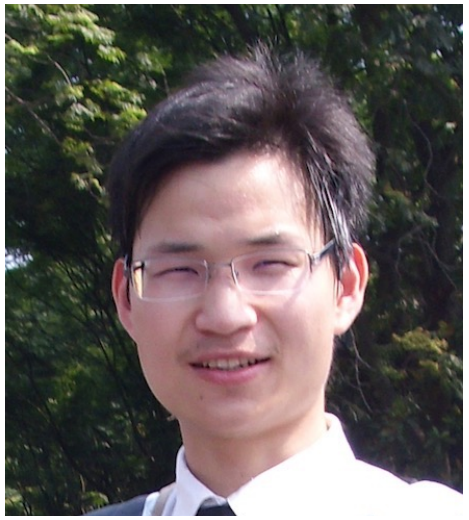
Topology from elementary band representations

Jennifer Cano
Princeton University

Collaborators

Barry Bradlyn (Princeton)



Zhijun Wang (Princeton)

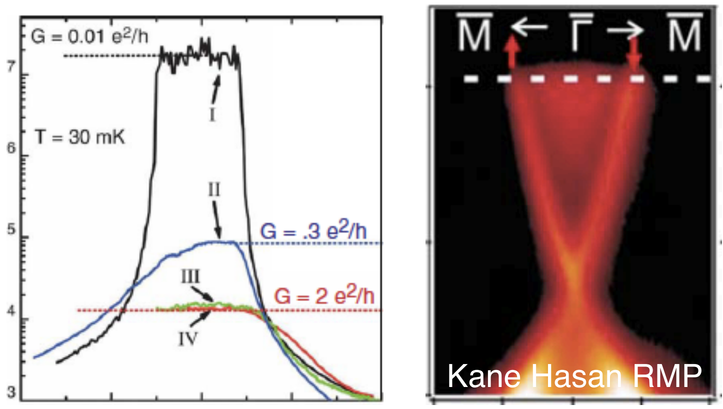
Maia Garcia Vergniory (DIPC, EHU)

Luis Elcoro (EHU)

Claudia Felser (Max Planck)

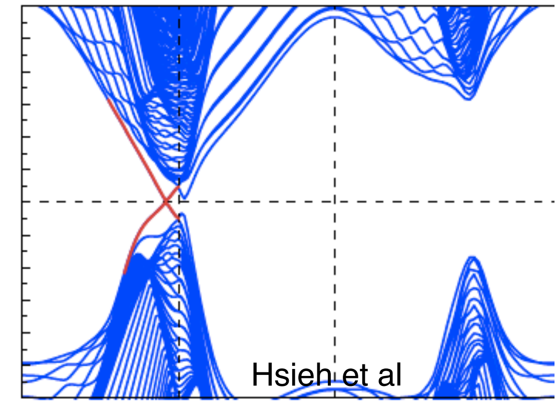
Mois Aroyo (EHU)

Andrei Bernevig (Princeton)



$\mathbb{Z}_2$

Topological insulators

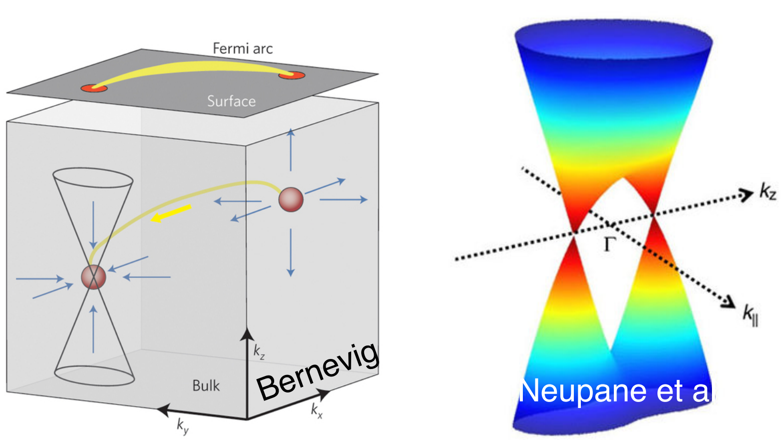


$\mathbb{Z}$

Mirror Chern Insulator

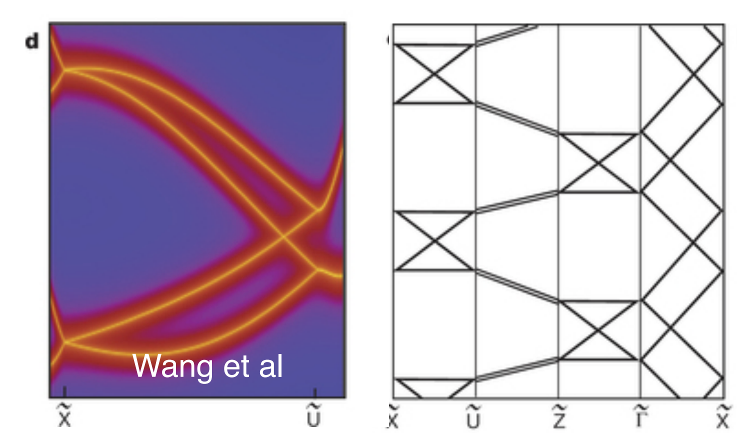
Topological Insulators and Topological Semimetals

$\mathbb{Z}$



$\mathbb{Z}_2$

Weyl and Dirac fermions



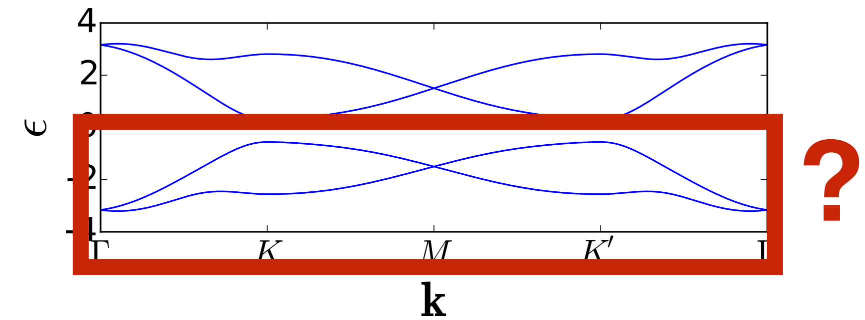
$\mathbb{Z}_4$

Hourglass fermions

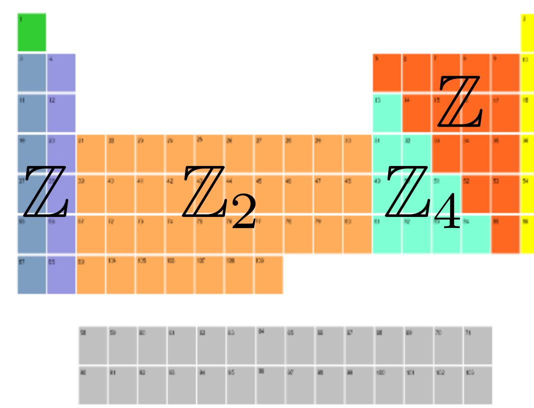
Piecewise classification of topological (crystalline) insulators

Open questions:

How do we know when the classification is complete?



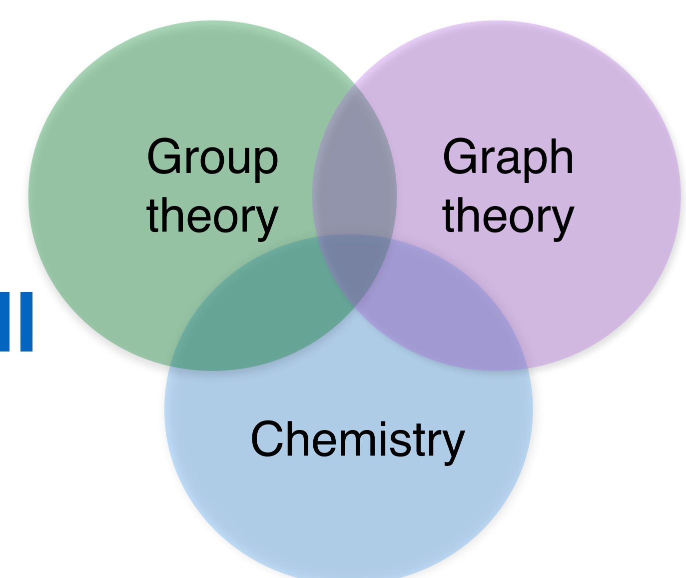
How can we find topological materials?



200000 materials in ICSD database:

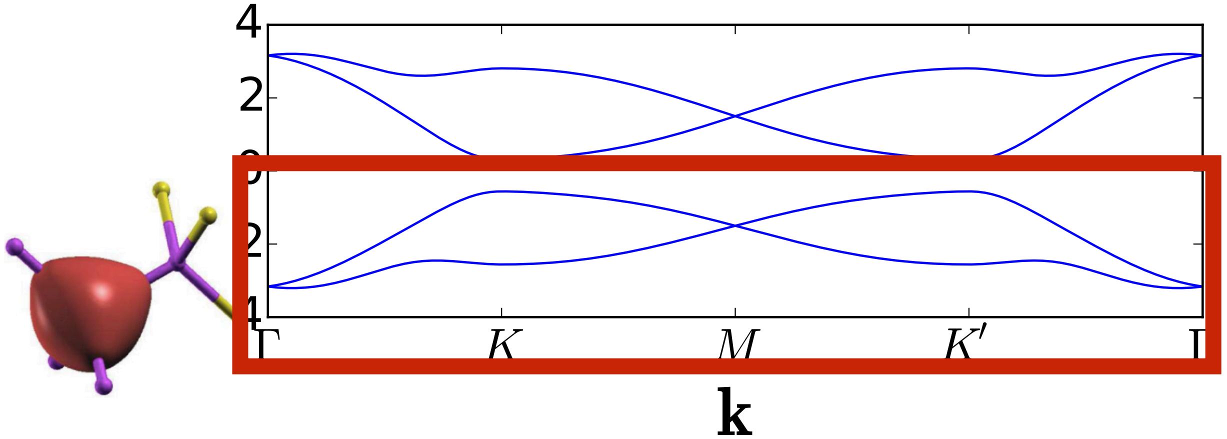
100 time reversal topological insulators
10 mirror Chern insulators
15 Weyl semimetals
15 Dirac semimetals
3 Non-Symmorphic topological insulators

Set of measure zero…
Are topological materials that esoteric?

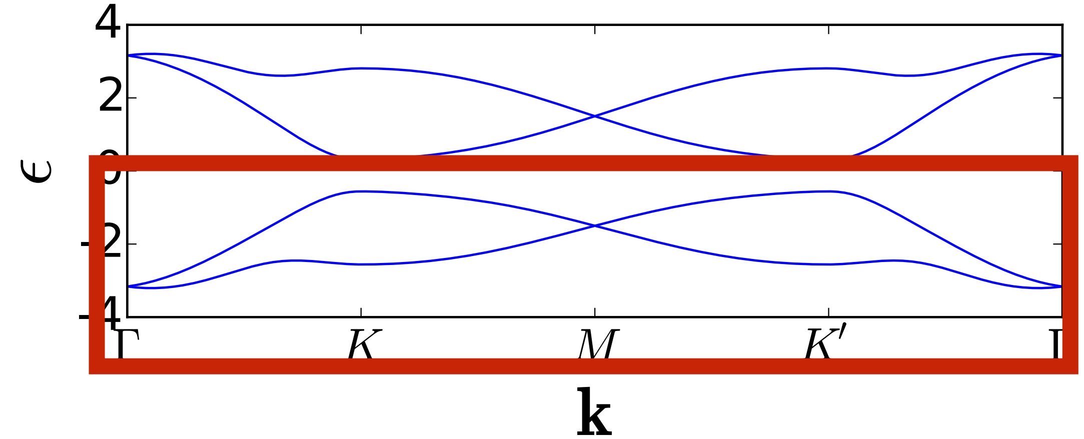


“Topological quantum chemistry”: captures all crystal symmetries and has predictive power

What distinguishes topological vs trivial band structures?



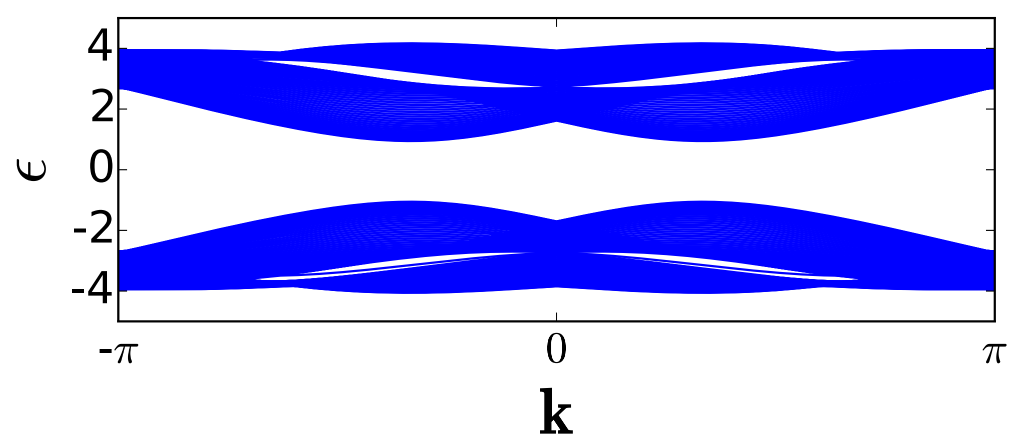
Localized Wannier functions exist
that obey crystal symmetry
(i.e., atomic limit)



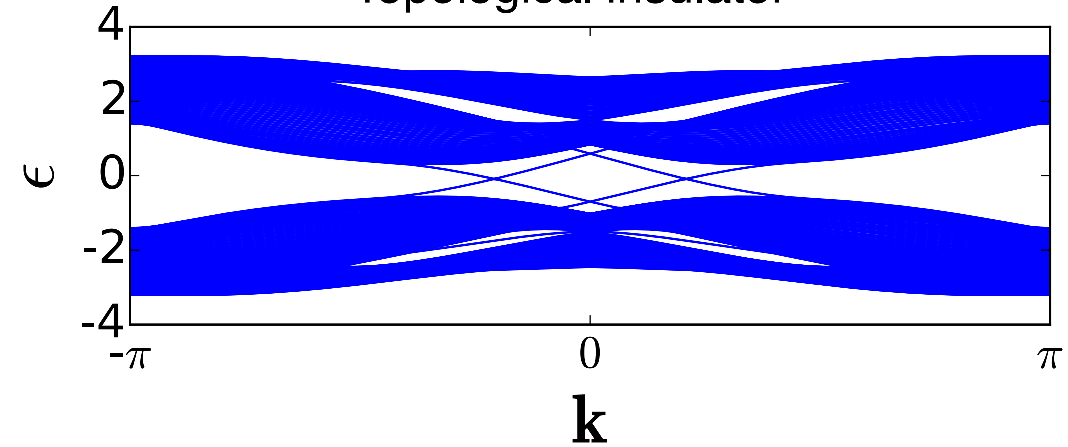
Localized Wannier functions do not exist
that obey crystal symmetry

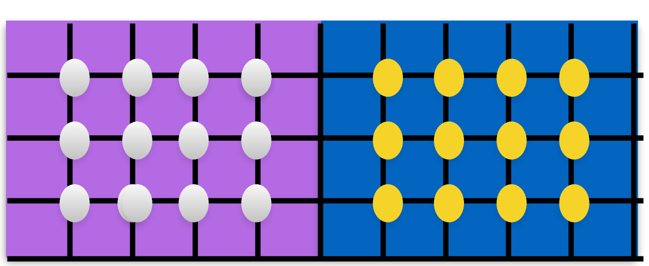
Fu, Kane (2007)
Soluyanov, Vanderbilt (2011)
Alexandradinata, et al (2014)

Atomic insulator



Topological insulator





If atomic limit exists
on both sides, then
no need for surface
states!

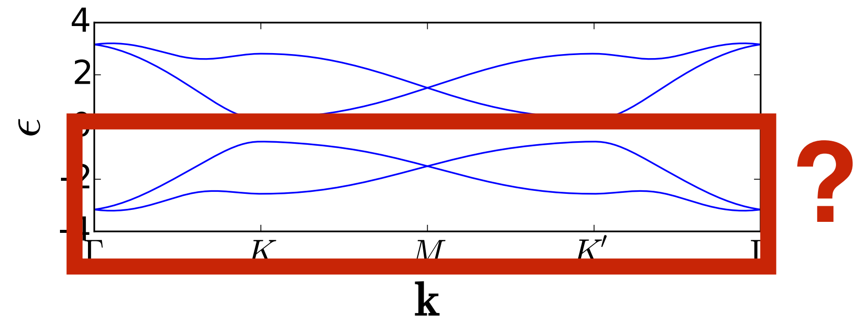
Diagnosing 3D topological phases: strategy

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

Topological phases lack an atomic limit

For each space group, enumerate all "atomic limits"

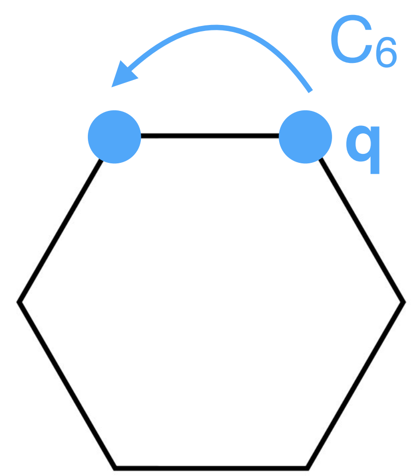
An arbitrary set of bands can be classified
by comparing to list



Connecting real space orbitals to topological properties ⇒ predictive power

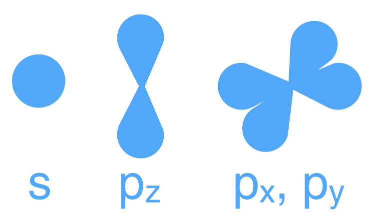
How to build an atomic limit

Consider one lattice site:



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

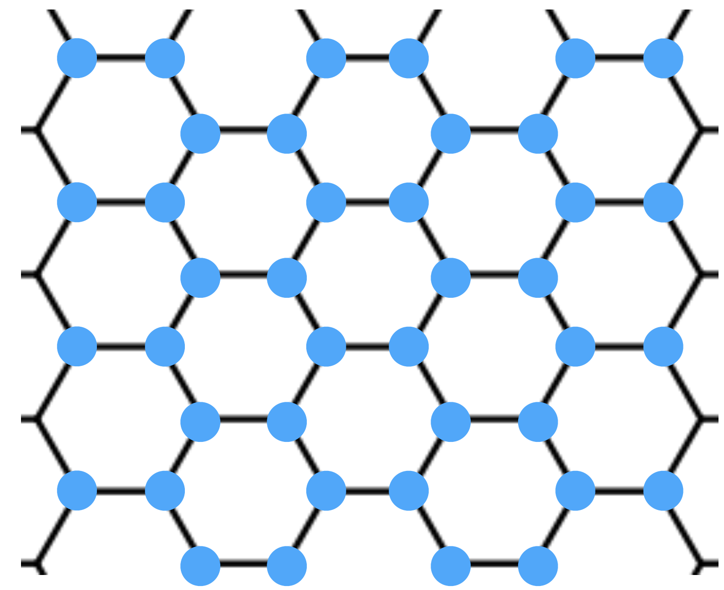
Orbitals at **q** transform under a rep, ρ, of $G_{\mathbf{q}}$



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

How to build an atomic limit

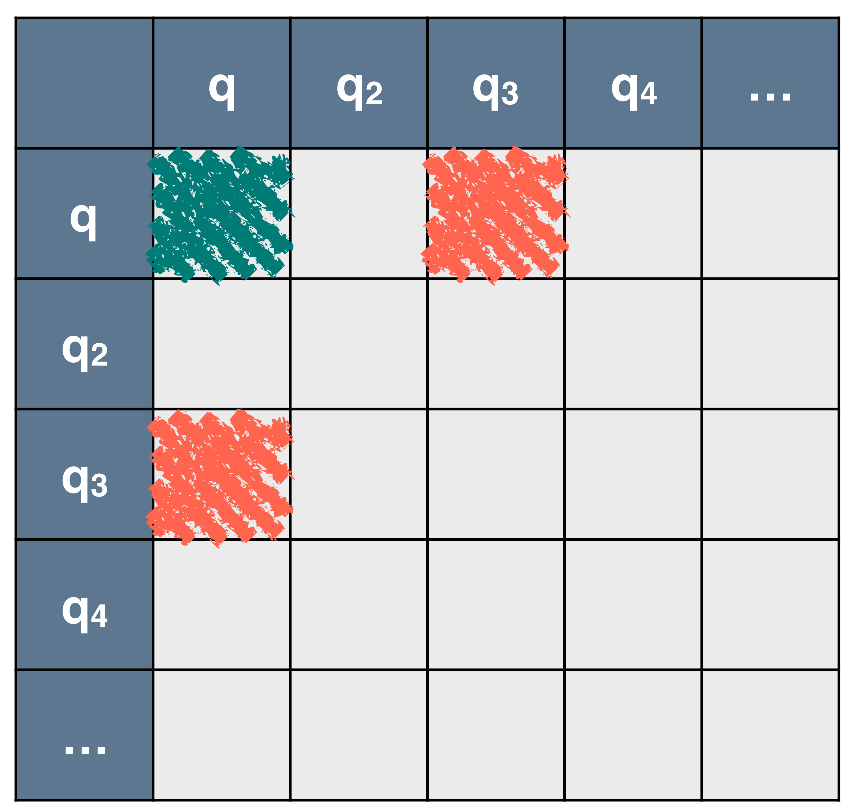
Act with full space group
➡ crystal symmetric atomic limit



Collection of all symmetry-related orbitals transforms under *induced representation*

$$\rho \uparrow S$$

Each symmetry operation represented by N x N matrix



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

Off-diagonal block if g interchanges sites

Atomic limit defines a “band representation”

Zak PRL 1980, PRB 1981, 1982

Fourier transformed representation

Diagonal blocks form representation of “little group of k”

gk = k+K

Each band representation has an atomic limit

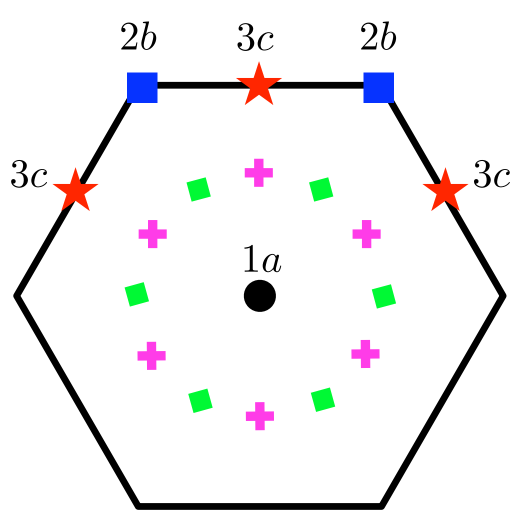
Elementary band reps cannot be decomposed into a sum of band representations

"Building bricks of band representations" - Zak

Necessary conditions for band rep to be elementary:

1. Orbitals transform as irrep of site-symmetry group

2. Atomic positions must be maximal: locally maximal symmetry



We have enumerated all elementary band reps and their symmetry labels

bilbao crystallographic server

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

Bradlyn et al, *Nature* 547, 298–305 (2017);
Vergniory et al, Phys Rev E 96, 023310 (2017);
Elcoro et al, J. Appl. Crys. 50, 1457 (2017);
Bradlyn, et al PRB 97, 035138 (2018);
Cano, et al PRB 97, 035139 (2018)

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

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

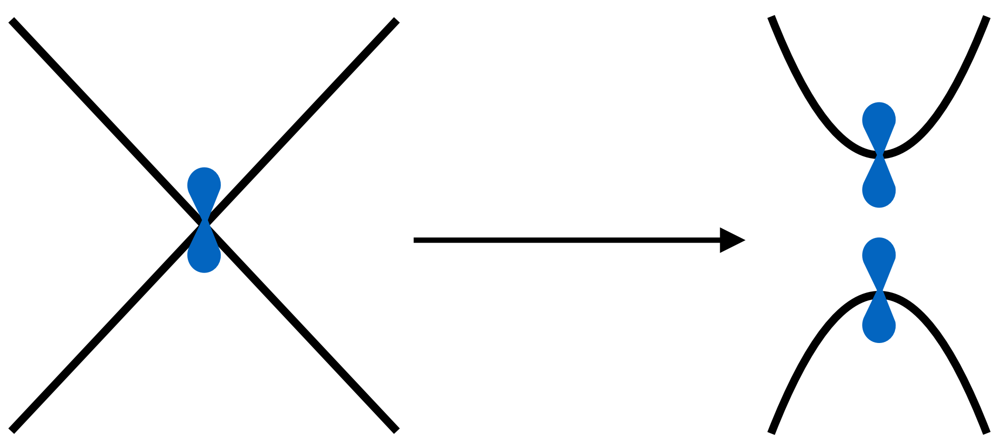
Atom arrangement

Orbital

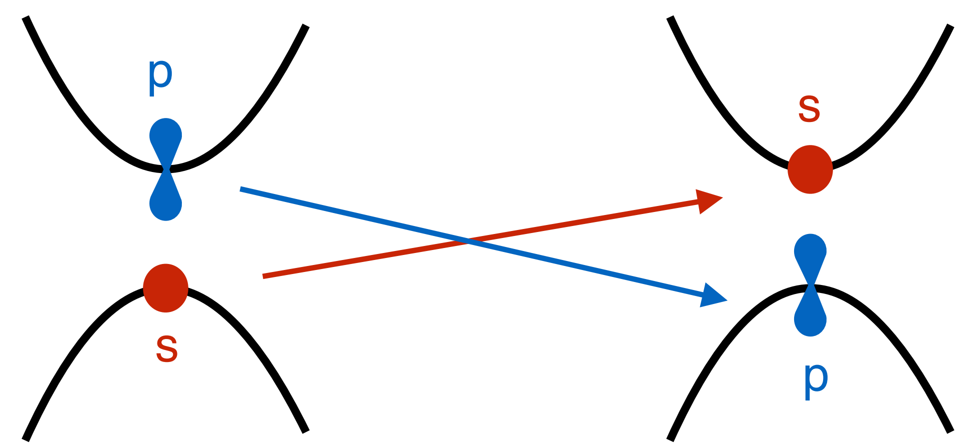
High-symmetry points

Topological bands are not band representations

Two routes to topological bands:



Disconnected elementary
band representation
(e.g., graphene)



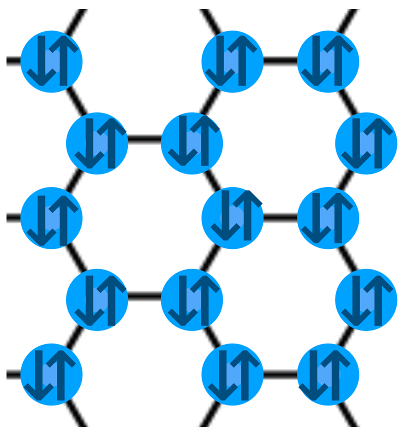
Multiple EBRs + band inversion

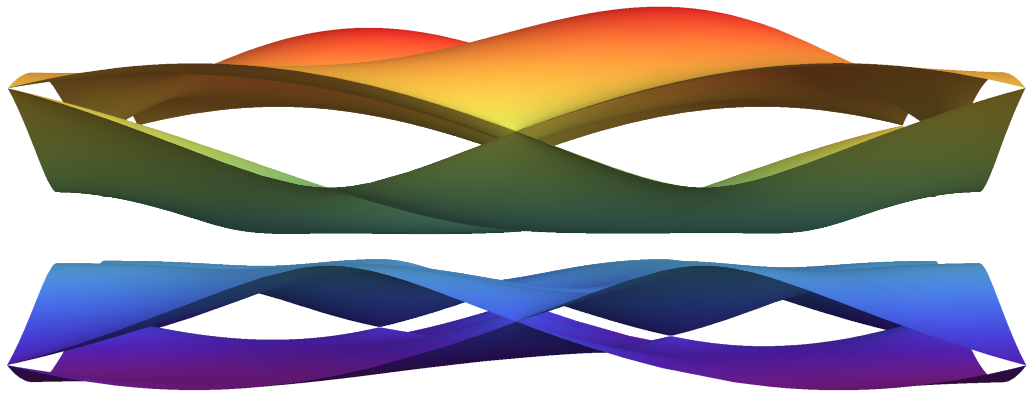
(e.g., HgTe)

Disconnected elementary bands are topological

JC et al., PRB 97, 035139 (2018), 1709.01935;
Bradlyn, **JC**, et al., *Nature* 547, 298–305 (2017), 1703.02050

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





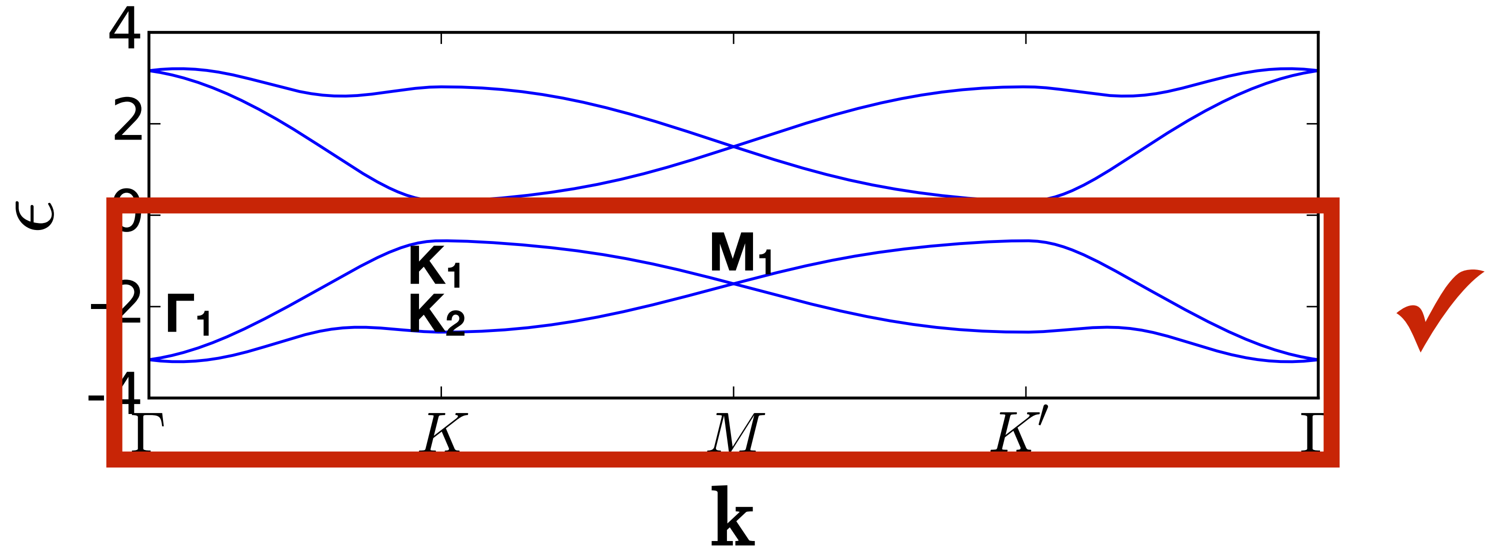
TR requires 4 sites per unit cell on honeycomb lattice

Two bands cannot have localized Wannier functions ⇒ topological!

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

We can identify topological bands by comparing to EBRs

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



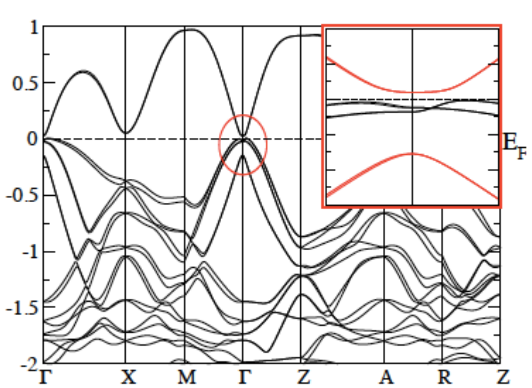
See also: Po, Vishwanath, Watanabe, Nature Comm. 8, 50 (2017),
Shiozaki, Sato, Gomi, PRB 95, 235425 (2017)

Steps to search for topological materials:

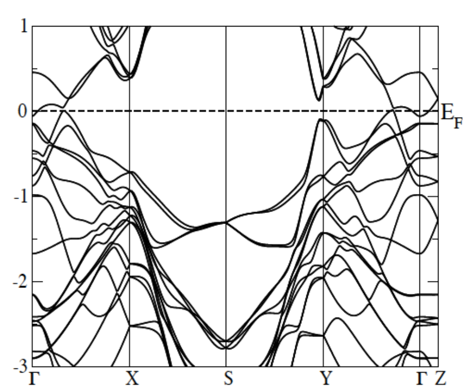
For every known chemical compound:

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

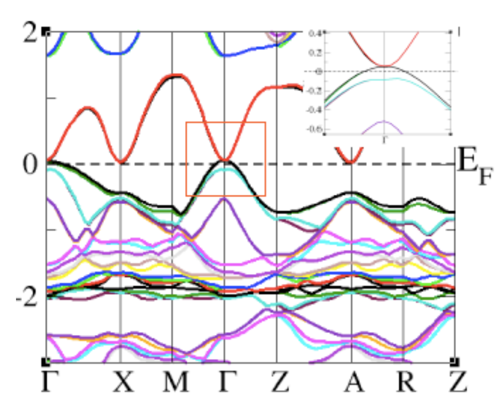
Other search algorithms: Bradlyn, JC, et al., *Nature* 547, 298–305



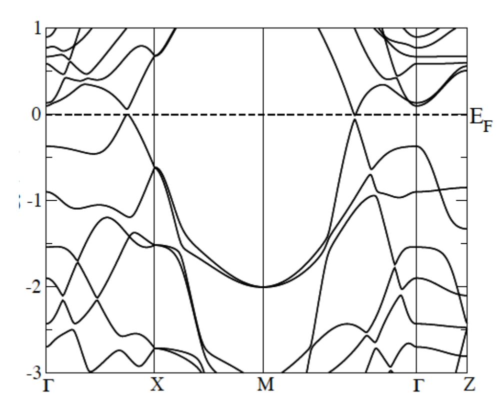
Cu_2SbCuS_4



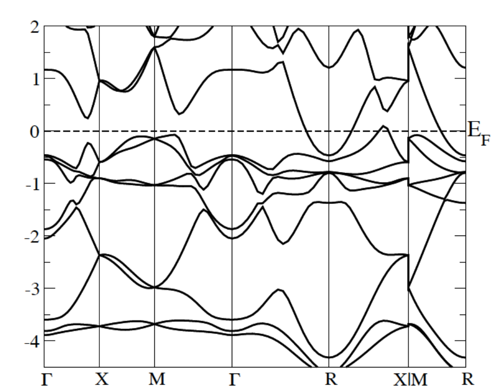
$SrZnSb_2$



$Cu_2SnHgSe_4$

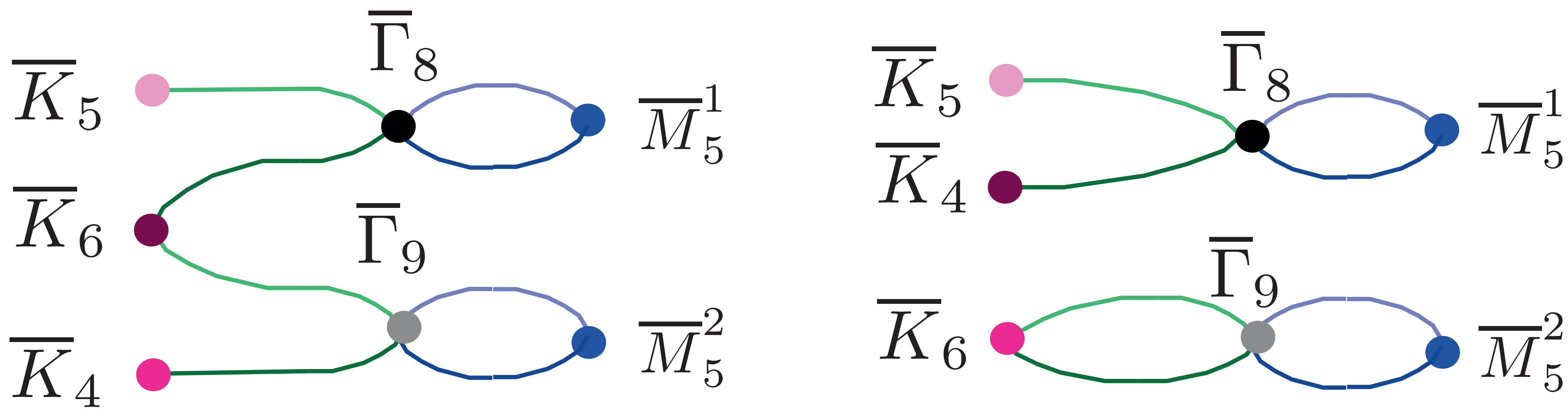


ZrSnTe



PbO_2

Symmetry does not uniquely determine connectivity



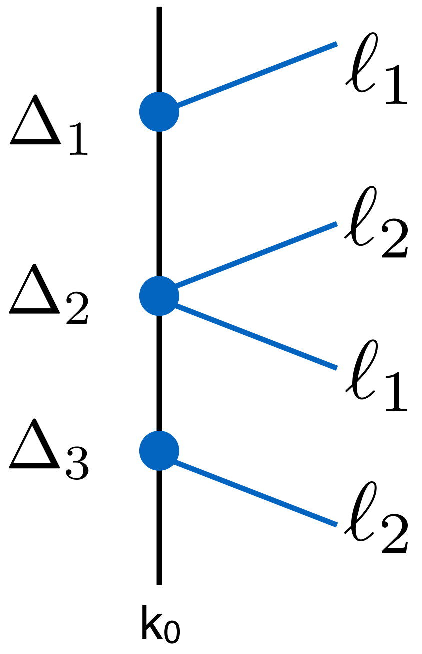
How to determine possible band connectivities?

Band connectivity is determined by irreps of little groups

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

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)

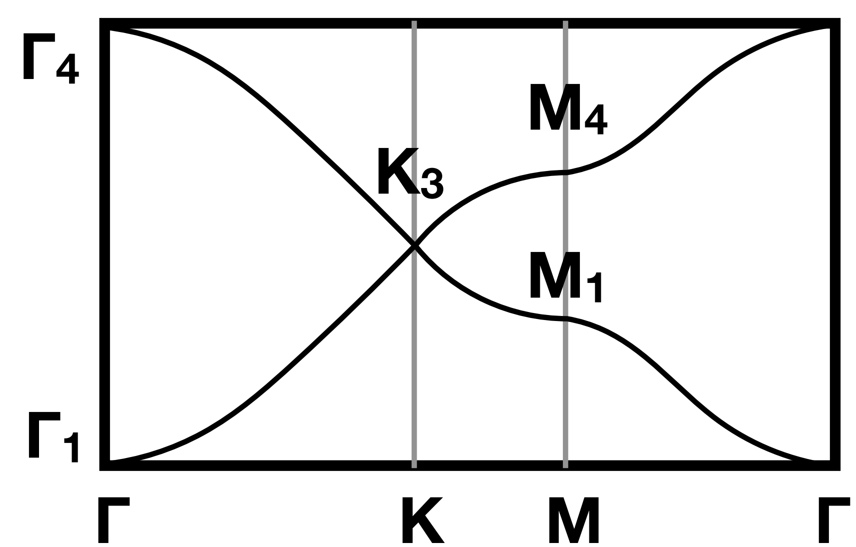
spinless s, p_z

Orbital → Band-Rep.

Can it gap? → Decomposable\Indecomposable

Band-Rep.	$A_1\uparrow G(2)$	$A_2\uparrow G(2)$	$E\uparrow G(4)$	$^1\bar{E}^2\bar{E}\uparrow G(4)$	$\bar{E}_1\uparrow G(4)$
Band-type	Elementary	Elementary	Elementary	Elementary	Elementary
Decomposable\Indecomposable	Indecomposable	Indecomposable	Decomposable	Decomposable	Decomposable
Γ:(0,0,0)	$\Gamma_1(1) \oplus \Gamma_4(1)$	$\Gamma_2(1) \oplus \Gamma_3(1)$	$\Gamma_5(2) \oplus \Gamma_6(2)$	$2\,\bar{\Gamma}_7(2)$	$\bar{\Gamma}_8(2) \oplus \bar{\Gamma}_9(2)$
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



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

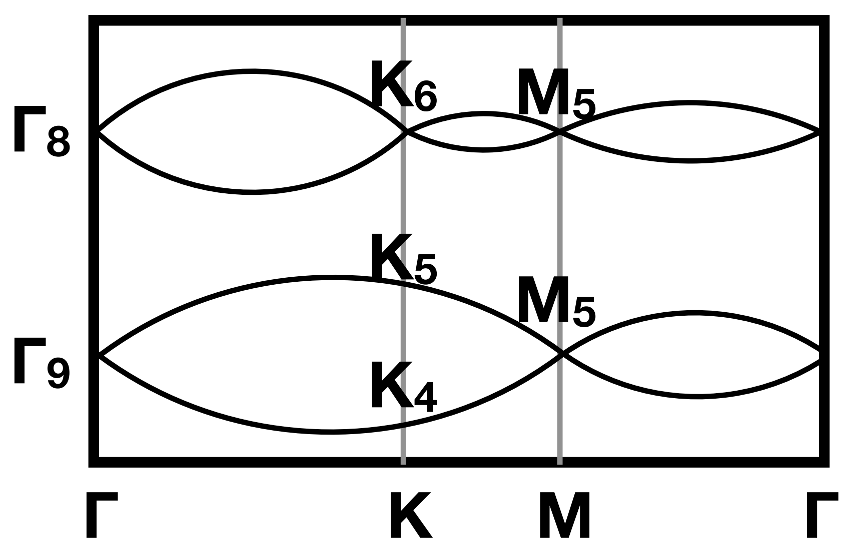
Band-representations with time-reversal symmetry of the Double Space Group *P6mm* (No. 183) and Wyckoff position 2b:(1/3,2/3,z)

spinful s, p_z

Orbital → Band-Rep.

Can it gap? → Decomposable\Indecomposable

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/

bilbao crystallographic server

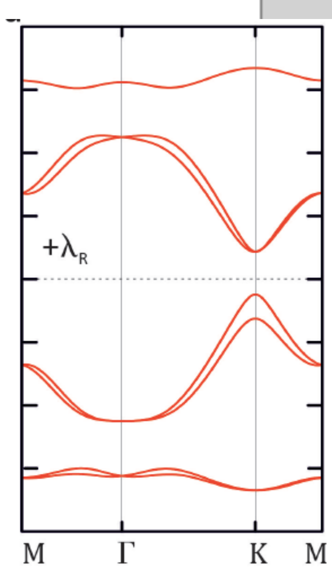
Band-representations with time-reversal symmetry of the Double Space Group *P6mm* (No. 183) and Wyckoff position 2b:(1/3,2/3,z)

spinful $p_{x,y}$

Orbital →

Can it gap? →

Band-Rep.	$A_1\uparrow G(2)$	$A_2\uparrow G(2)$	$E\uparrow G(4)$	$^1\bar{E}^2\bar{E}\uparrow G(4)$	$\bar{E}_1\uparrow G(4)$
Band-type	Elementary	Elementary	Elementary	Elementary	Elementary
Decomposable\ Indecomposable	Indecomposable	Indecomposable	Decomposable	Decomposable	Decomposable
Γ:(0,0,0)	$\Gamma_1(1) \oplus \Gamma_4(1)$	$\Gamma_2(1) \oplus \Gamma_3(1)$	$\Gamma_5(2) \oplus \Gamma_6(2)$	$2\,\bar{\Gamma}_7(2)$	$\bar{\Gamma}_8(2) \oplus \bar{\Gamma}_9(2)$
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)	$H_3(2)$	$H_3(2)$	$H_1(1) \oplus H_2(1) \oplus H_3(2)$	$2\,\bar{H}_6(2)$	$\bar{H}_4(1) \oplus \bar{H}_5(1) \oplus \bar{H}_6(2)$
[illegible]	[illegible]	[illegible]	$M_1(1) \oplus M_2(1) \oplus M_3(1) \oplus M_4(1)$	$2\,\bar{M}_5(2)$	$2\,\bar{M}_5(2)$
[illegible]	[illegible]	[illegible]	$L_1(1) \oplus L_2(1) \oplus L_3(1) \oplus L_4(1)$	$2\,\bar{L}_5(2)$	$2\,\bar{L}_5(2)$



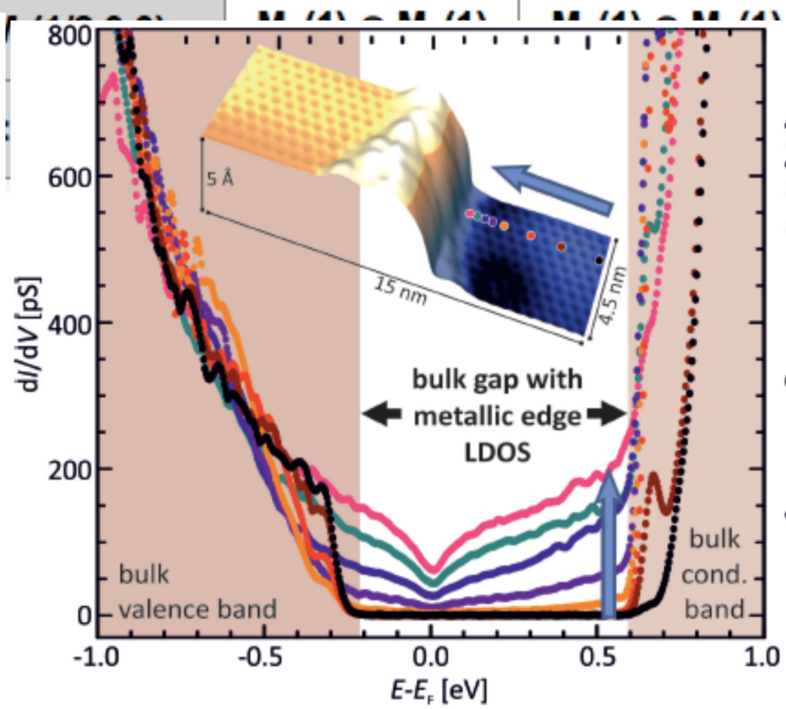


Figure 4 Spectroscopy of the Edge State

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)

Gapped elementary band representations are a place to look for topological materials

Lets try to understand them

1. Topological materials without SOC
2. Insulating gap = topological gap
3. Theoretical understanding

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 $p_{x,y}$

Orbital →

Can it gap? →

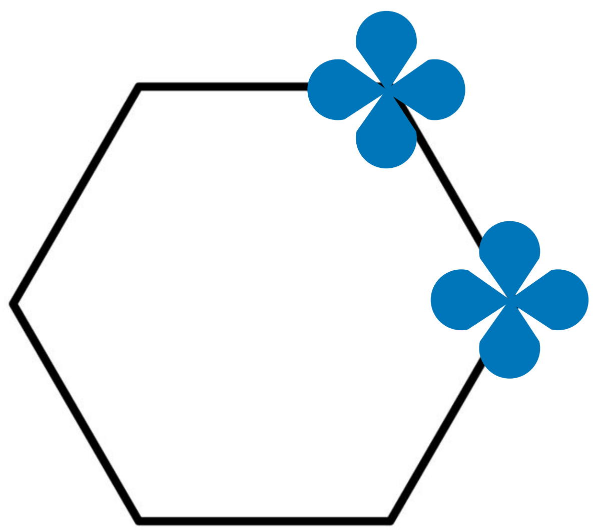
Band-Rep.	$A_1\uparrow G(2)$	$A_2\uparrow G(2)$	$E\uparrow G(4)$	$^1\bar{E}^2\bar{E}\uparrow G(4)$	$\bar{E}_1\uparrow G(4)$
Band-type	Elementary	Elementary	Elementary	Elementary	Elementary
Decomposable\ Indecomposable	Indecomposable	Indecomposable	Decomposable	Decomposable	Decomposable
Γ:(0,0,0)	$\Gamma_1(1) \oplus \Gamma_4(1)$	$\Gamma_2(1) \oplus \Gamma_3(1)$	$\Gamma_5(2) \oplus \Gamma_6(2)$	$2\ \bar{\Gamma}_7(2)$	$\bar{\Gamma}_8(2) \oplus \bar{\Gamma}_9(2)$
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)	$L_1(1) \oplus L_4(1)$	$L_2(1) \oplus L_3(1)$	$L_1(1) \oplus L_2(1) \oplus L_3(1) \oplus L_4(1)$	$2\ \bar{L}_5(2)$	$2\ \bar{L}_5(2)$

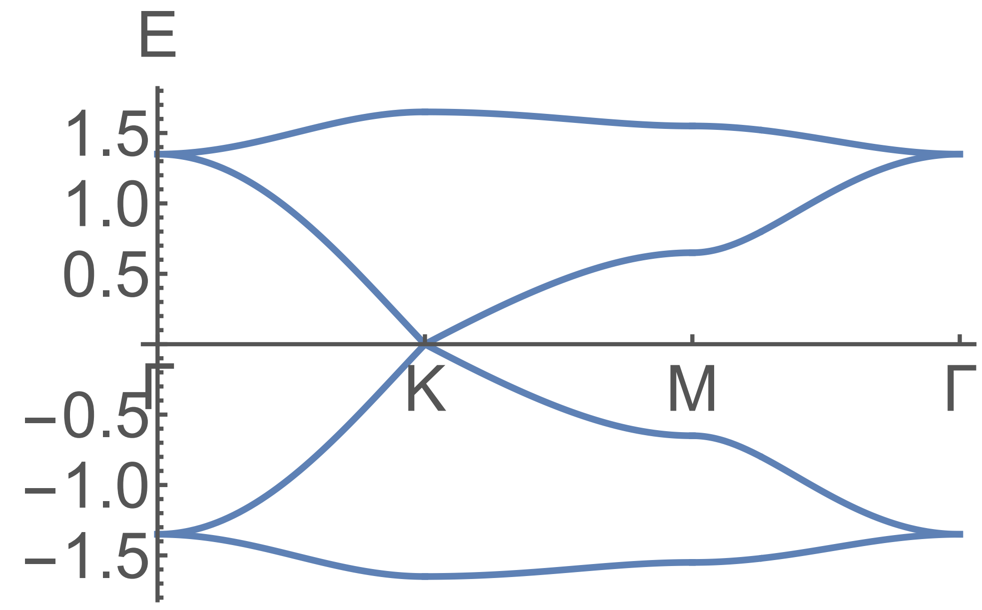
↓

Spinless topological crystalline insulator?

Ex 1: p_x, p_y orbitals on honeycomb

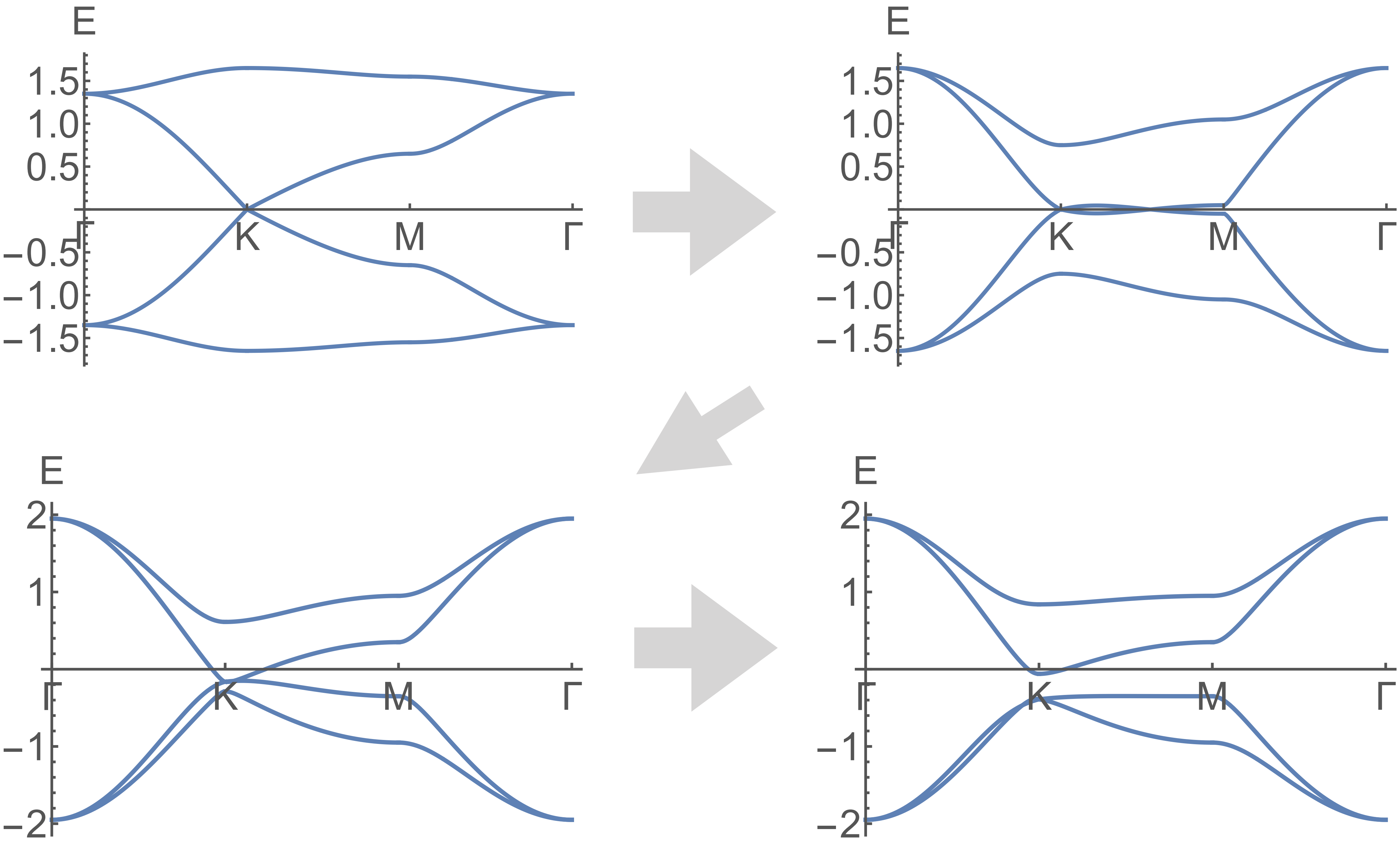
JC et al., PRL 120, 266401 (2018)



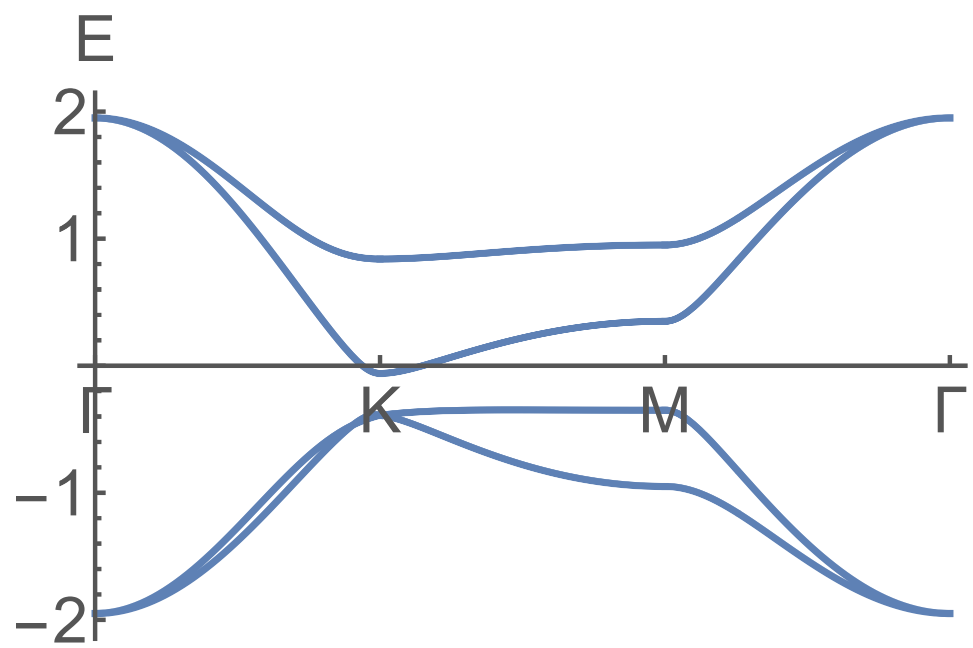


Nearest neighbor Hamiltonian

Ex 1: p_x, p_y orbitals on honeycomb



Ex 1: p_x, p_y orbitals on honeycomb

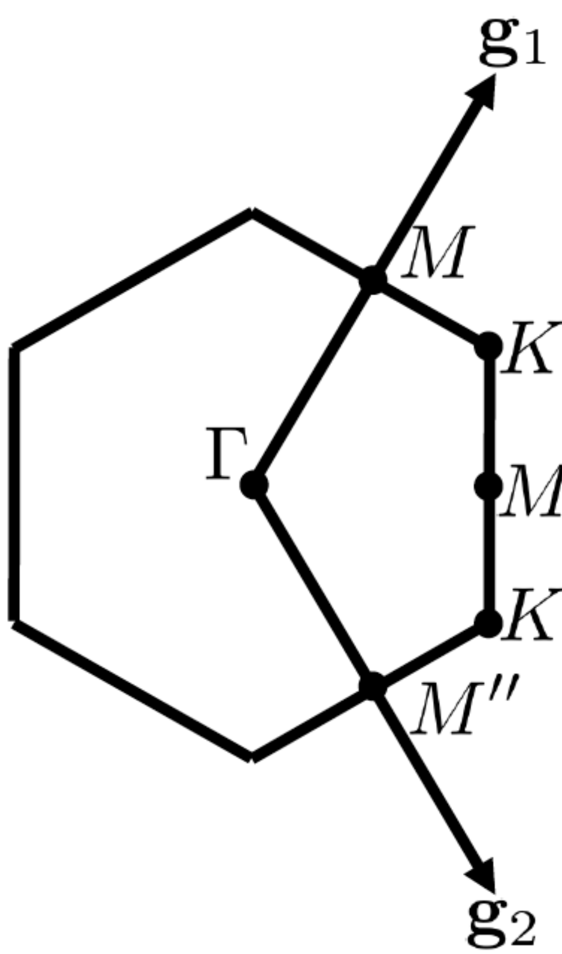


Gapped elementary band representation ⇒ topological!

What is the topological invariant?

Wilson loop yields gauge-invariant Berry phases

Alexandradinata, Wang, Bernevig PRX 6, 021008 (2016)



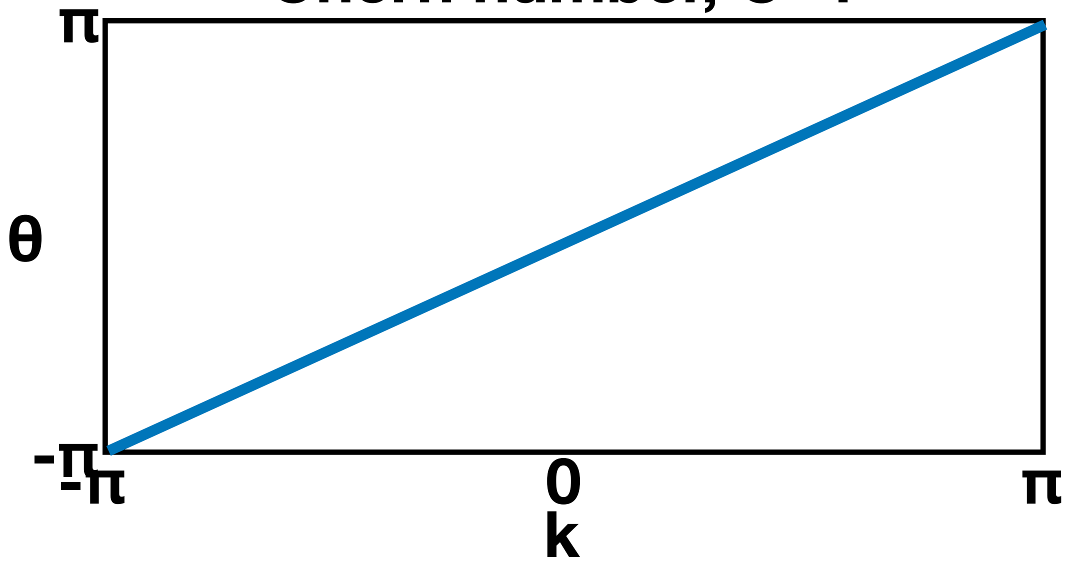
$$\mathcal{W}(k_2) = P e^{i \int_0^{2\pi} dk_1 A(k_1, k_2)}$$

$$[A]_{ij} = i \langle u_i(\mathbf{k}) | \partial_{k_1} u_j(\mathbf{k}) \rangle$$

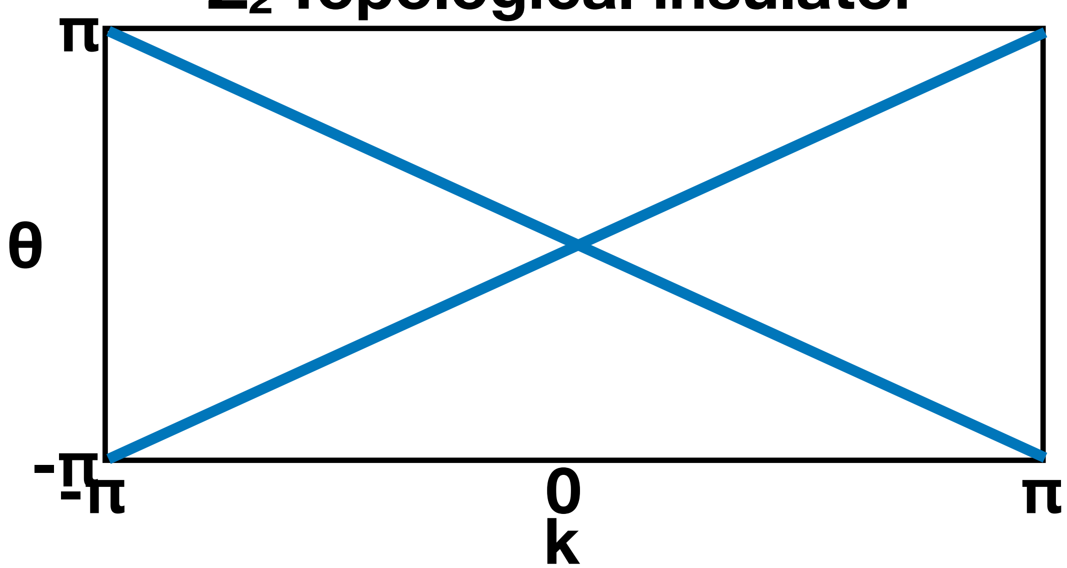
Winding Berry phase ⇒ topological bands

Topological examples:

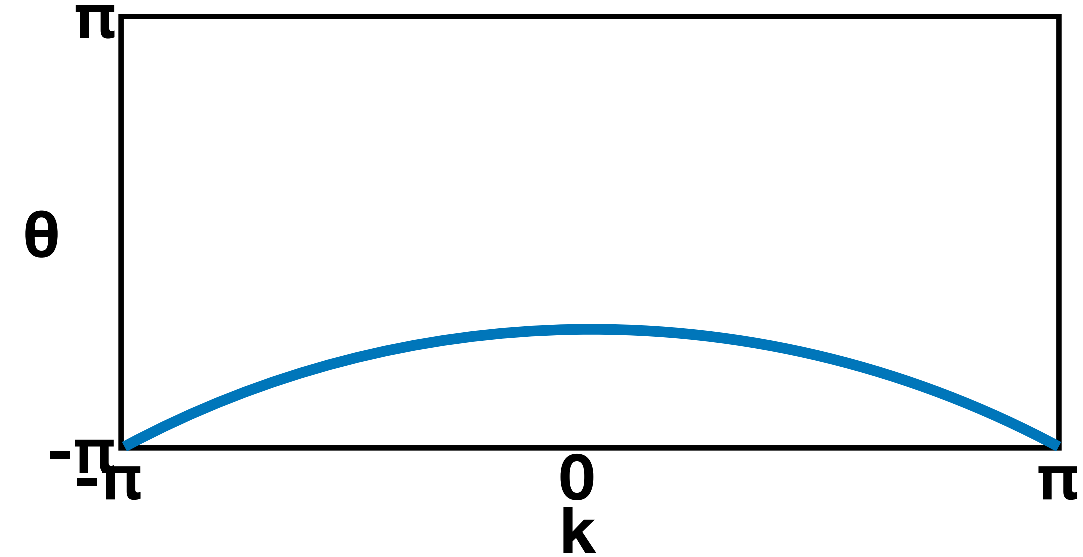
Chern number, C=1

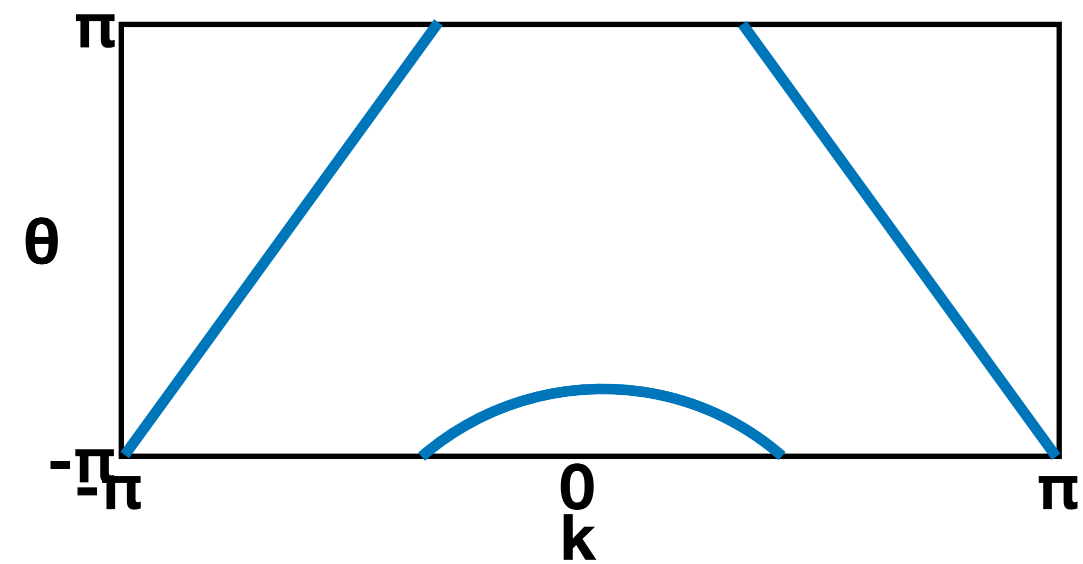


Z_2 Topological insulator



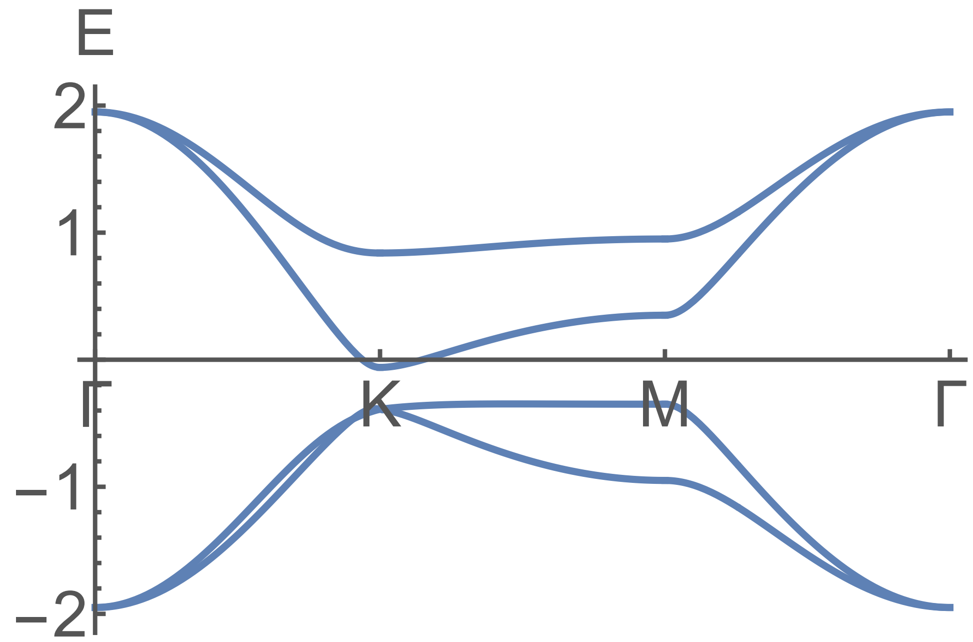
Deformable to atomic limit (trivial):





Bulk-edge correspondence

Back to our example: p_x, p_y orbitals on honeycomb

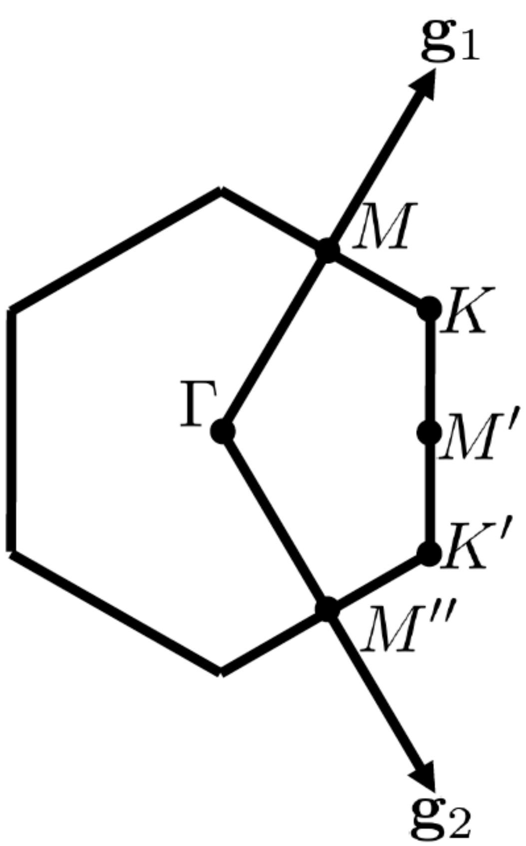


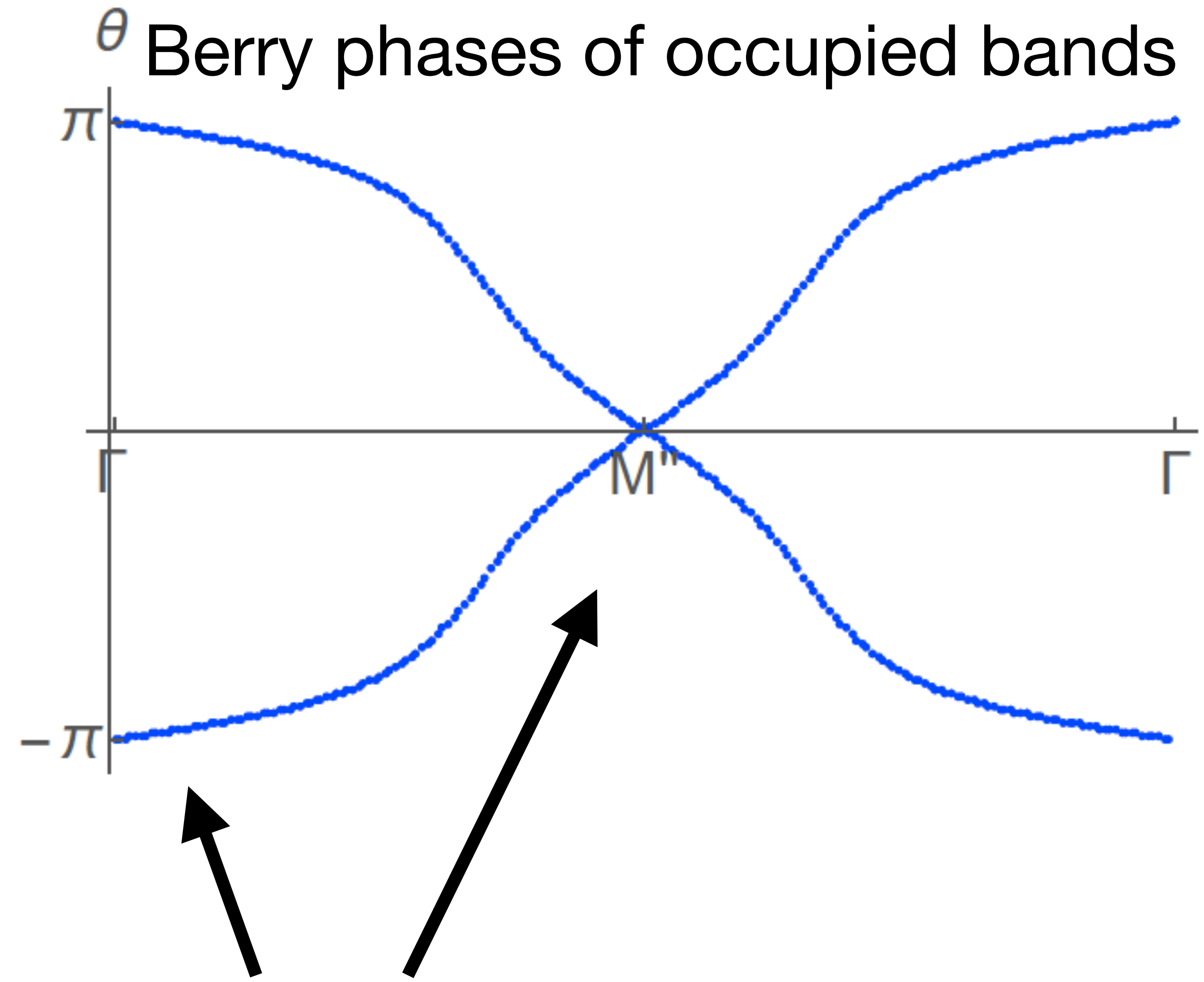
Gapped elementary band representation ⇒ topological!

What is the topological invariant?

Winding Berry phase ⇒ topological

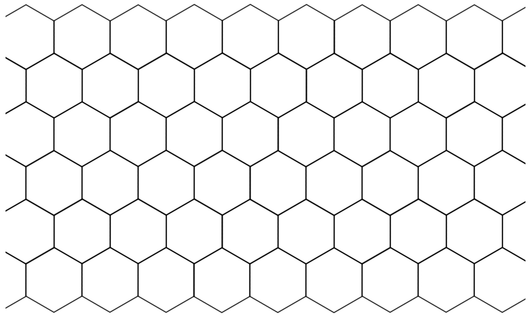
JC et al., PRL 120, 266401 (2018)



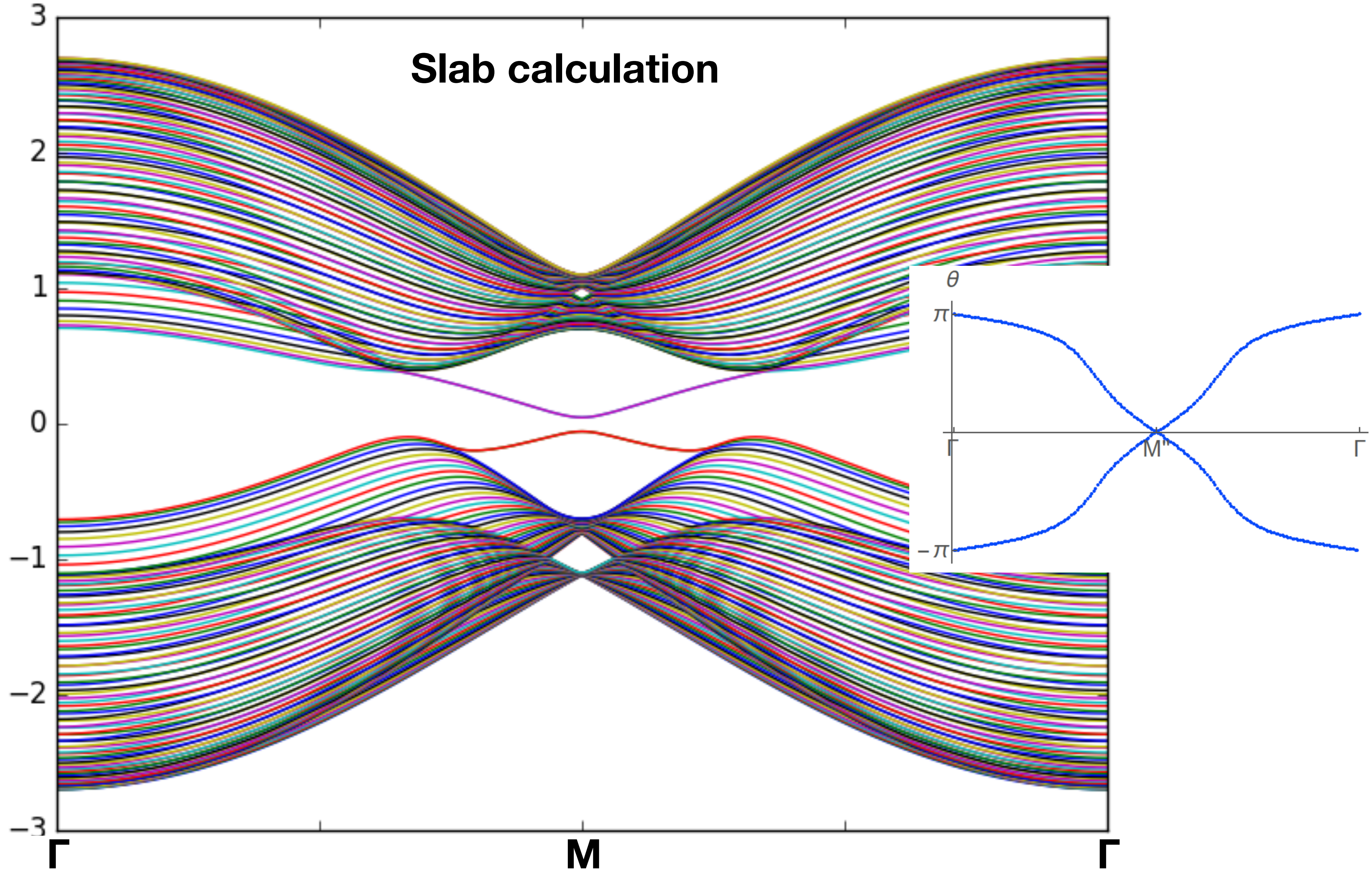


Crossings pinned by C_{2z} symmetry

(Alexandradinata, Dai, Bernevig, PRB 89, 155114 (2014))



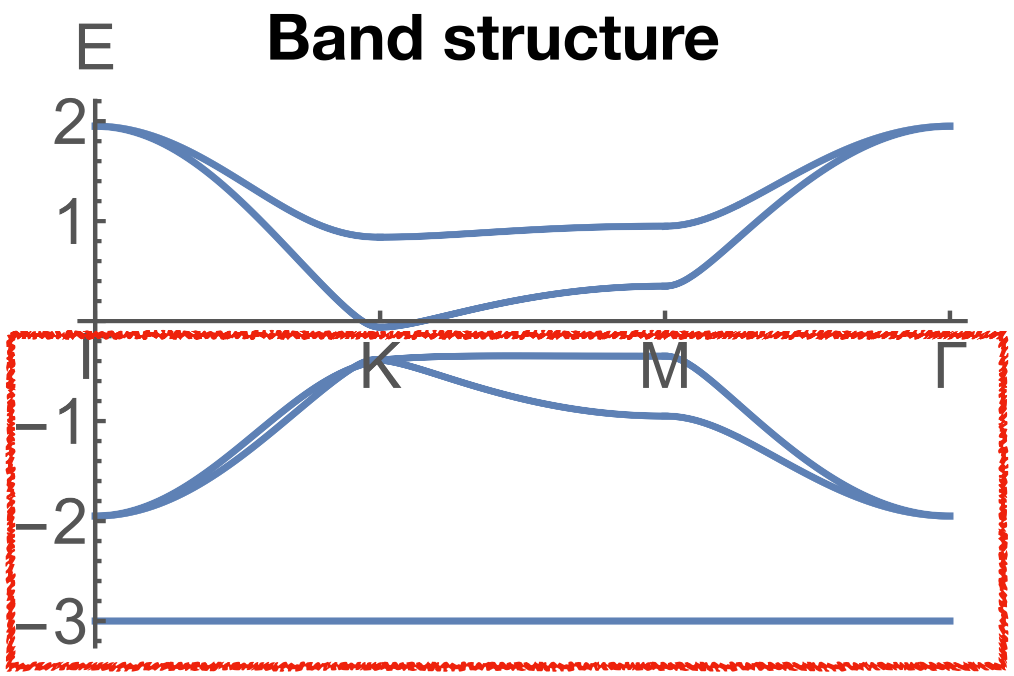
Edge not invariant under C_{2z}

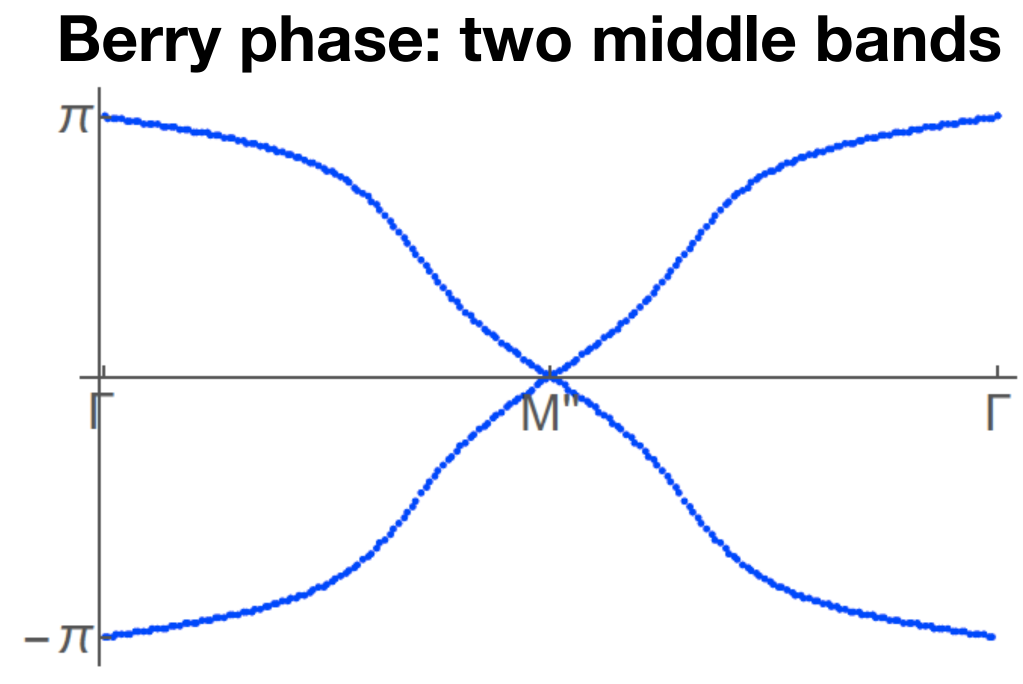


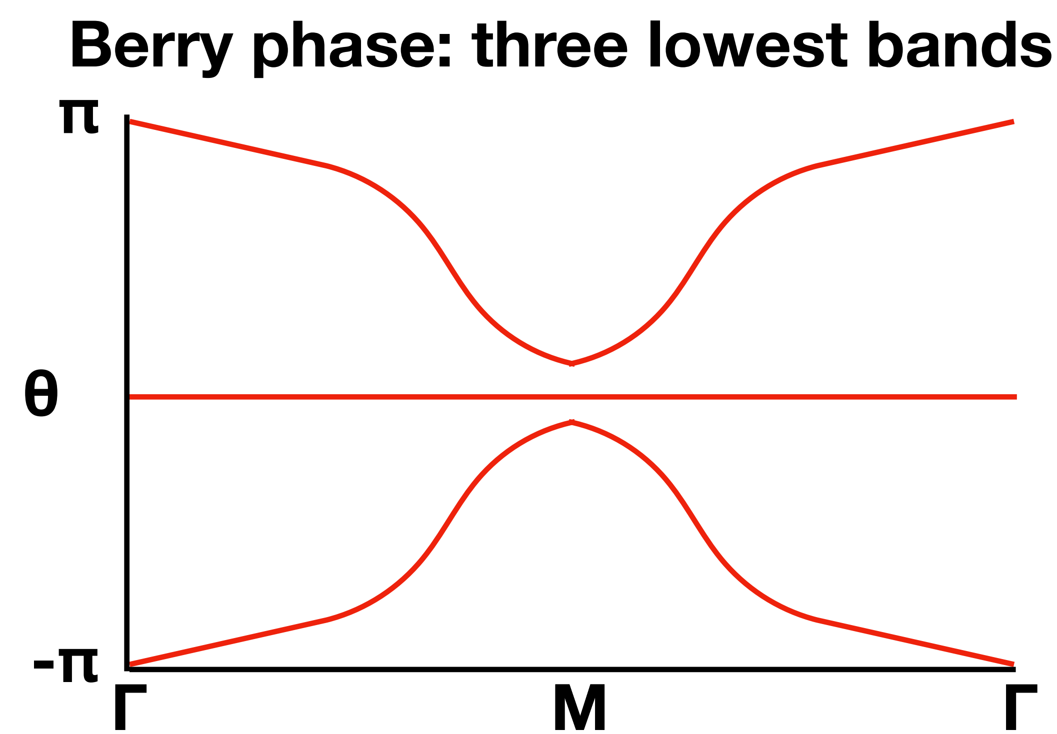
⇒ edge states not required

Berry phase trivialized by extra band

JC et al., PRL 120, 266401 (2018)

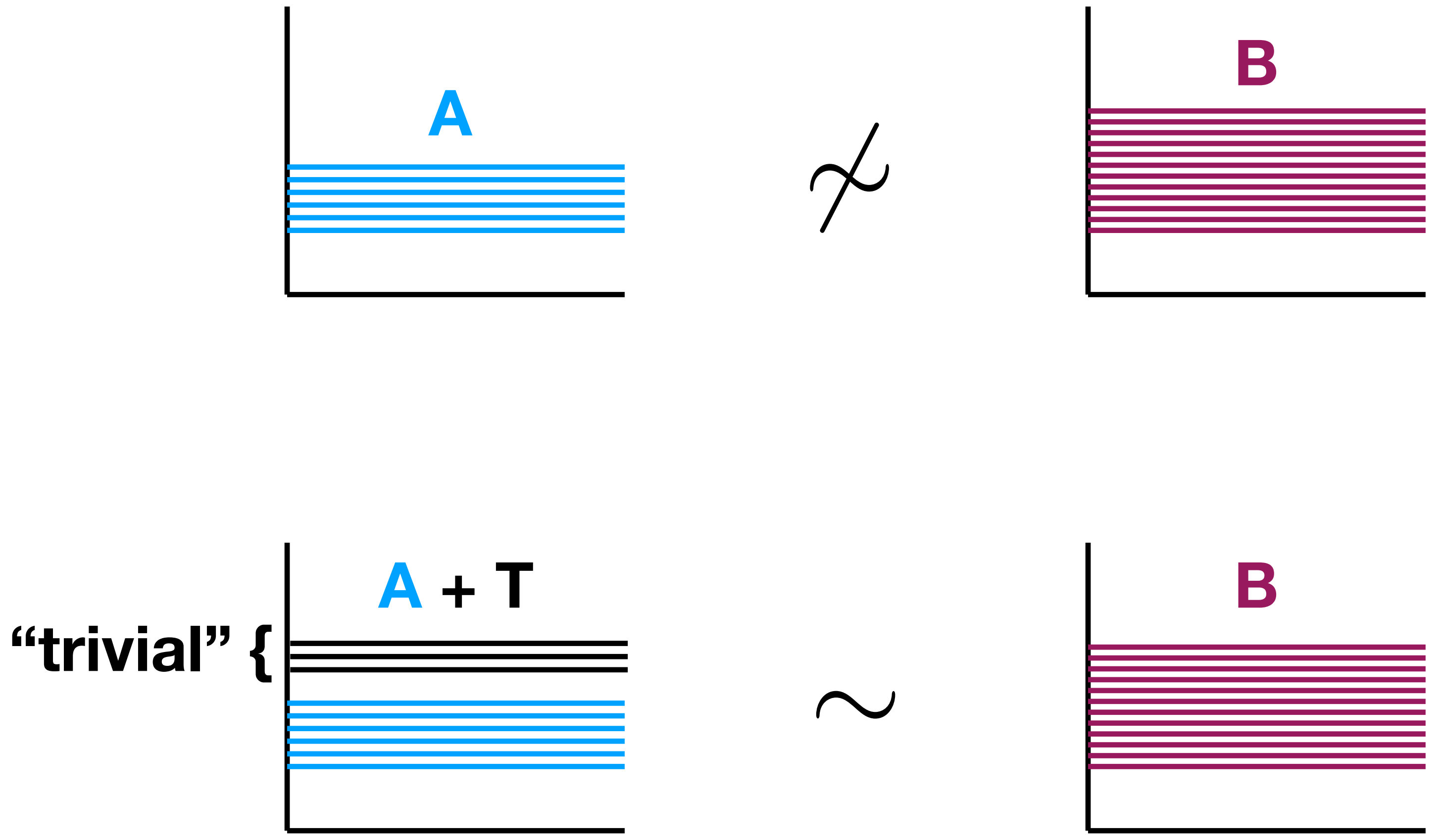






Topological + trivial = trivial ???

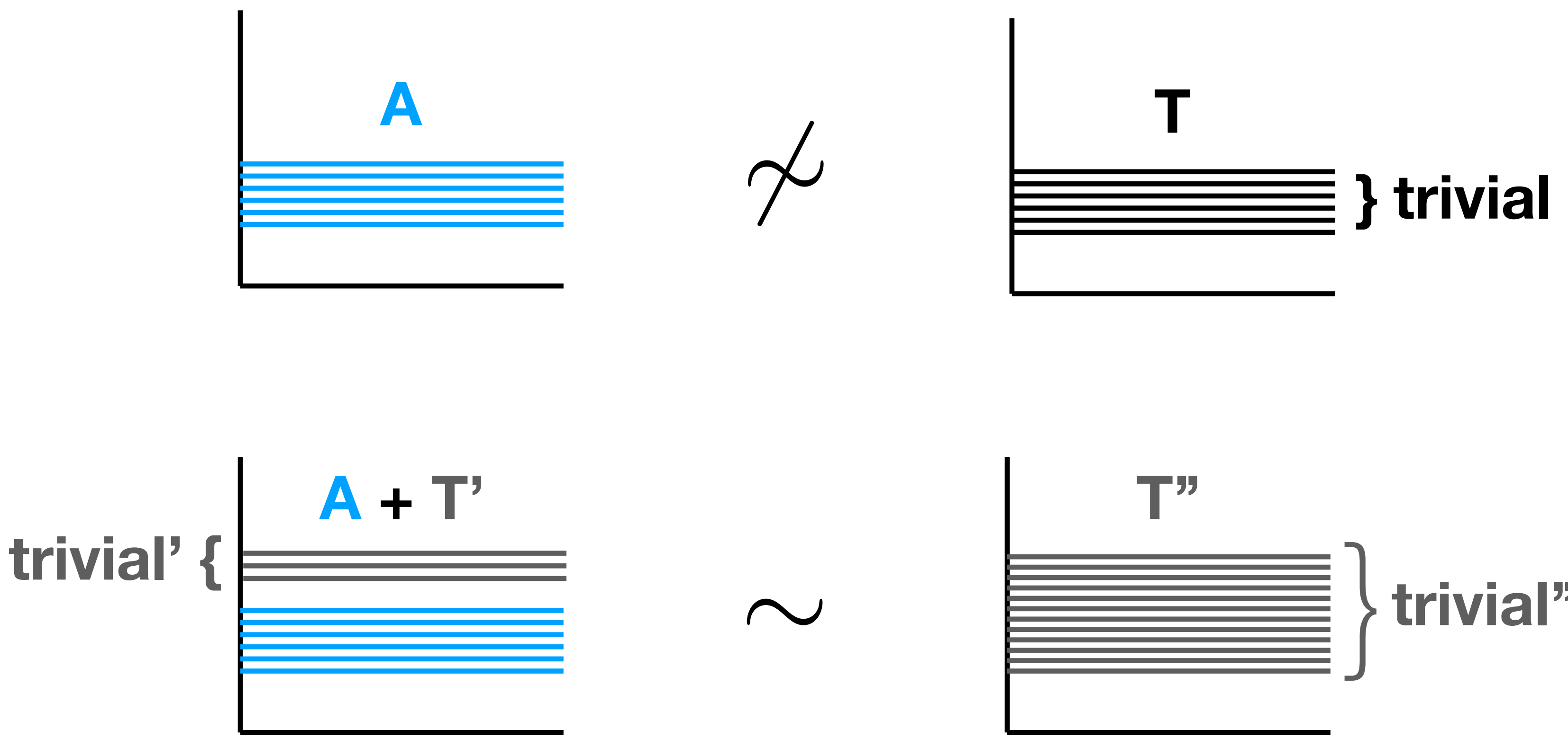
Stable equivalence:
K-theory classification of topological phases



A and B are stably equivalent

“Fragile” topological phase

Po and Vishwanath, ArXiv: 1709.06551



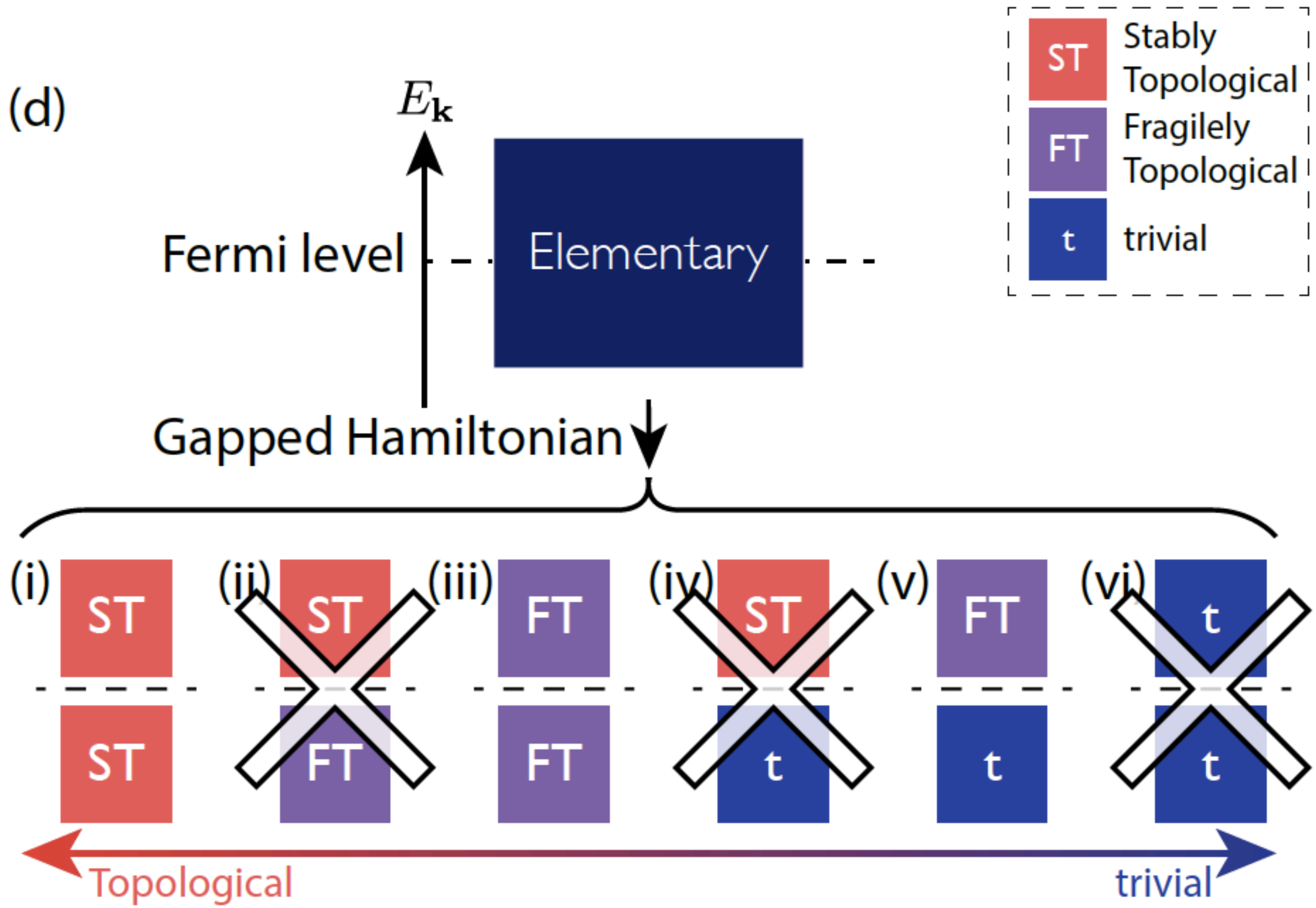
A is stably equivalent to T”

A is fragile topological

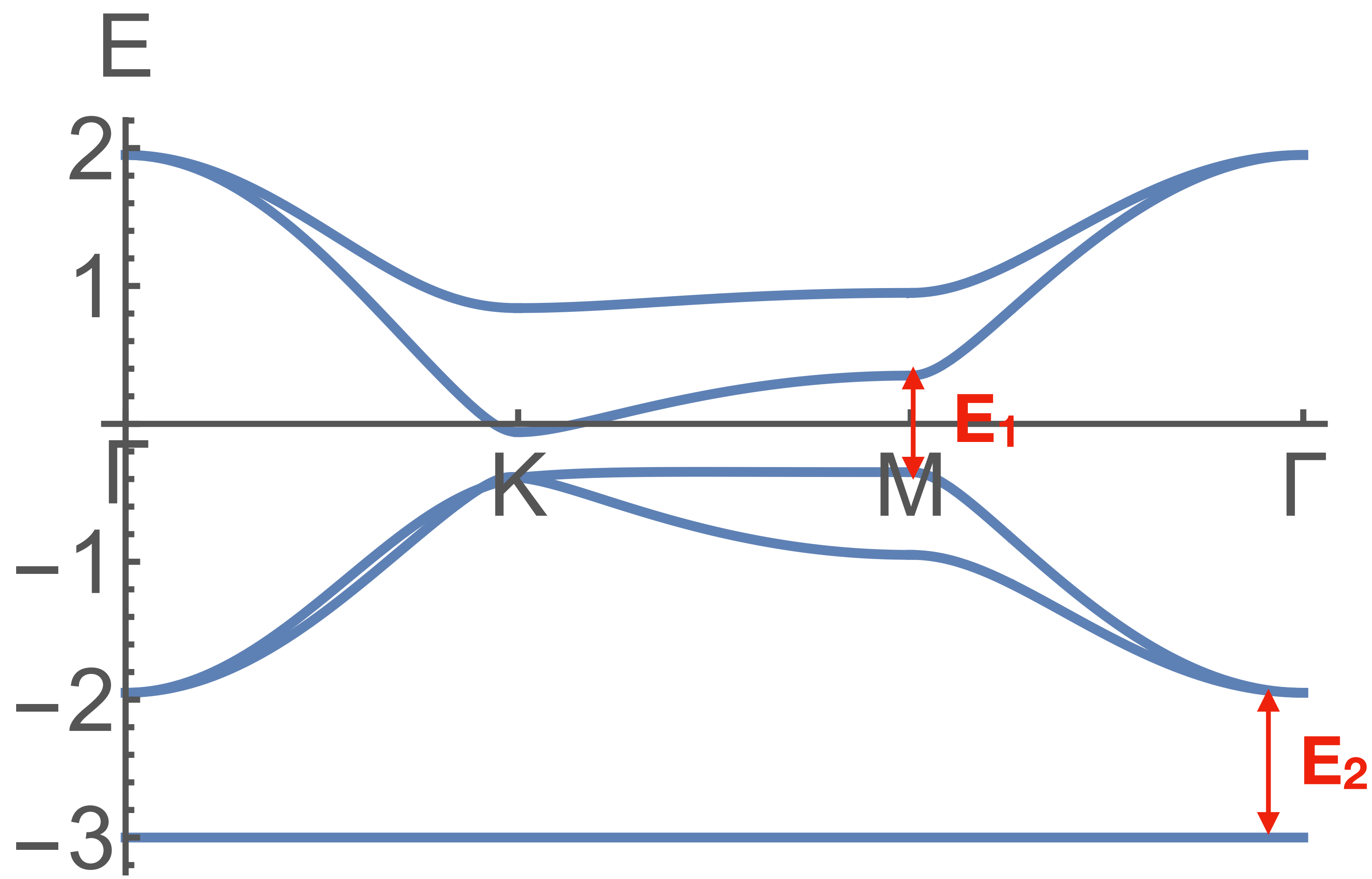
Fragile topological + trivial = trivial

What does this mean for gapped EBRs?

Po and Vishwanath, ArXiv: 1709.06551



As long as topological bands are gapped, Wilson loop eigenvalues constitute a physical observable!



Experimental signature: measure fragile topological bands by Berry phase?

Bloch oscillations (thy): Höller and Alexandradinata, ArXiv:1708.02943

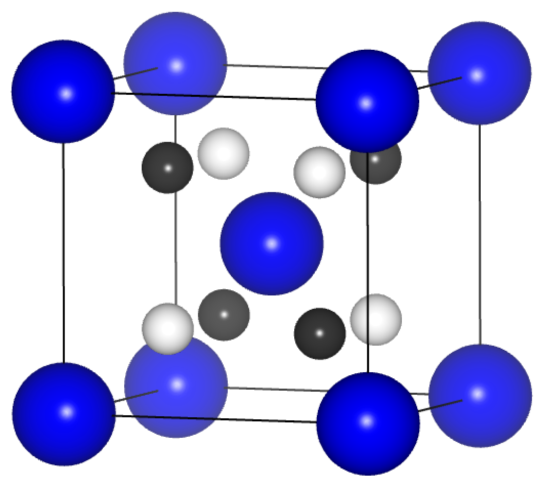
Zak phase (cold atoms): Atala, et al, Nature Physics 9, 795 (2013)

Non-Abelian Zak phase (cold atoms): Li, et al, Science 352, 1094 (2016)

Dynamical birefringence (electronic): Banks, et al, PRX 7, 041042 (2017)

Ex 2: d orbitals in non-symmorphic $P4_232$

Unit cell



Generators:

$\{C_{2x} \mid 0\}$

$\{C_{3,111} \mid 0\}$

$\{C_{2,110} \mid ½\ ½\ ½\}$

Atoms:

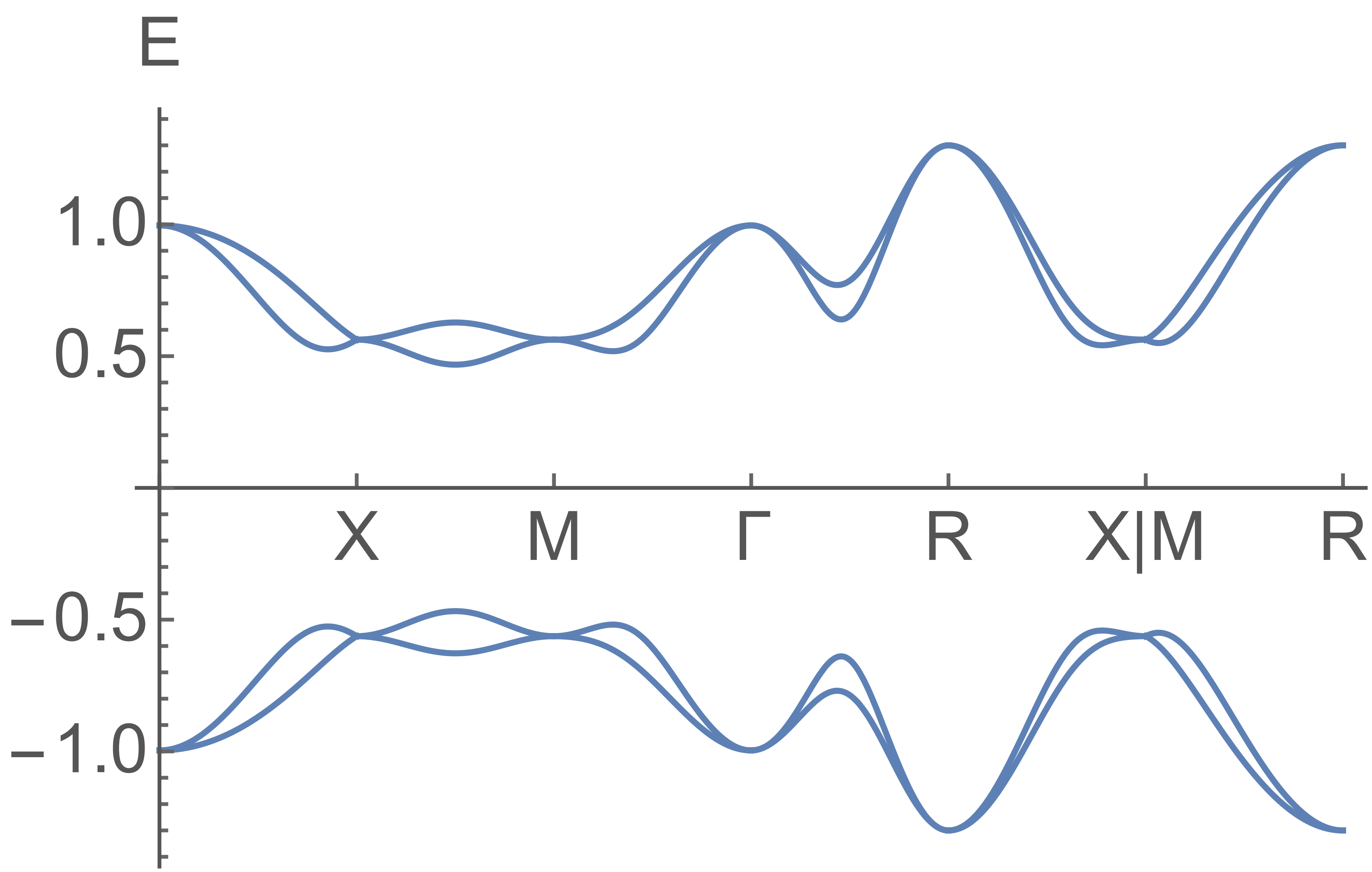
2a: (0,0,0), (½,½,½)

4b: (¼, ¼, ¼), (¾, ¾, ¼), (¾, ¼, ¾), (¼, ¾, ¾)

4c: (¾, ¾, ¾), (¼, ¼, ¾), (¼, ¾, ¼), (¾, ¼, ¼)

Ex 2: d orbitals in non-symmorphic $P4_232$

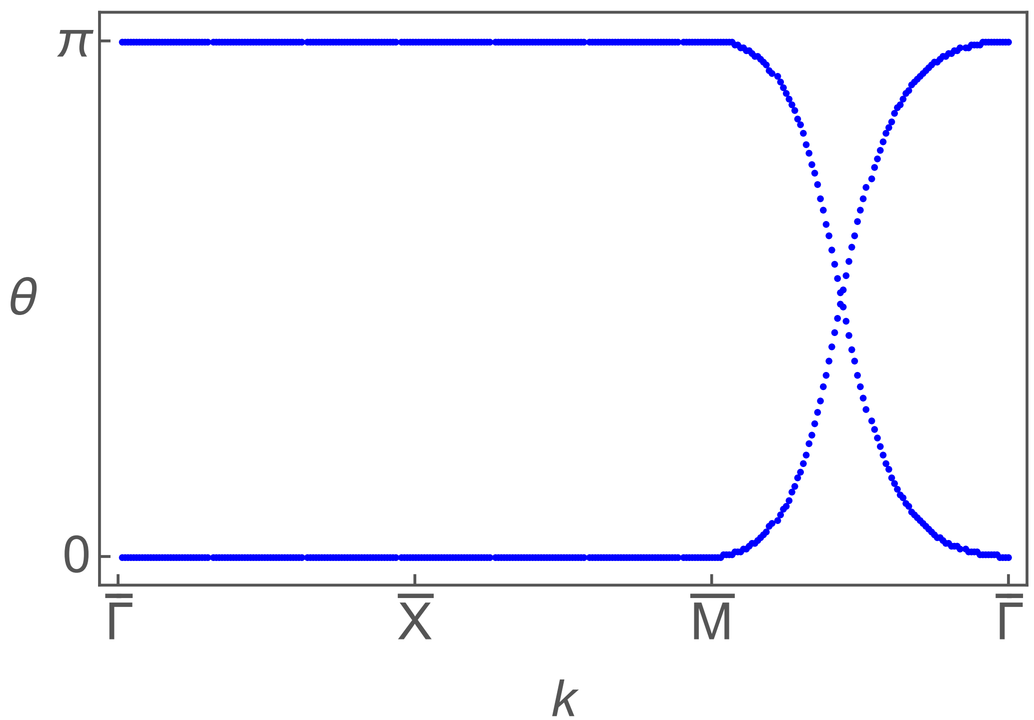
JC et al., PRL 120, 266401 (2018)

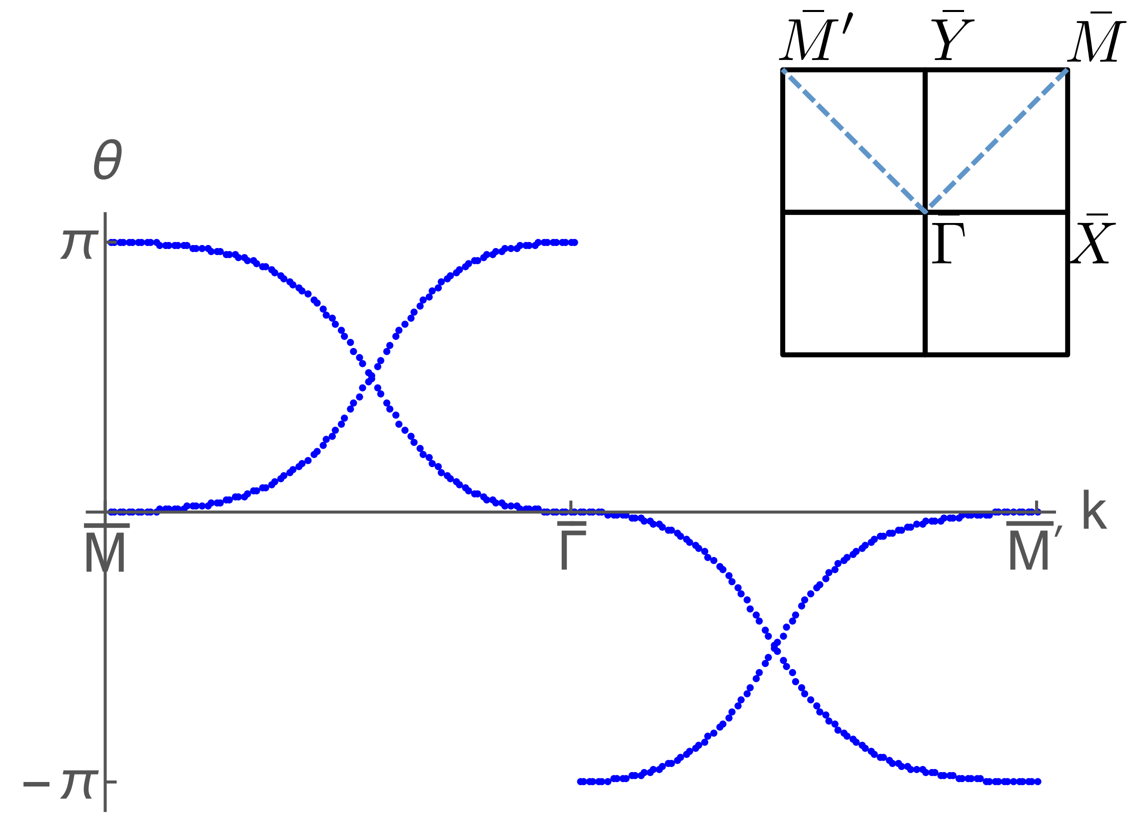


Gapped elementary band representation ⇒ topological

Winding Berry phase yields topological invariant

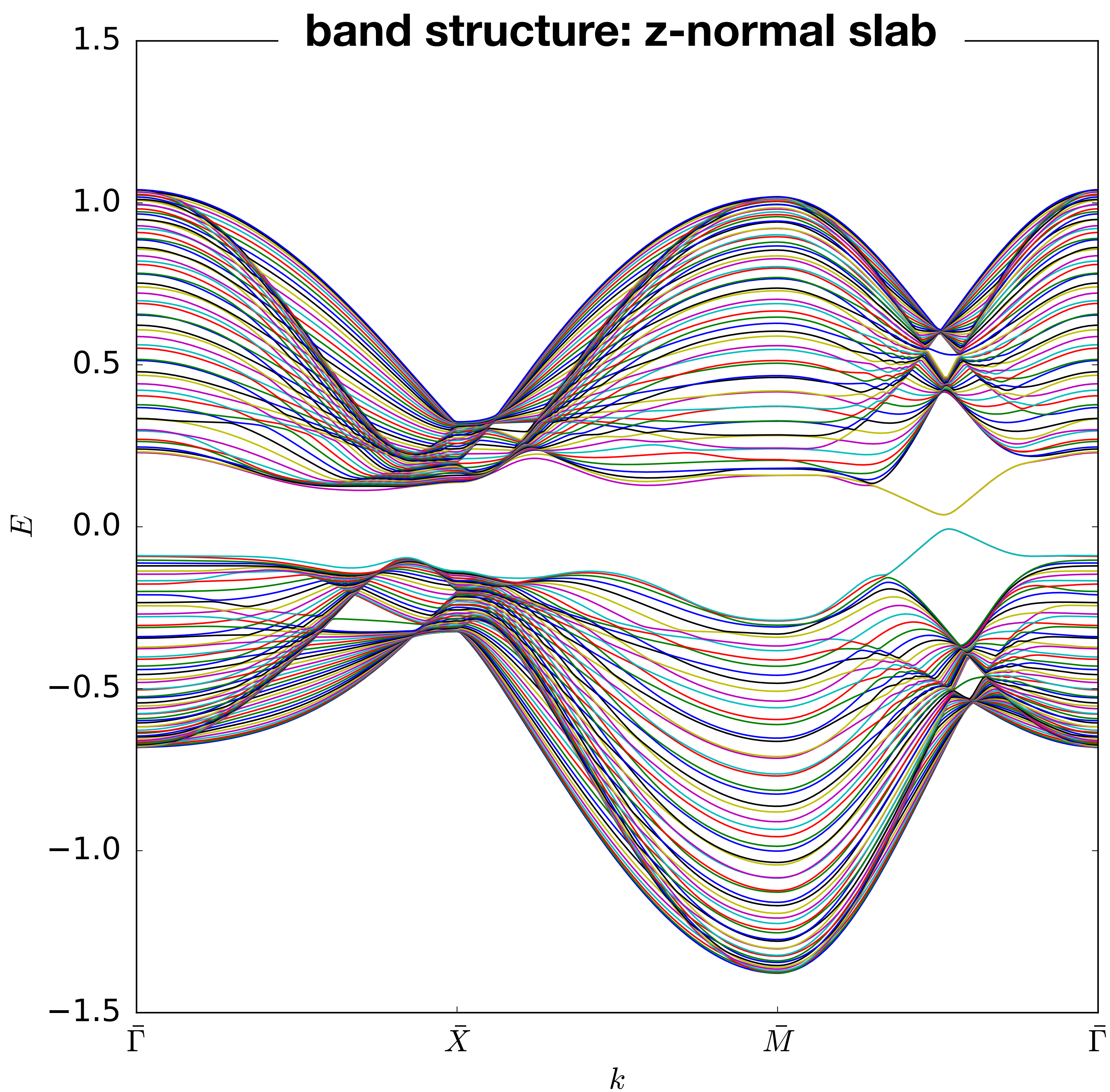
JC et al., PRL 120, 266401 (2018)

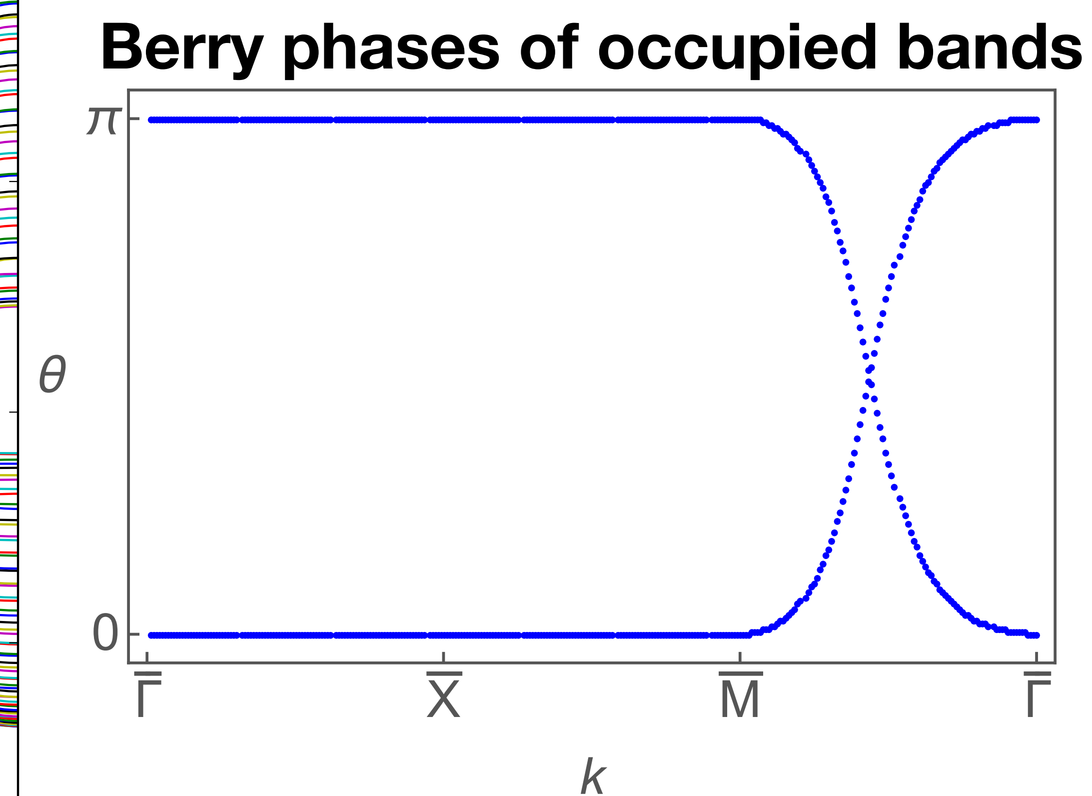




Dirac points along Γ — M: moveable but unremovable

No screw symmetry on surface ⇒ no surface states





Summary

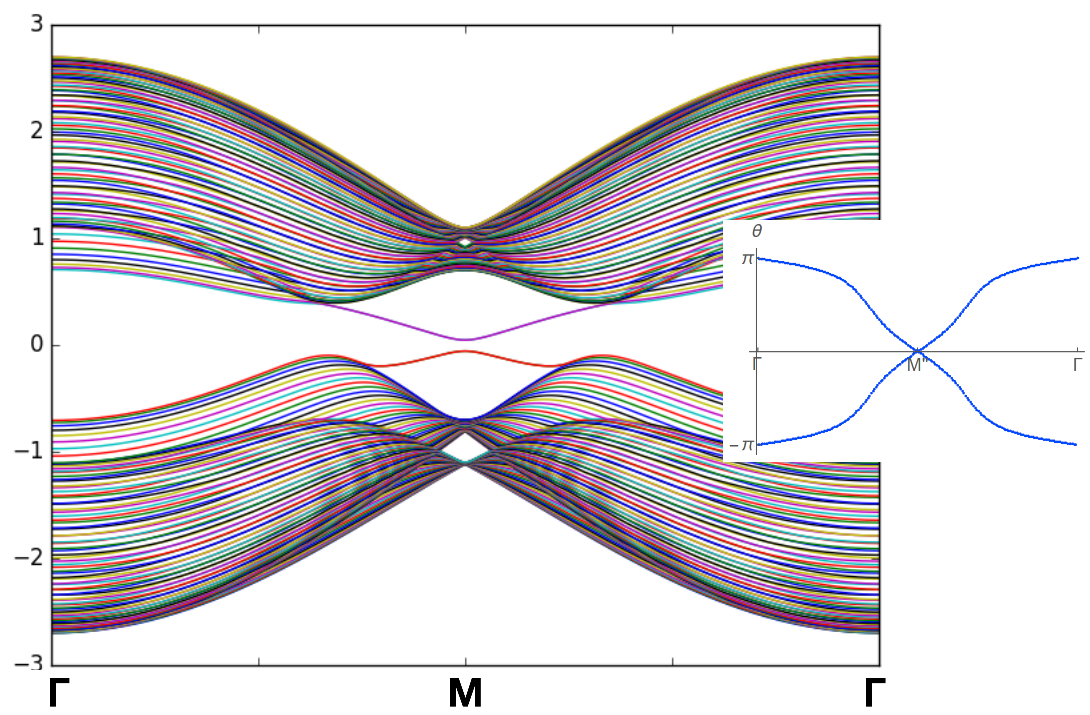
JC et al., PRB 97, 035139 (2018), 1709.01935;
Bradlyn, **JC**, et al., *Nature* 547, 298–305 (2017), 1703.02050
JC et al., PRL 120, 266401 (2018)

Disconnected EBRs realize topological phases

Spinless or spinful | **Stable or "fragile" topological**

Framework for classifying/predicting topological materials

New questions about definition of topological phase



What are the signatures and how should we classify fragile topological phases?