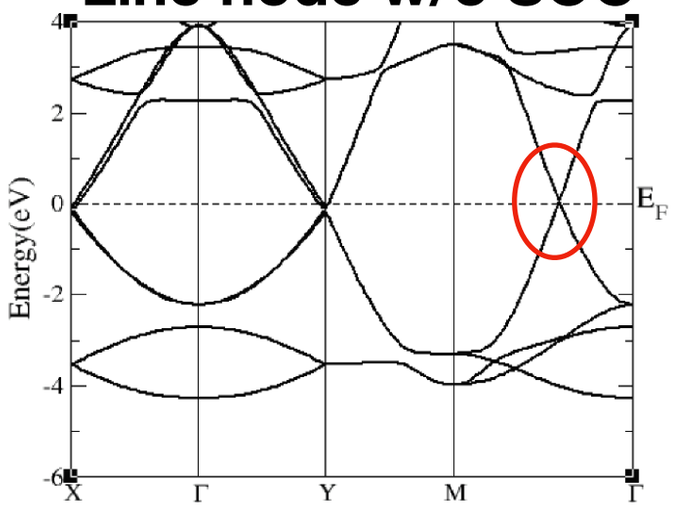
(Very) small gap, strong TI



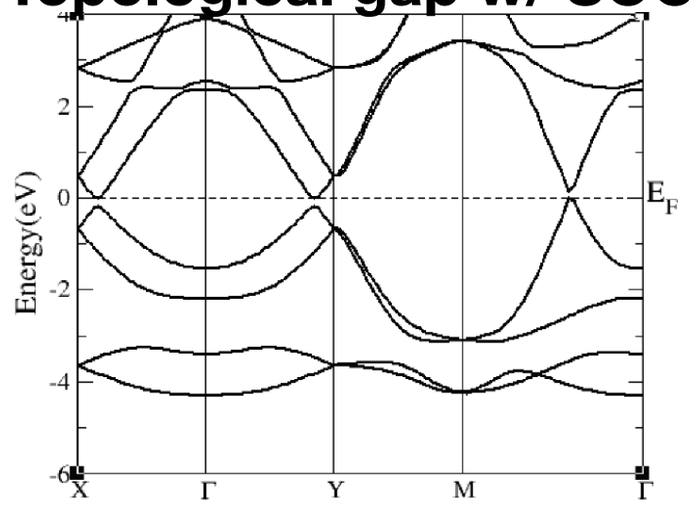
Weak topological insulators with infinitesimal SOC

Bands at E_F from Bi square net

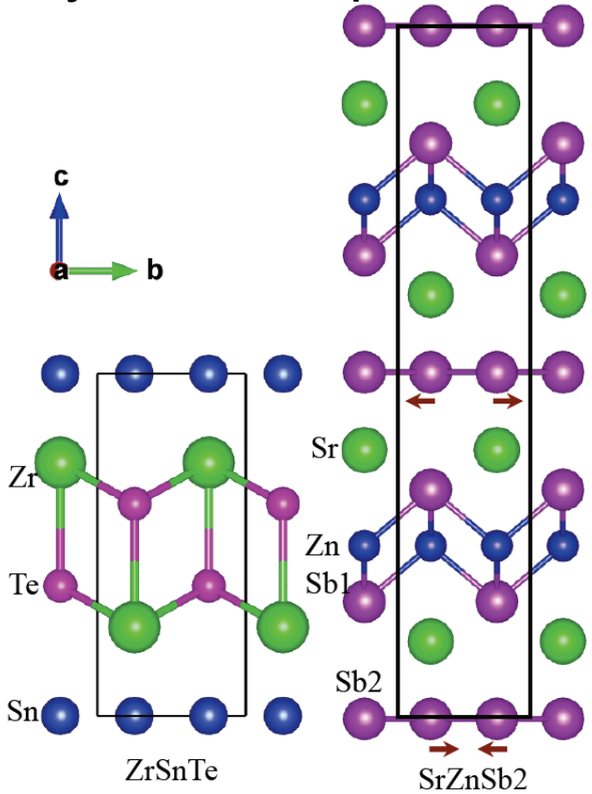
Line node w/o SOC



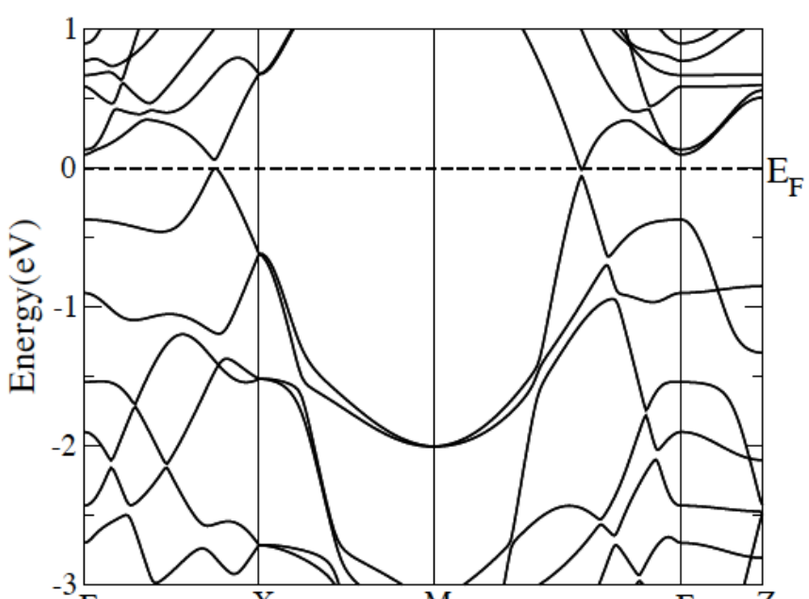
Topological gap w/ SOC



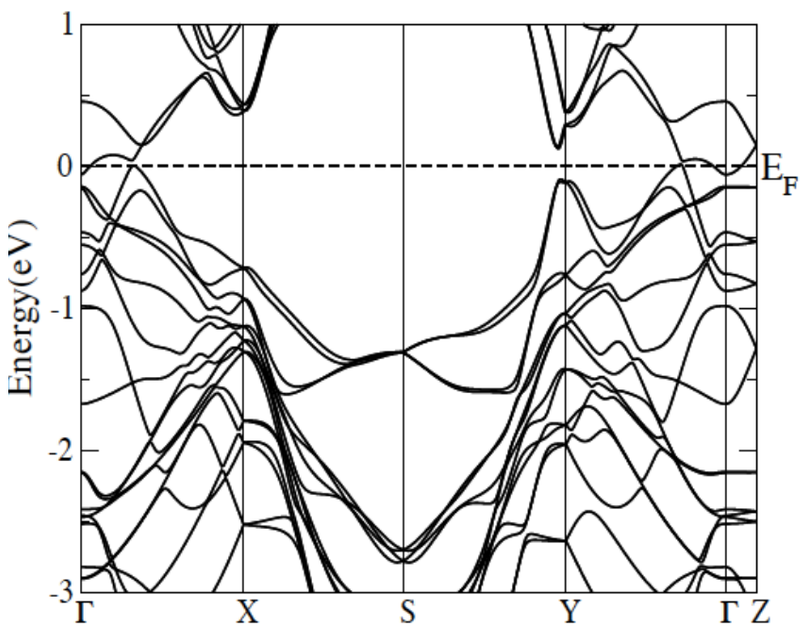
Layered compounds



a=b (P4/nmm) a≠b (P4/nma)



ZrSnTe

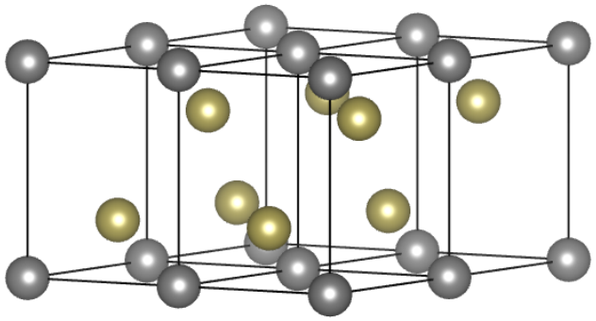


$SrZnSb_2$

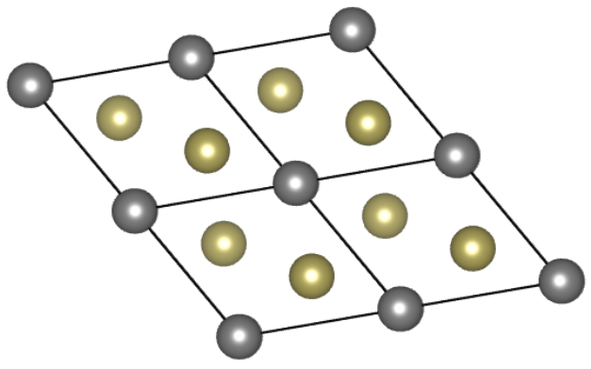
Many other compounds with this structure type

Type-II Dirac points in buckled honeycomb compounds

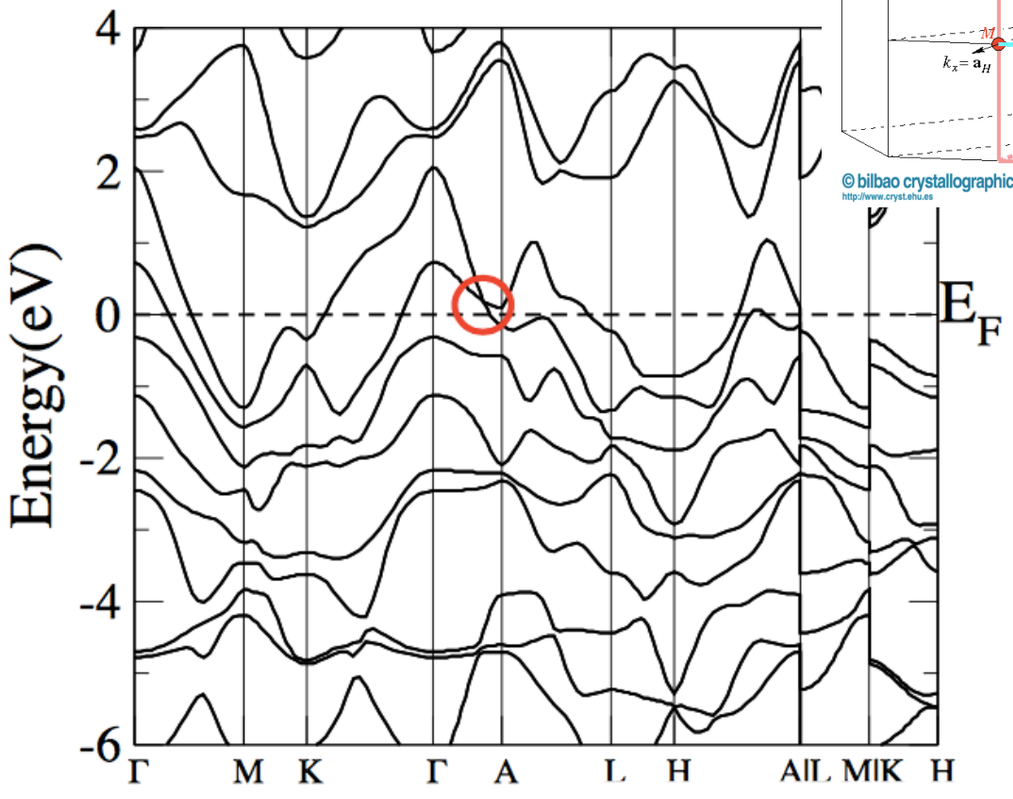
Bent honeycomb

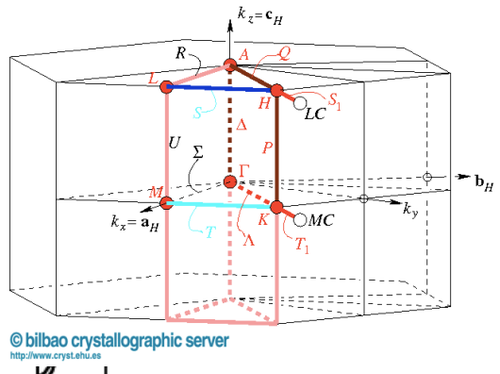


Top view

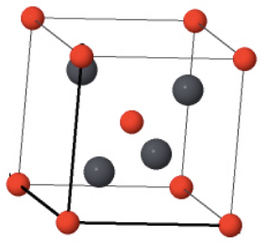


$IrTe_2$, P-3m1

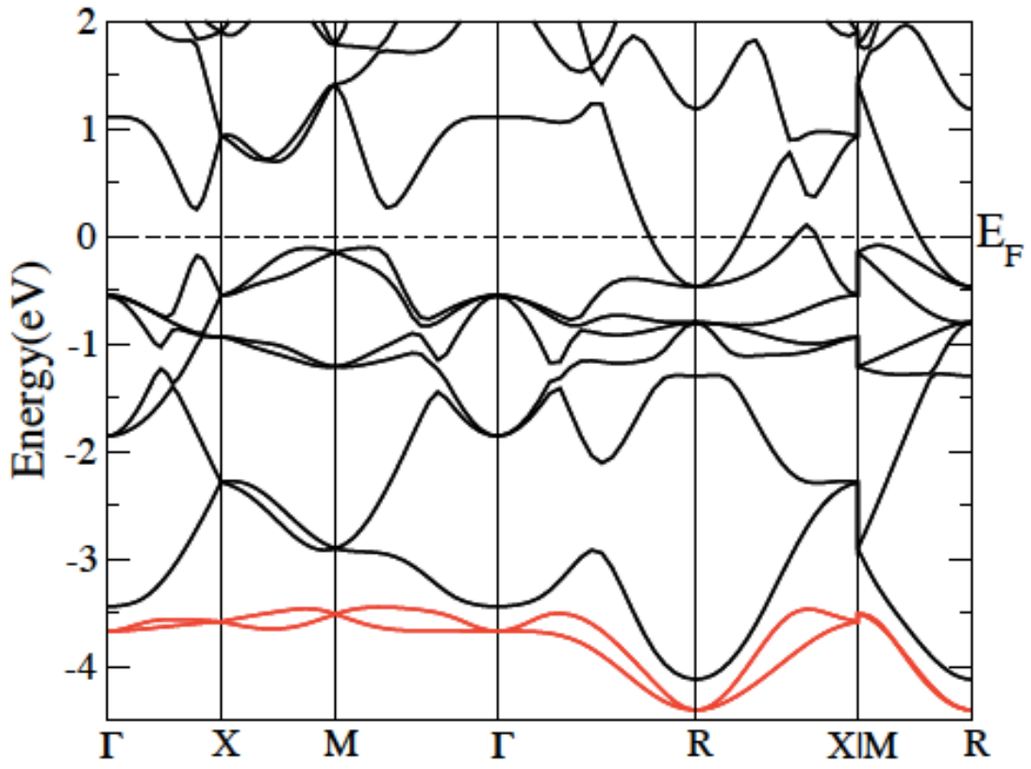




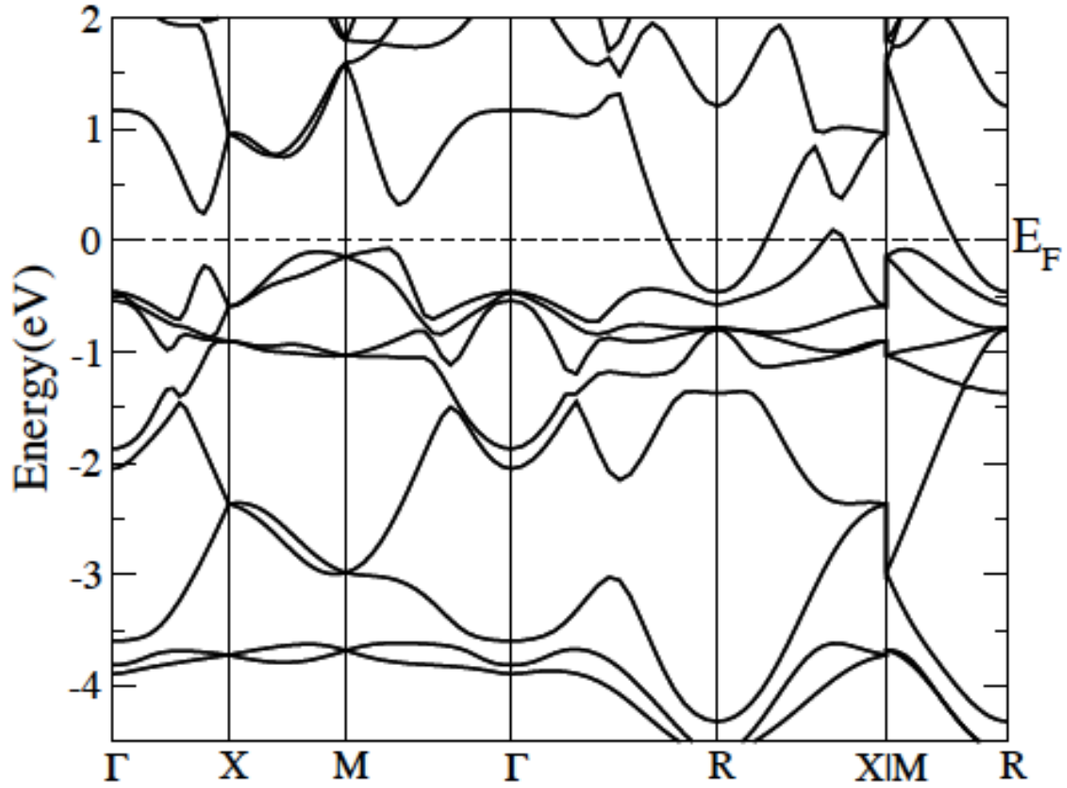
Strained PbO_2



(pic: ICSD)



Strain



Semi-metal; topological bands -3.5eV

Uniaxial strain opens topological gap near E_F

Topological quantum chemistry can diagnose and predict topological materials

JC et al., PRB 97, 035139 (2018); BB, **JC**, et al., *Nature* 547, 298–305 (2017)

Key: topological bands are not deformable to an atomic limit

1. Identify atomic limit band structures with symmetry ✓
2. Systematic search for topological bands ✓
3. New topological materials ✓