Topological Crystalline Insulators and Semimetals, Part 2

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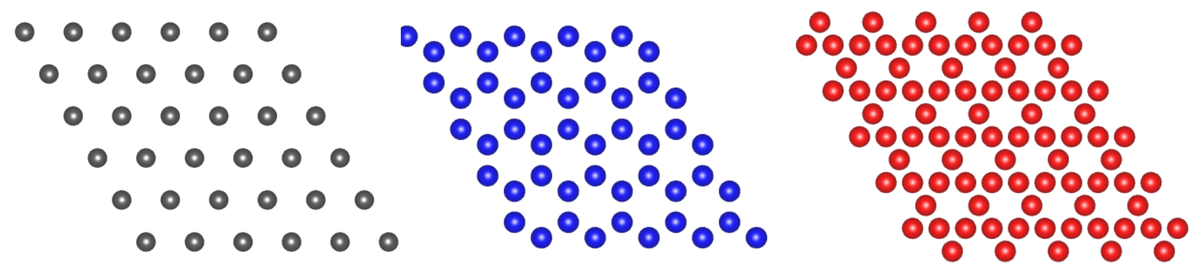
Last time:



- We seek a unified description of topological crystalline insulators in all space groups by enumerating atomic limits

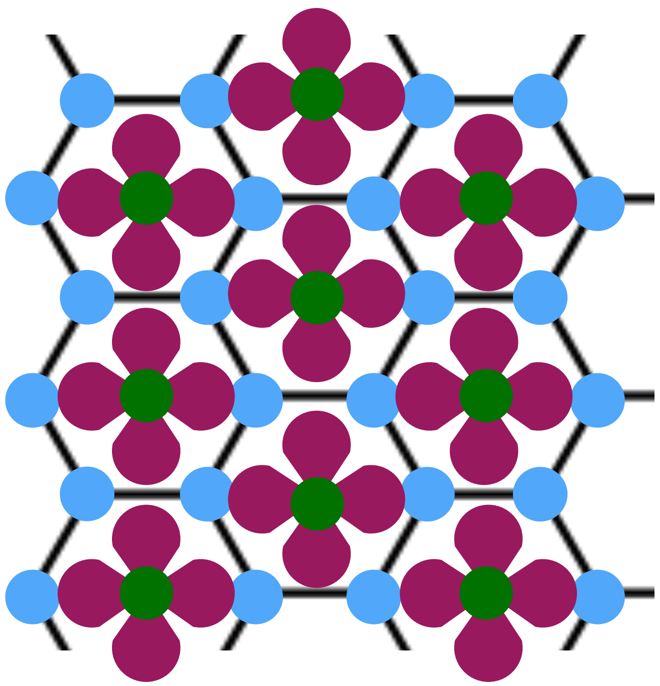
- “Atomic limits” are defined by their space group, Wyckoff position and orbital

    - Uniquely specifies symmetry in real space and momentum space “band representation”

- Example: inversion eigenvalues

Goal: compute <u>all</u> atomic limit phases for <u>all</u> space groups

Problem: there are infinitely many atomic limits!



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

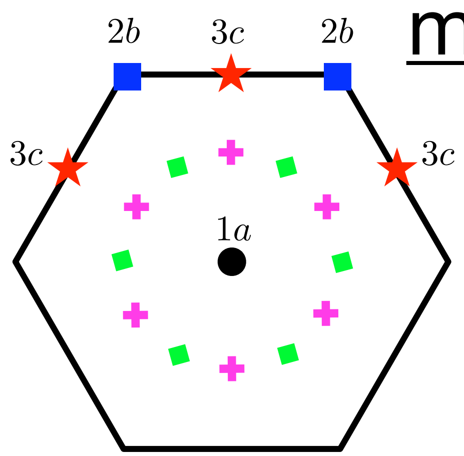
Elementary band representations do not decompose into sum of band representations

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)

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

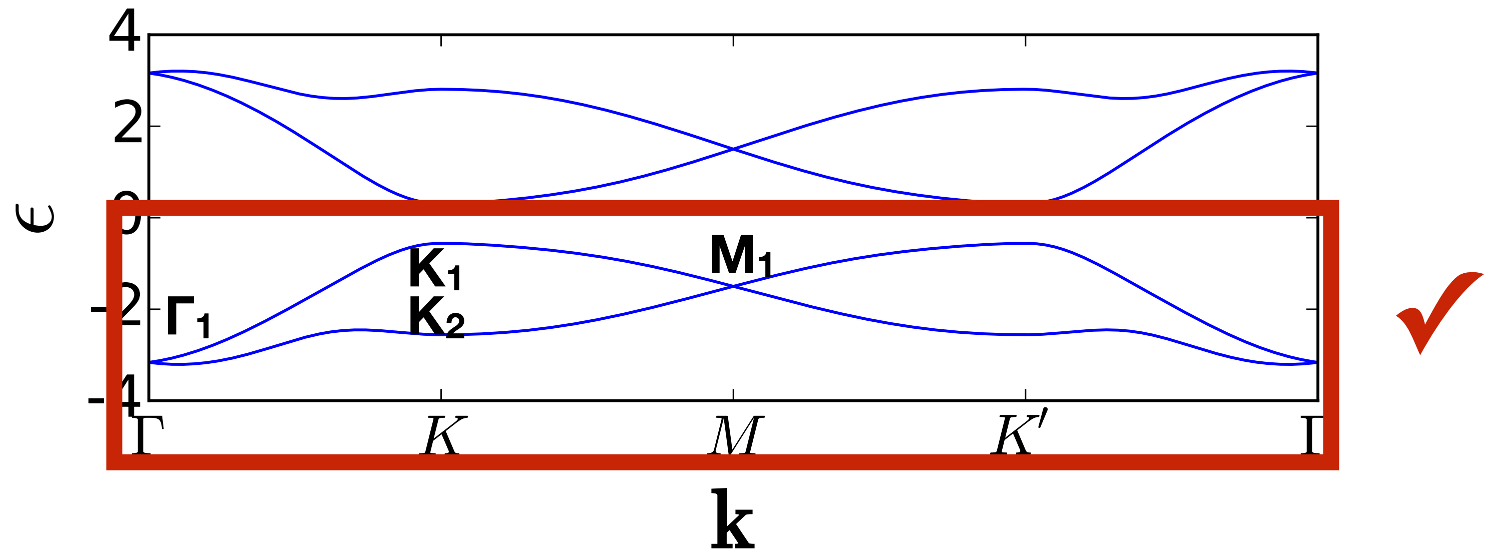
Atom arrangement

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

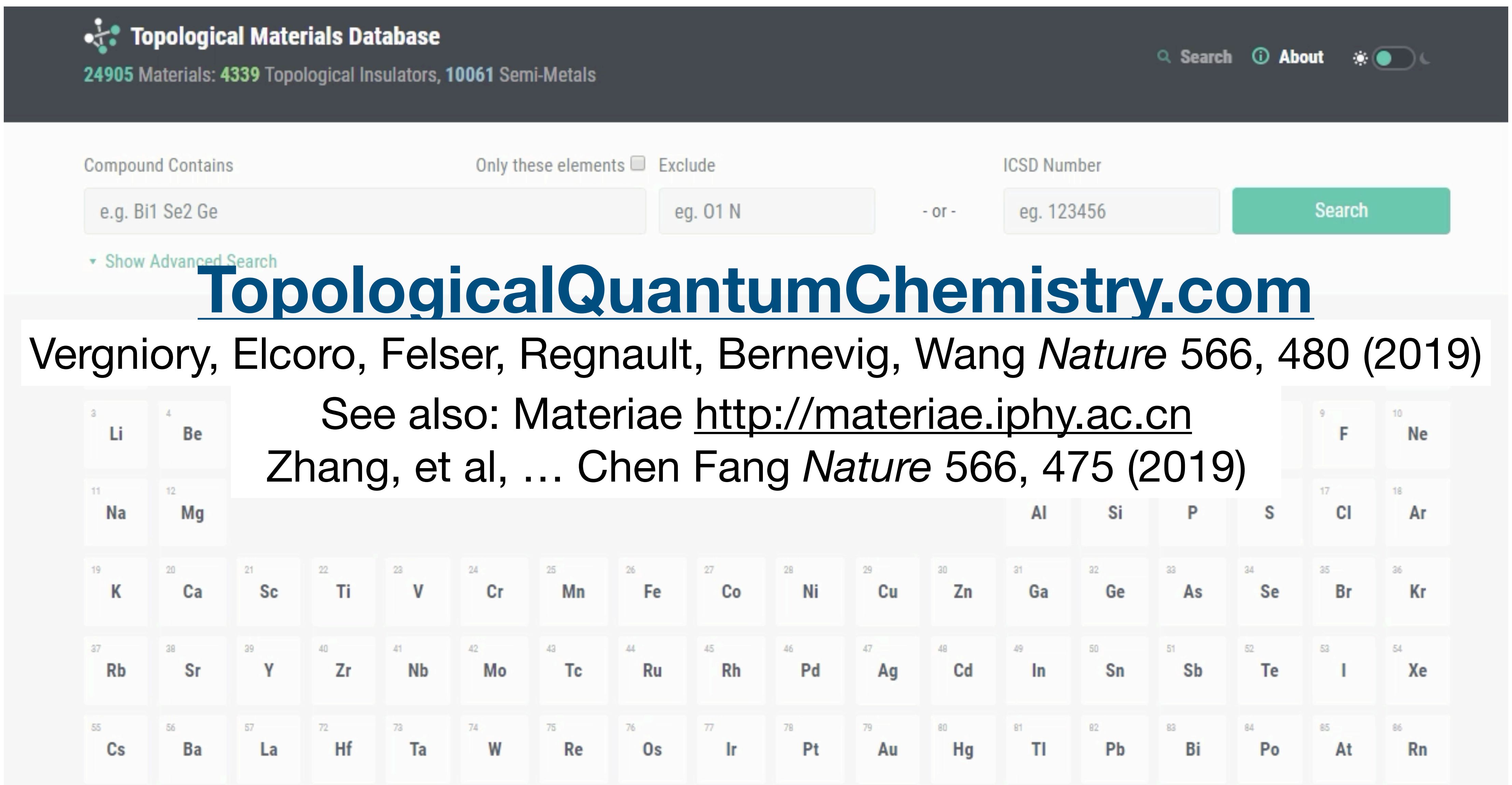
Topological bands are not a “sum” of elementary band representations

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



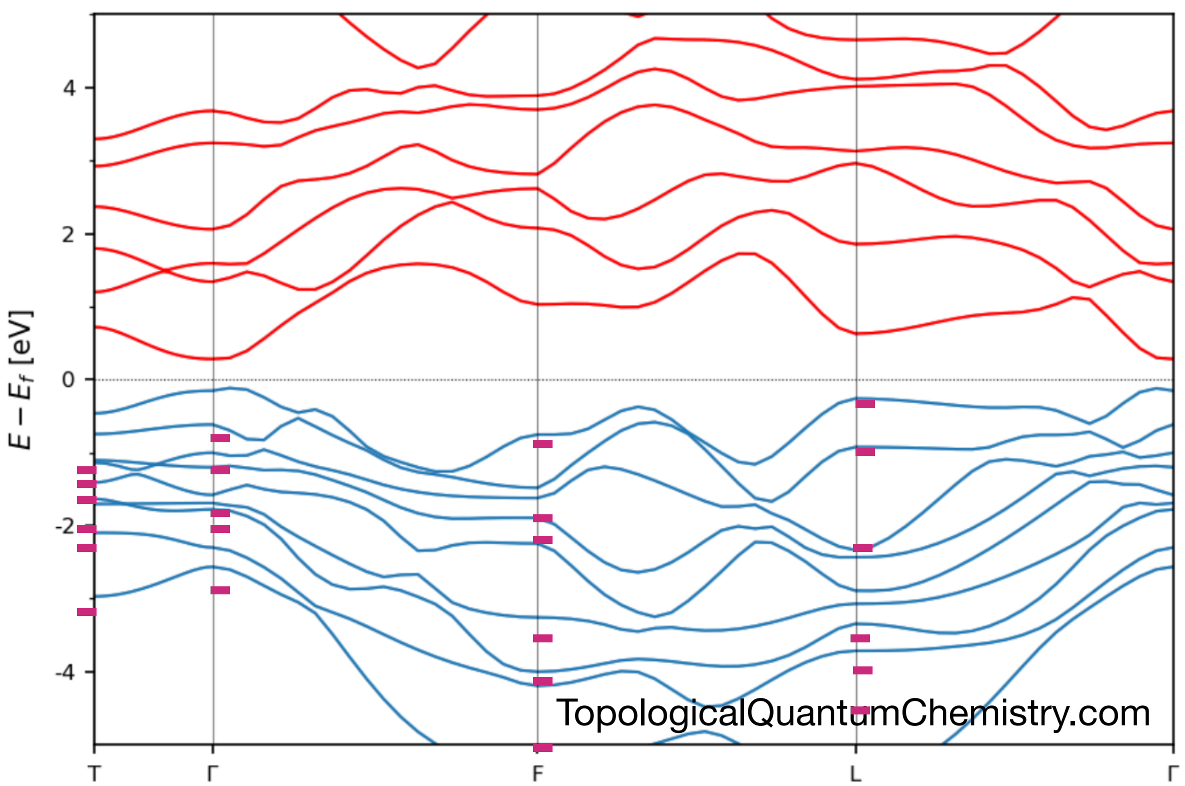
TopologicalQuantumChemistry.com

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

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

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

Summary



Crystal symmetry can protect and identify topological phases

Exs: mirror Chern, inversion eigenvalue formula, hourglass fermion, …

Symmetry indicators — generalizations of inversion eigenvalue invariant — have been derived for every space group and can be determined from elementary band reps

Part 2: topological semimetals

What is a Weyl fermion?

$$H = k \cdot \sigma$$

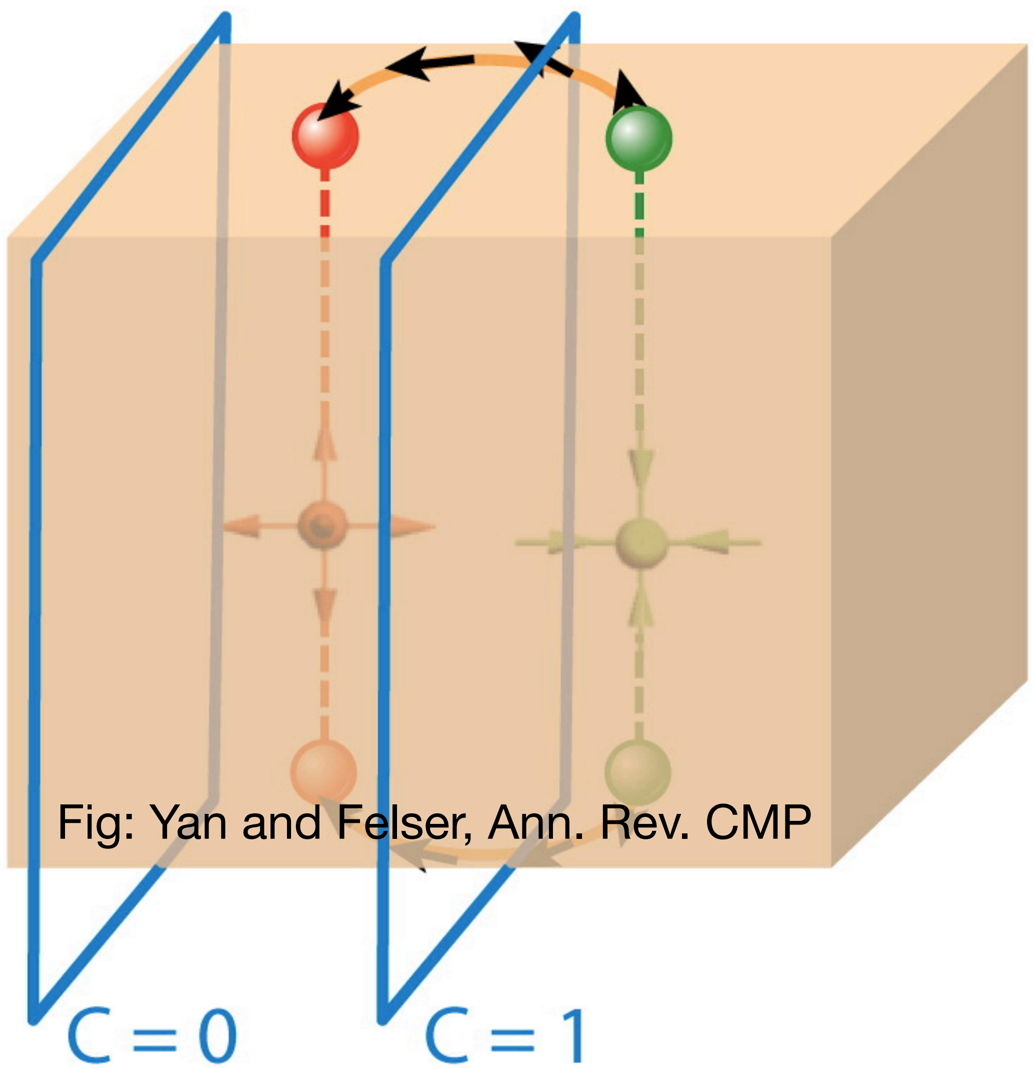


Fig: Yan and Felser, Ann. Rev. CMP

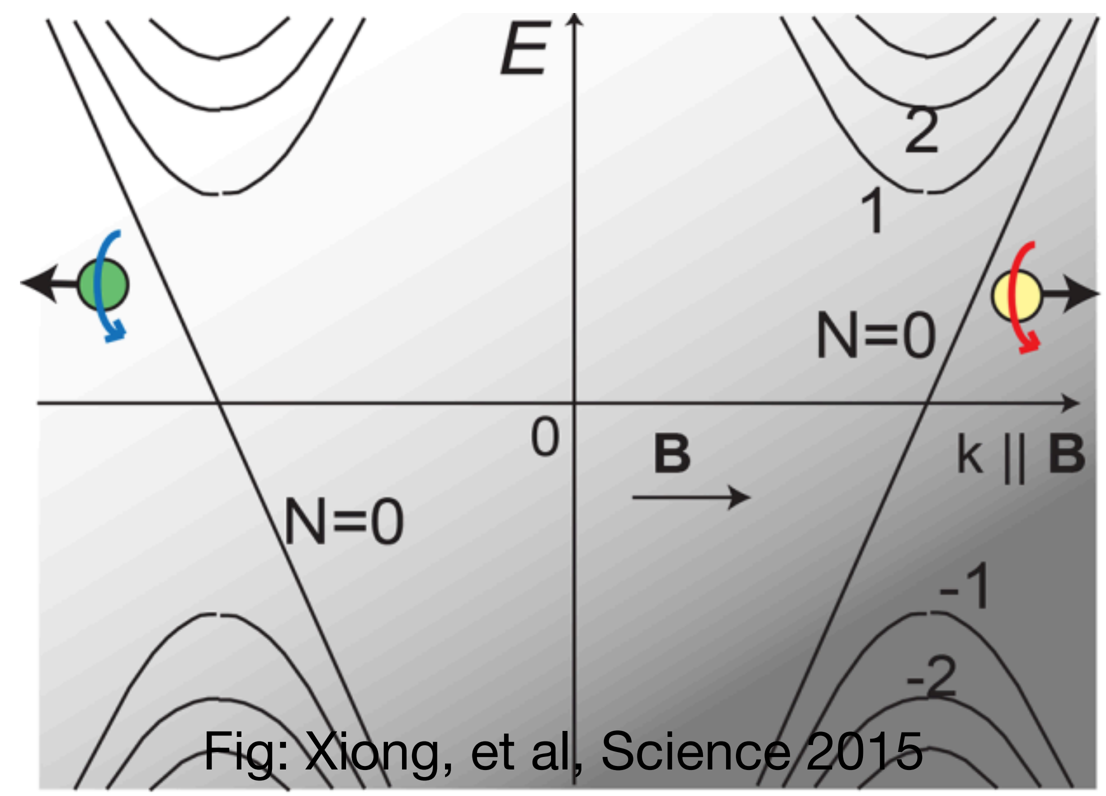
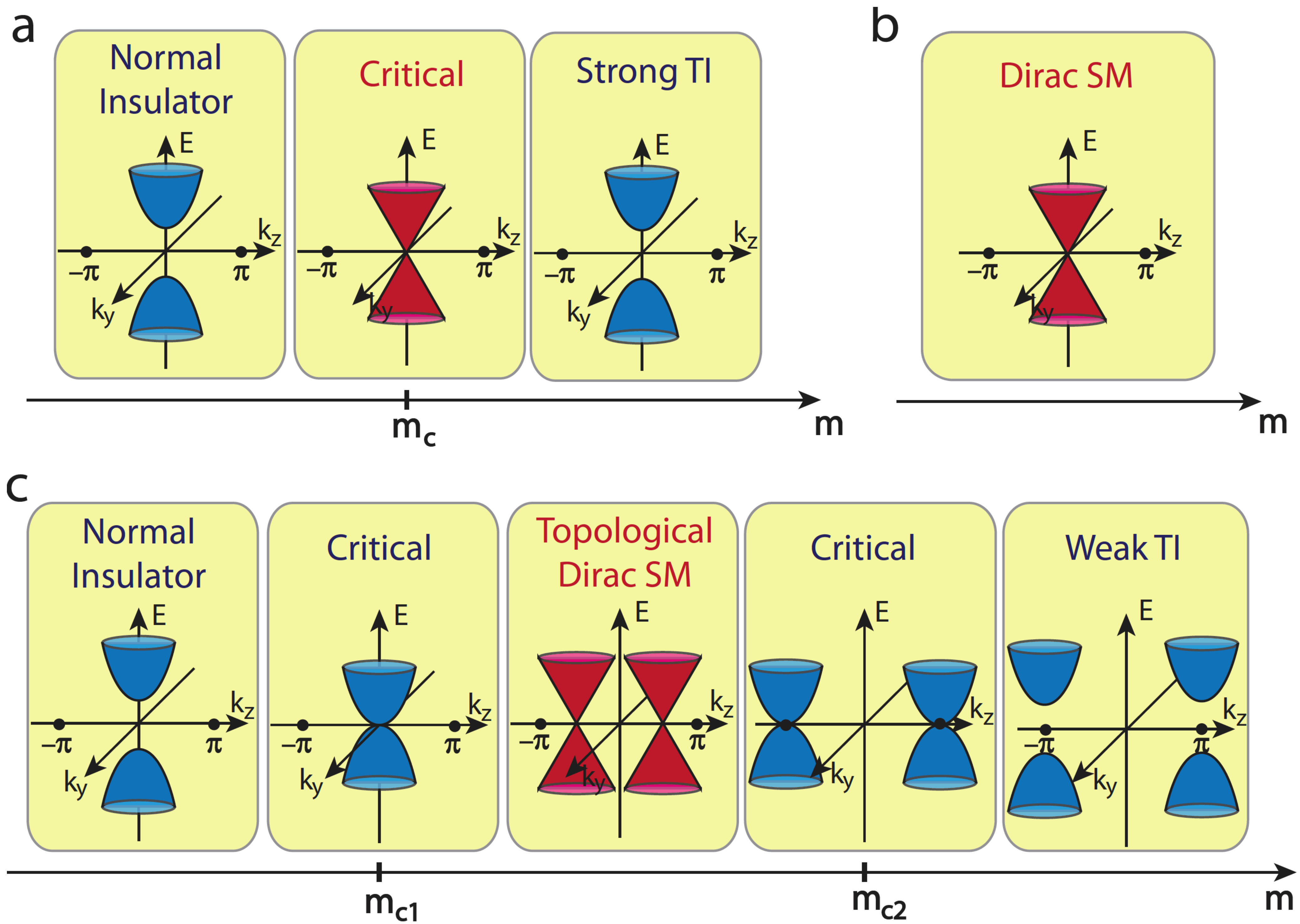


Fig: Xiong, et al, Science 2015

Dirac fermions: stabilized by crystal symmetry

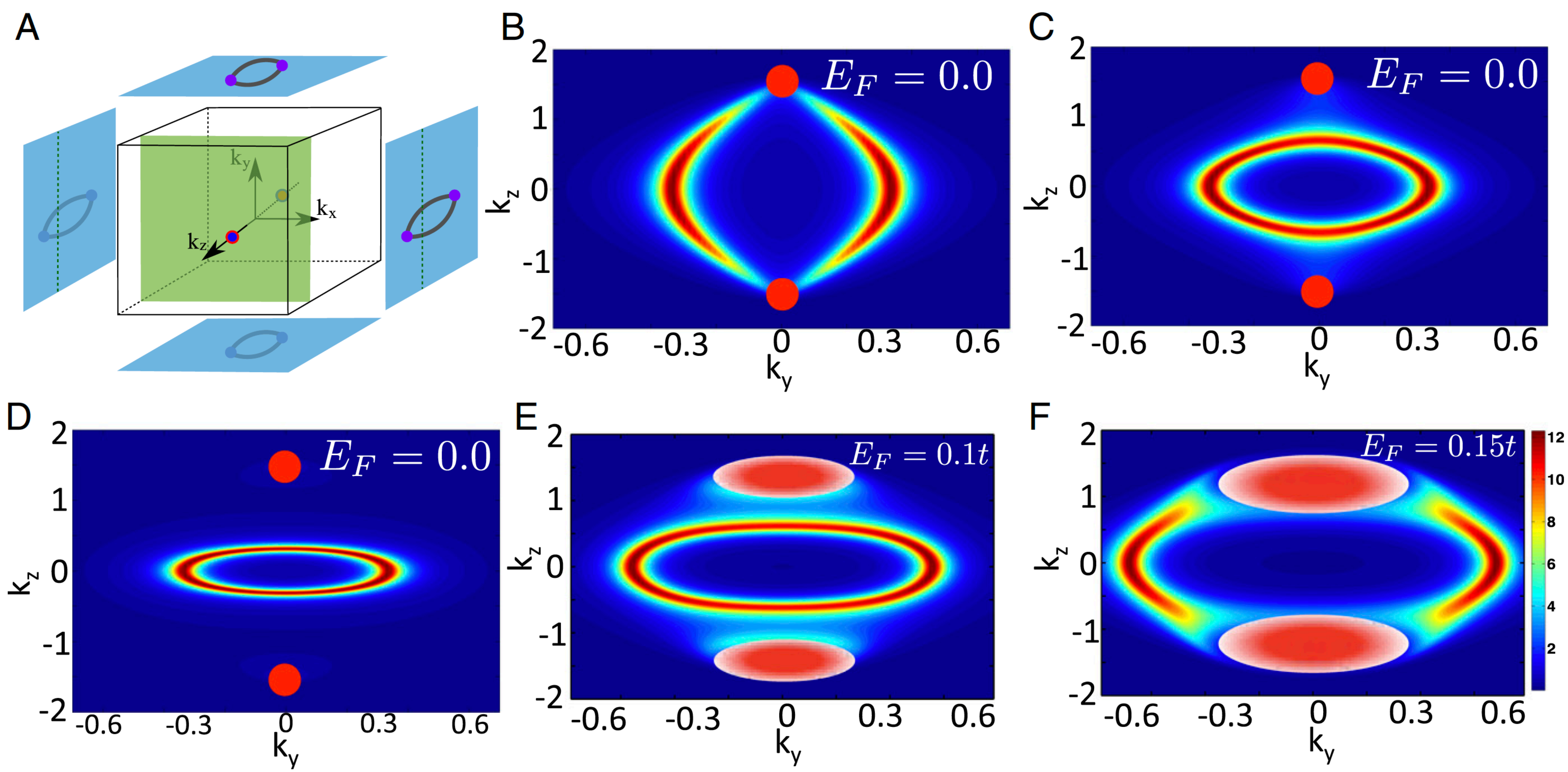
Classification: Yang and Nagaosa, Nature Comm. (2014)



Is a Dirac fermion topological?

Argument against: lack of Fermi arc

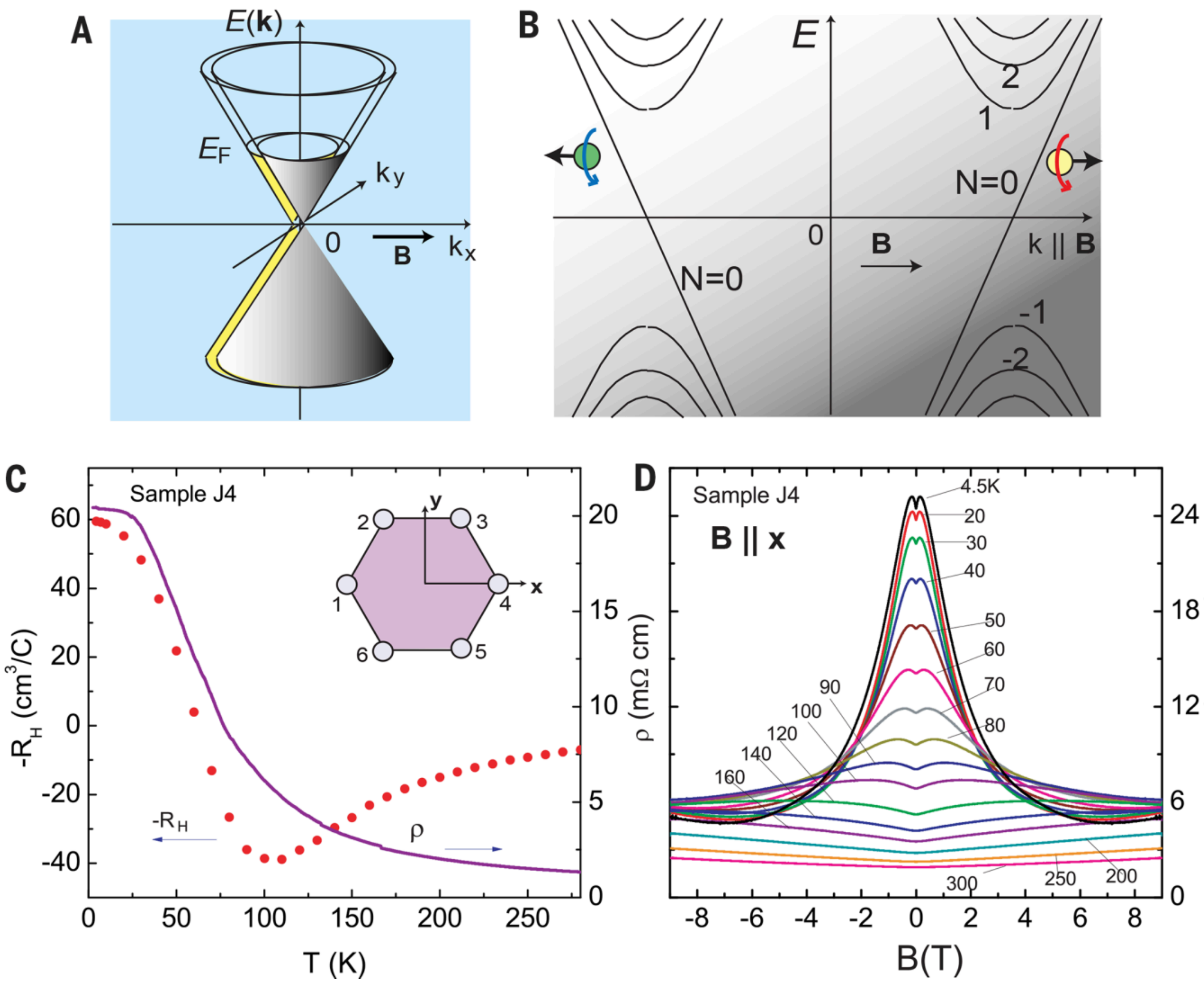
Kargarian, Randeria, Lu PNAS 2016



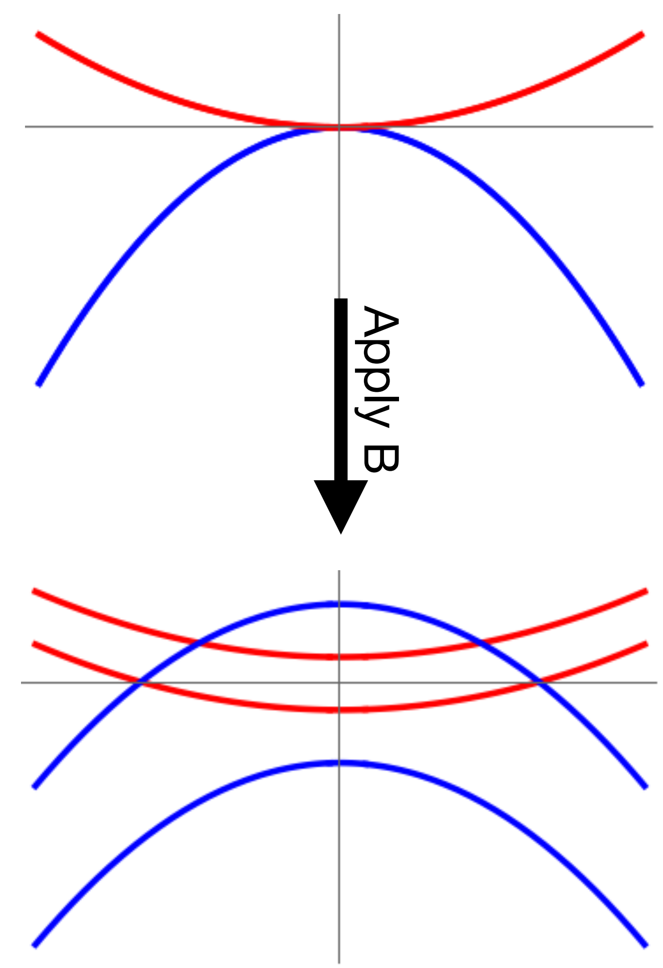
Is a Dirac fermion topological?

Argument for: applied field splits into two Weyl fermions

Chiral anomaly in Na_3Bi
Xiong, et al, Science 2015



"Chiral anomaly factory"
JC et al, PRB 2017, ArXiv:1604.08601

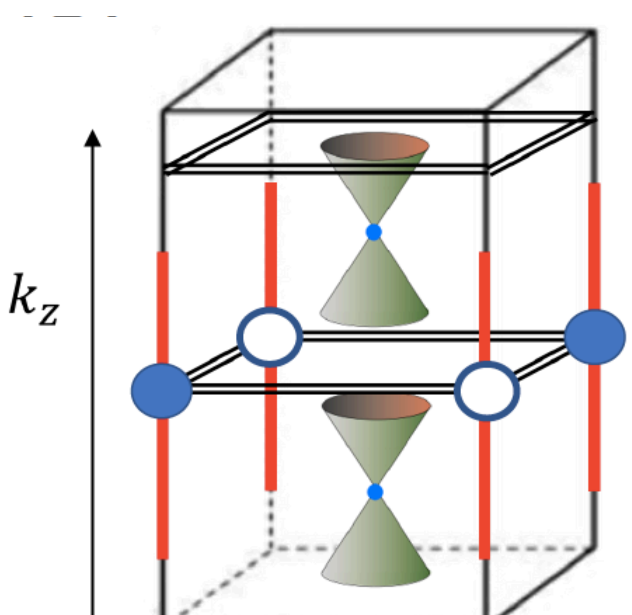


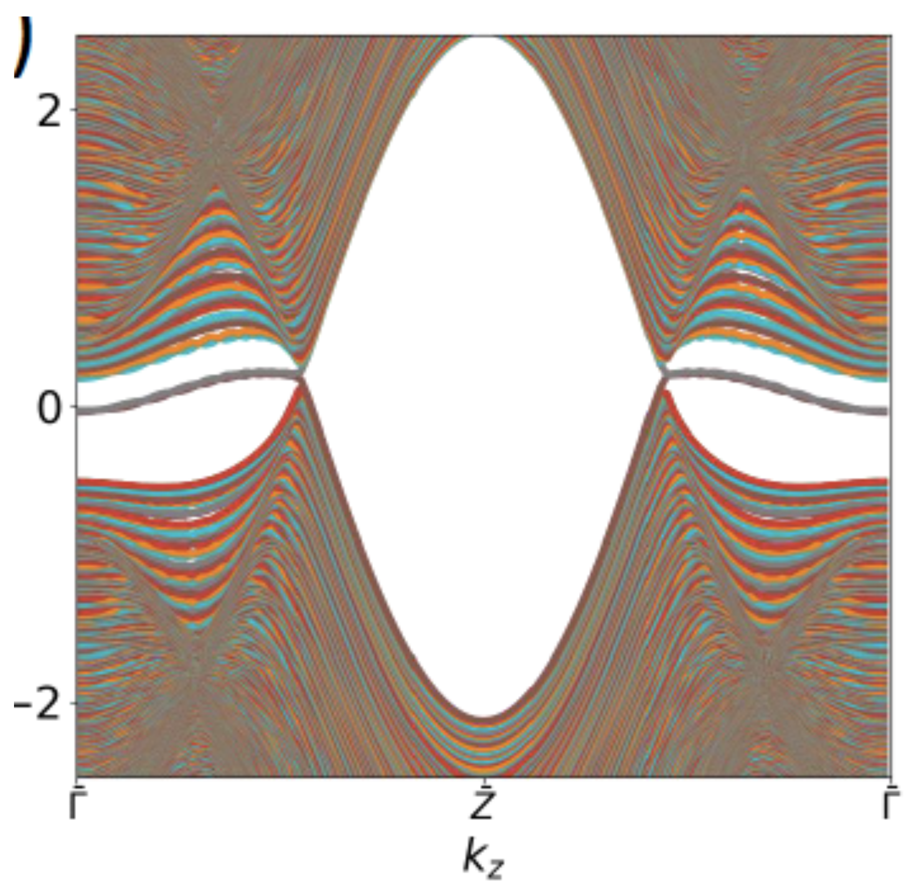
Distinct scaling of magnetoresistance

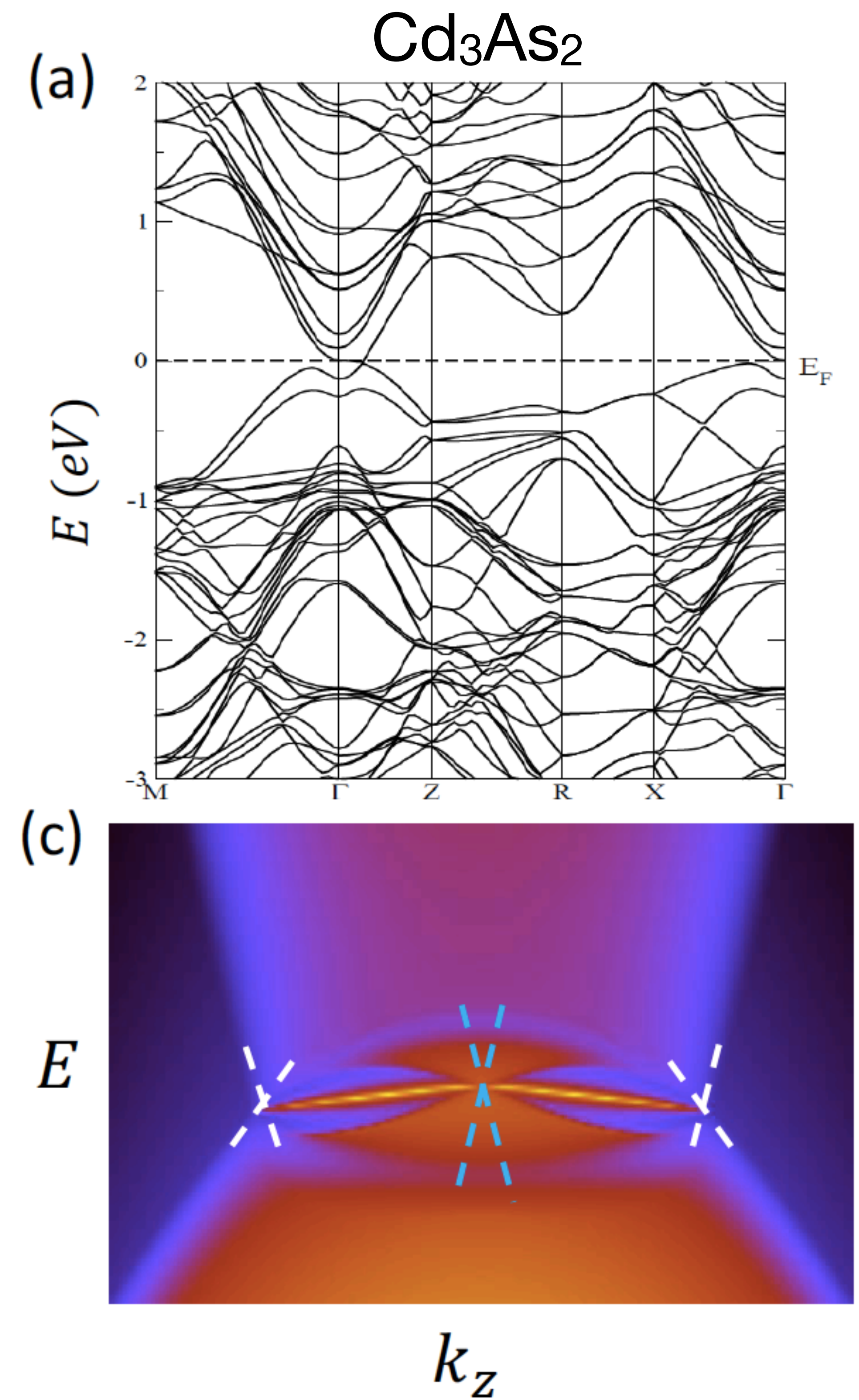
Is a Dirac fermion topological?

Argument for: “higher order Fermi arcs”

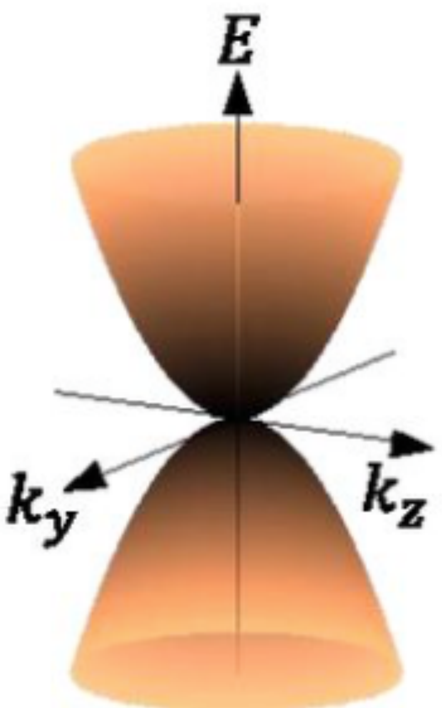
Wieder, Wang, JC, Dai, Schoop, Bradlyn, Bernevig, ArXiv: 1908.00016
also: Lin & Hughes, PRB 98, 241103 (2018)







More symmetry-protected topological band crossings

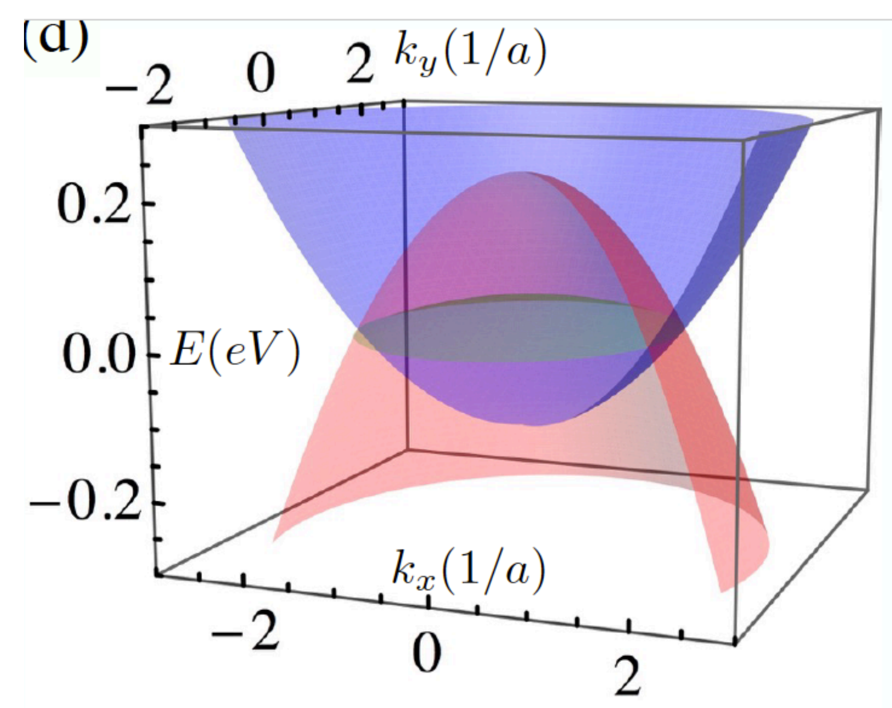


Double/triple Weyls protected by rotational symmetry

Huang et al PNAS 113, 1180 (2015),
Fang et al PRL 108, 266802 (2012)

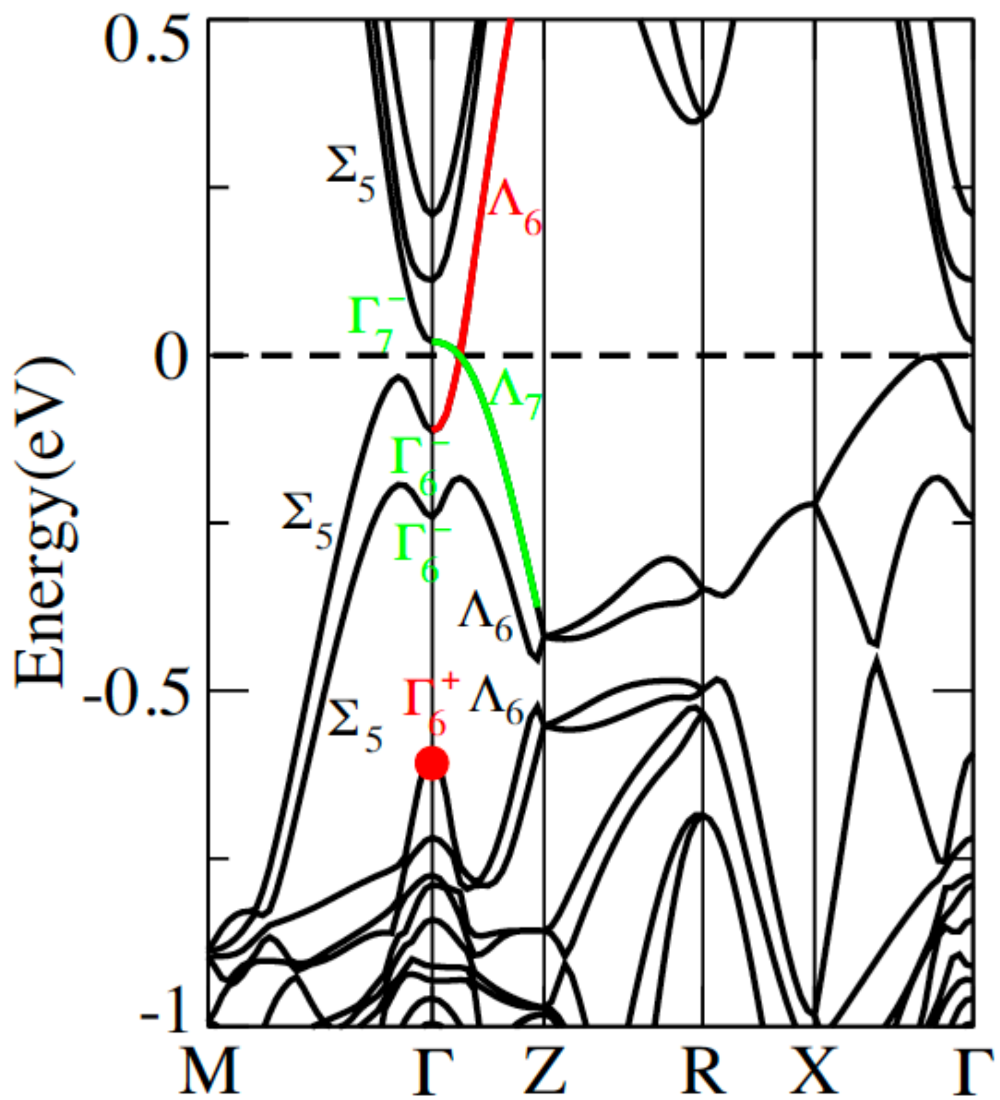
Line nodes protected by mirror symmetry

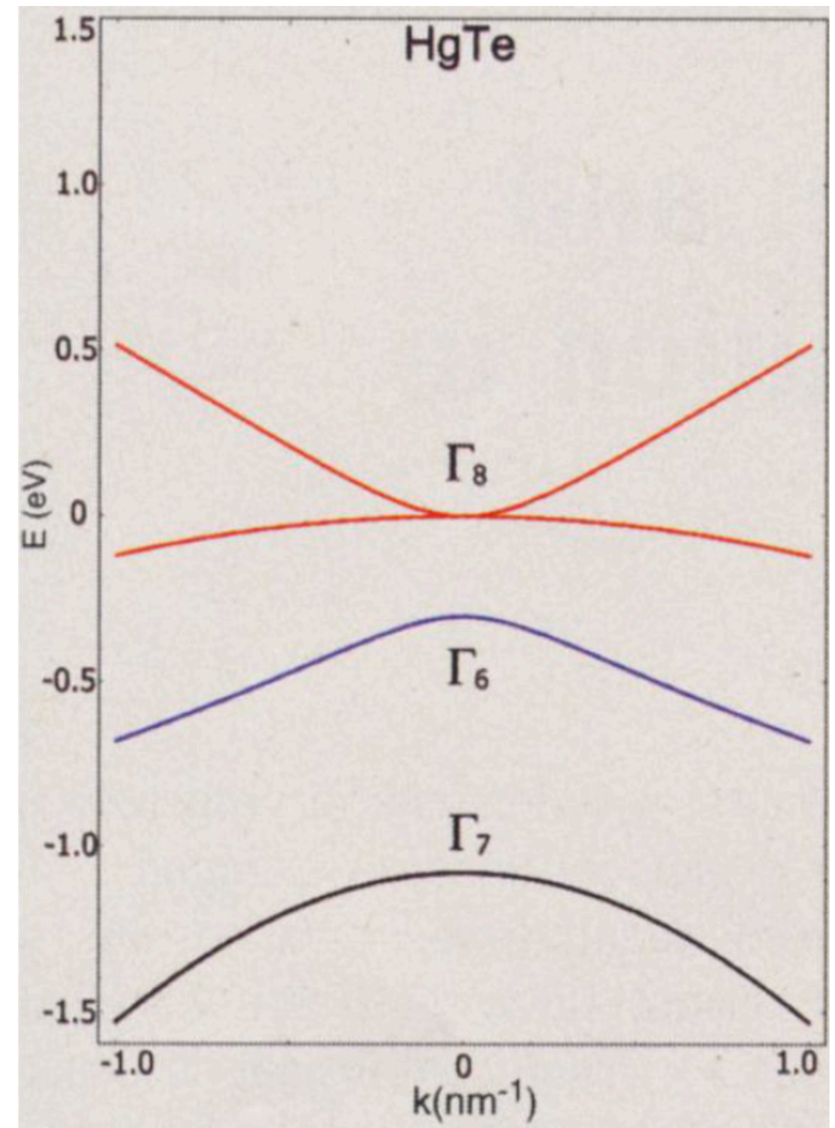
Chan, et al Phys. Rev. B 93, 205132 (2016)



Two types of symmetry-protected crossings

High-symmetry line vs High-symmetry point





Ex: Dirac fermions in Cd_3As_2 (also Na_3Bi)
Wang, et al, PRB 88, 125427 (2013)

Ex: HgTe, GdPtBi
Fig: Bernevig, Hughes, Zhang, Science 2006

Symmetry-protected topological fermions beyond Dirac and Weyl

What types of fermions can be protected at high-symmetry points?

Topological signatures

Role of non-symmorphic symmetries

Experimental realizations

Non-magnetic: Bradlyn, **JC**, Wang, Vergniory, Felser, Cava, Bernevig: Science **343**, 6299 (2016)

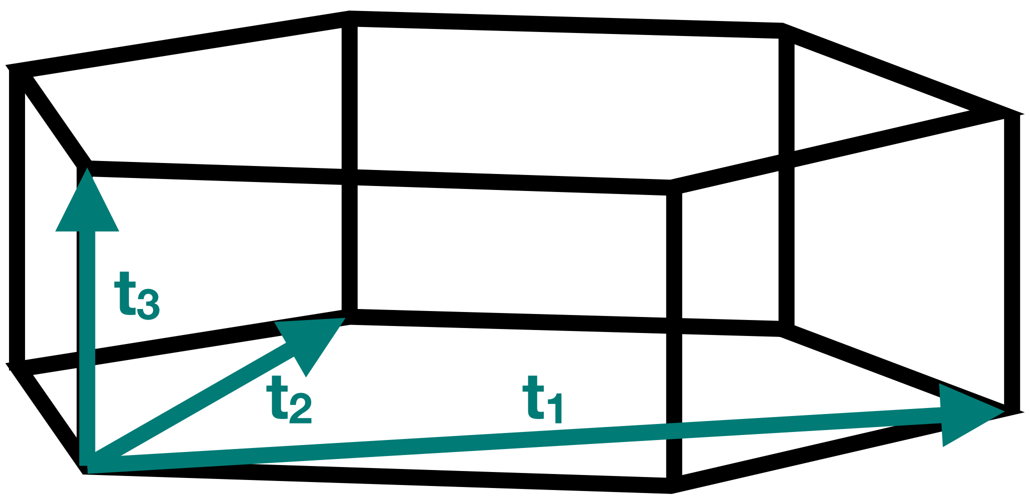
Magnetic: **JC**, Bradlyn, Vergniory: ArXiv: 1904.12867

Recall: space groups describe the symmetry of crystals in 3D

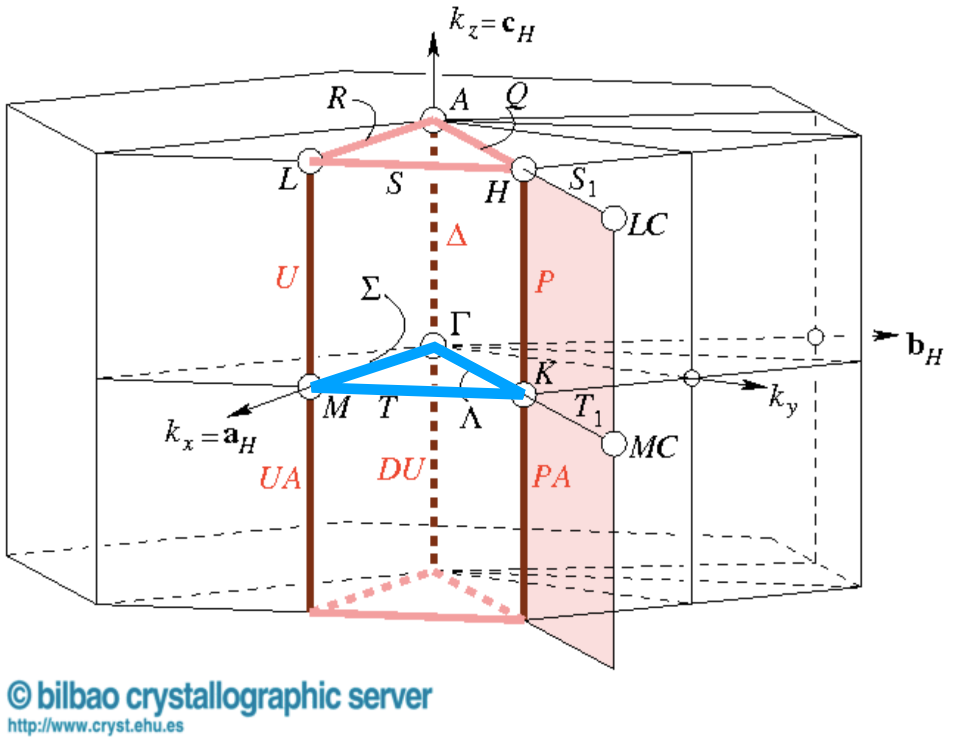
Ex: P6mm, (#183)

C_{6z}, m_x, lattice translations

Real space



Brillouin zone



230 space groups with time-reversal;
1191 space groups without time-reversal!!

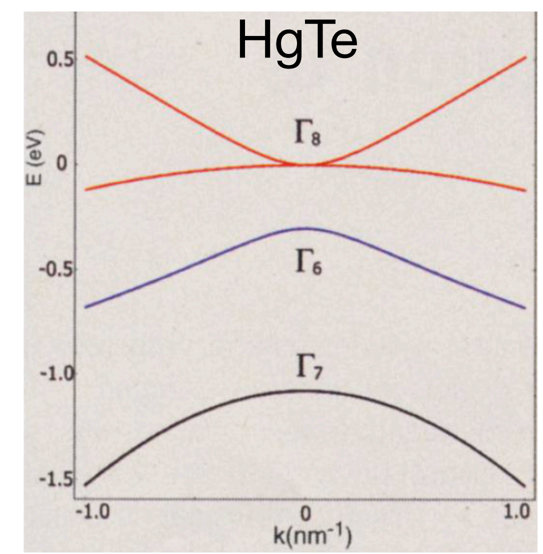
Method: enumerate representations at high-symmetry points

In each space group, at each **k**,

1. Symmetries that leave **k** invariant comprise "little group" at **k**

$$g\mathbf{k} = \mathbf{k} + \mathbf{G}$$

2. Bands at **k** transform as irrep of little group at **k**



$$\Downarrow$$

3. An n-fold degeneracy exists if and only if little group has n-dim irrep

2016: look up in textbook (Bradley and Cracknell)
2017: we added to Bilbao Crystallographic Server
(see Topological Quantum Chemistry, Nature 547, 298—305 (2017))

Method: enumerate representations at high-symmetry points

Deg.	SG	$\mathbf{k}$	Deg.	SG	$\mathbf{k}$
3	$I2_13$ (199)	P	8	$P4/ncc$ (130)	A
3	$I4_132$ (214)	P	8	$P4_2/mbc$ (135)	A
3	$I\bar{4}3d$ (220)	P	8	$P\bar{4}3n$ (218)	R
6	$P2_13$ (198)	R	8	$I\bar{4}3d$ (220)	H
6	$Pa\bar{3}$ (205)	R	8	$Pn\bar{3}n$ (222)	R
6	$Ia\bar{3}$ (206)	P	8	$Pm\bar{3}n$ (223)	R
6	$P4_332$ (212)	R	8	$Ia\bar{3}d$ (230)	H
6	$P4_132$ (213)	R			
6	$Ia\bar{3}d$ (230)	P			

Take-aways:

Only 2-, 3-, 4-, 6-, and 8-fold degeneracies are possible

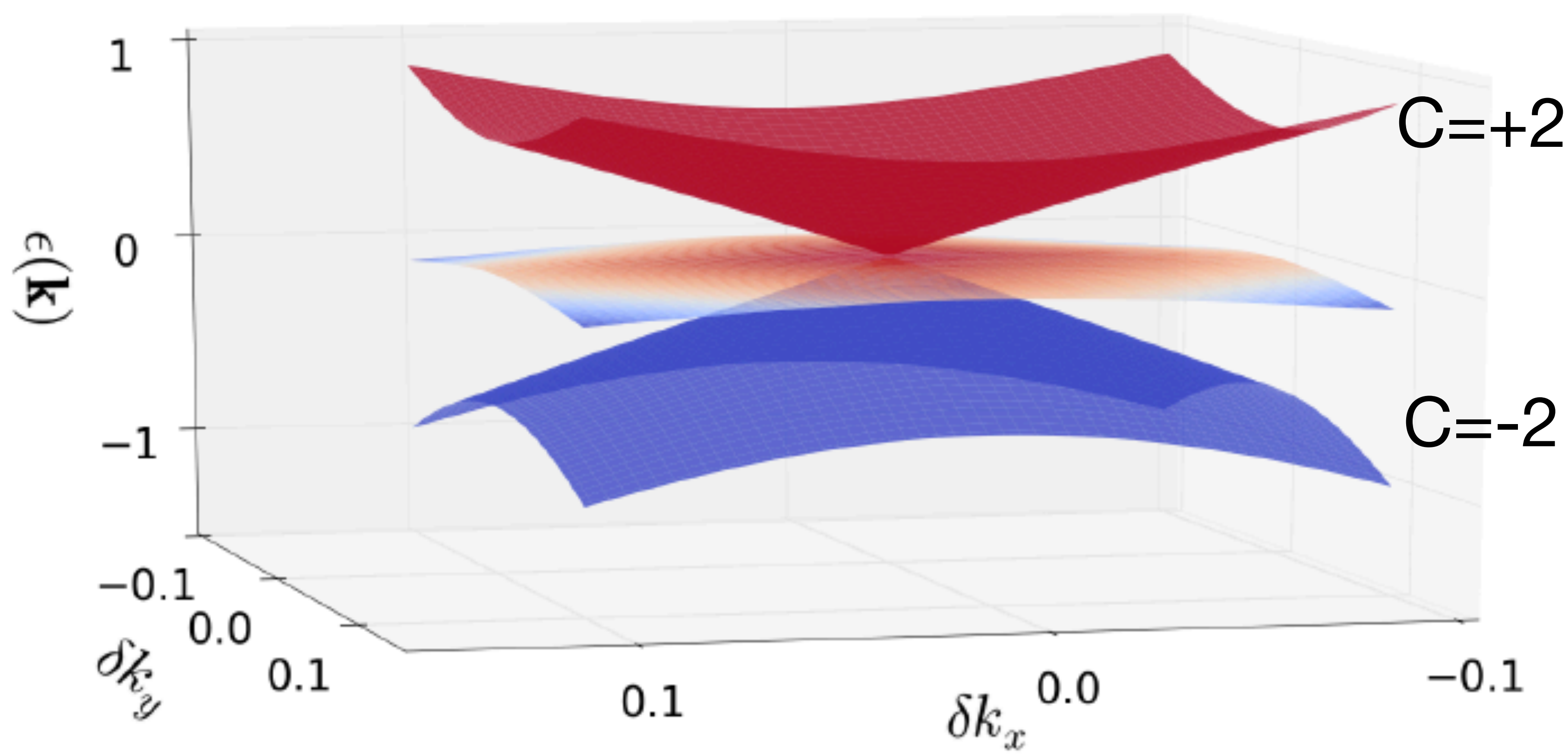
“Multifold fermions” only available in certain space groups

"Spin-1 Weyl"

$$H = \mathbf{k} \cdot \mathbf{S}$$

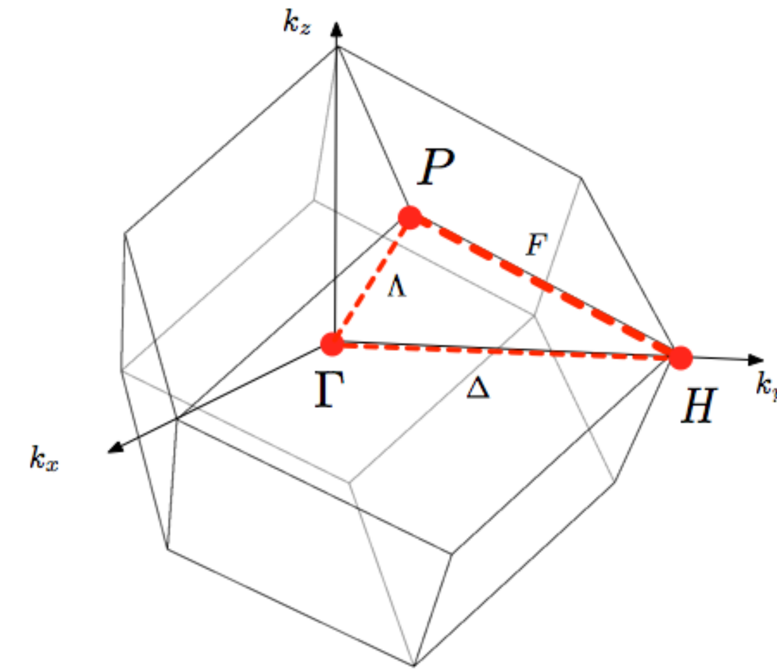
S_i are spin-1 matrices

$$E = 0, \pm\sqrt{\sum k_i^2}$$



Charge-2 monopole of Berry curvature!

“Spin-1 Weyl”



Occurs in space groups 199 and 214 (bcc)
at P = (¼, ¼, ¼)

Not time-reversal invariant point!

Derive 3-fold degeneracy: irreps of the “little group” at P

$$\{C_{2x}|\frac{1}{2}\frac{1}{2}0\}^2 = \{C_{3,\bar{1}1\bar{1}}|\frac{1}{2}\frac{1}{2}0\}^3 \neq 1$$

Non-symmorphic!

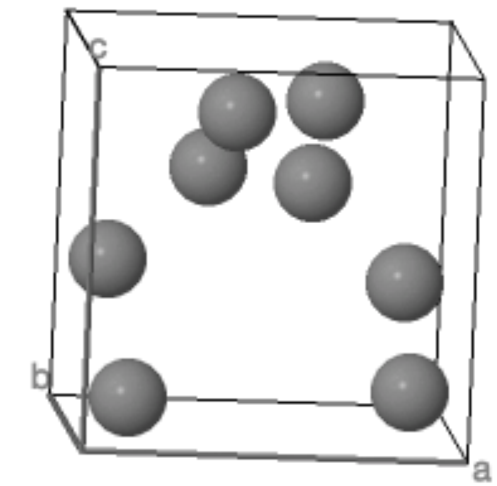
Rules:

- 2π rotations represented by -1
- Translation t represented by $e^{iP.t}$

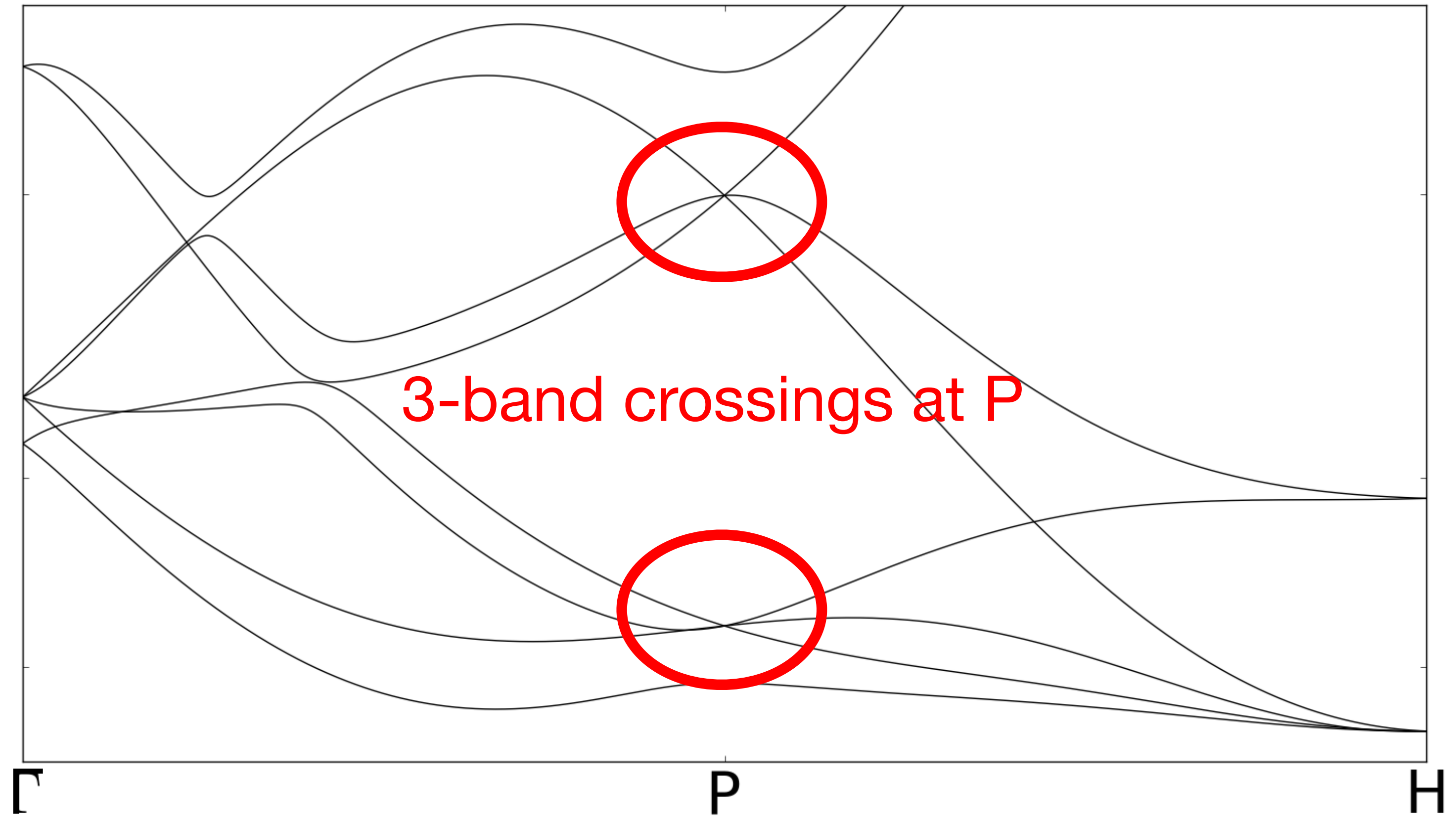
Result: 3d and 1d irreps

“Spin-1 Weyl”

Ex: tight-binding model for SG 214



Conv. unit cell (ICSD)

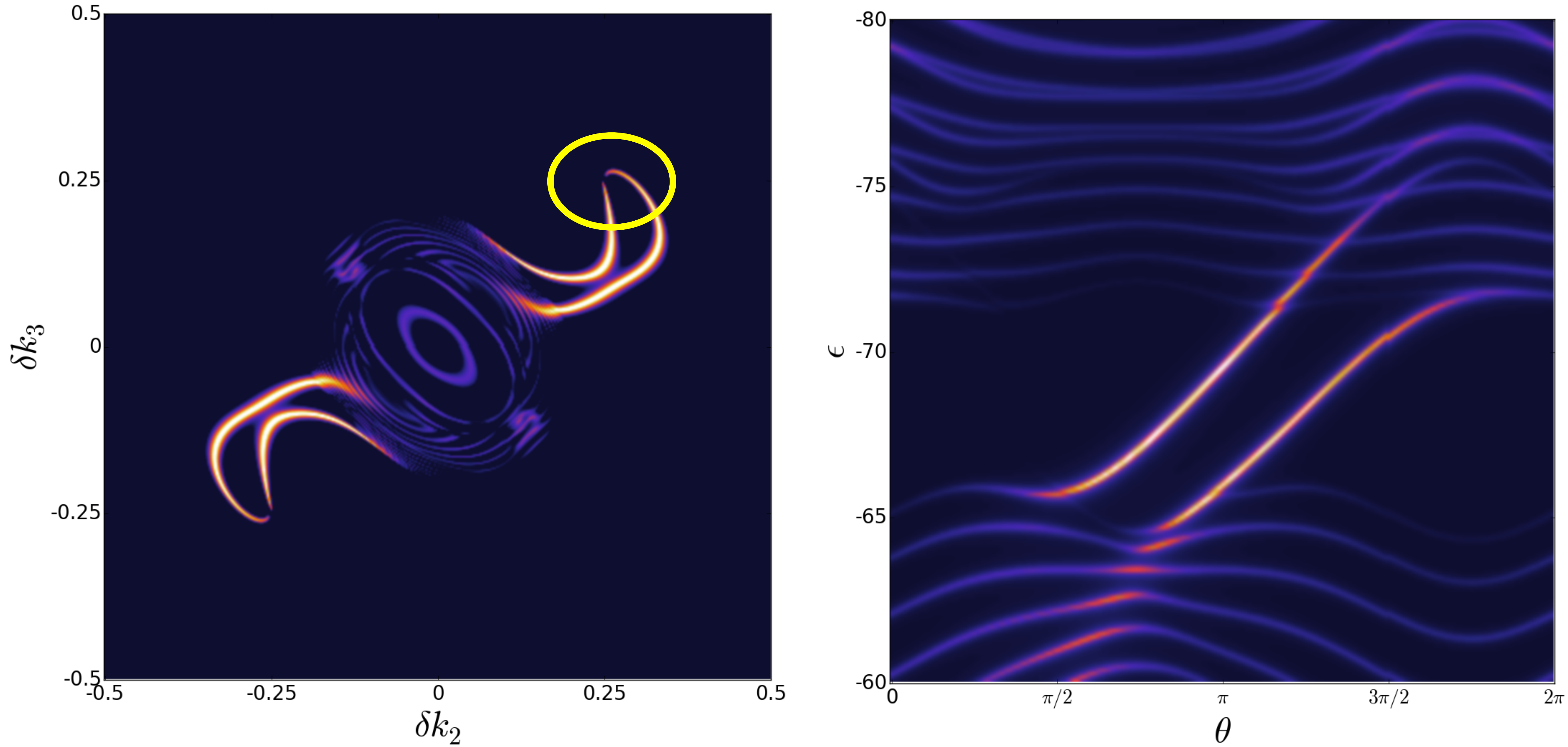


“Spin-1 Weyl”

Experimental signature: surface Fermi arc

Wan, Turner, Vishwanath, Savrasov (2011)

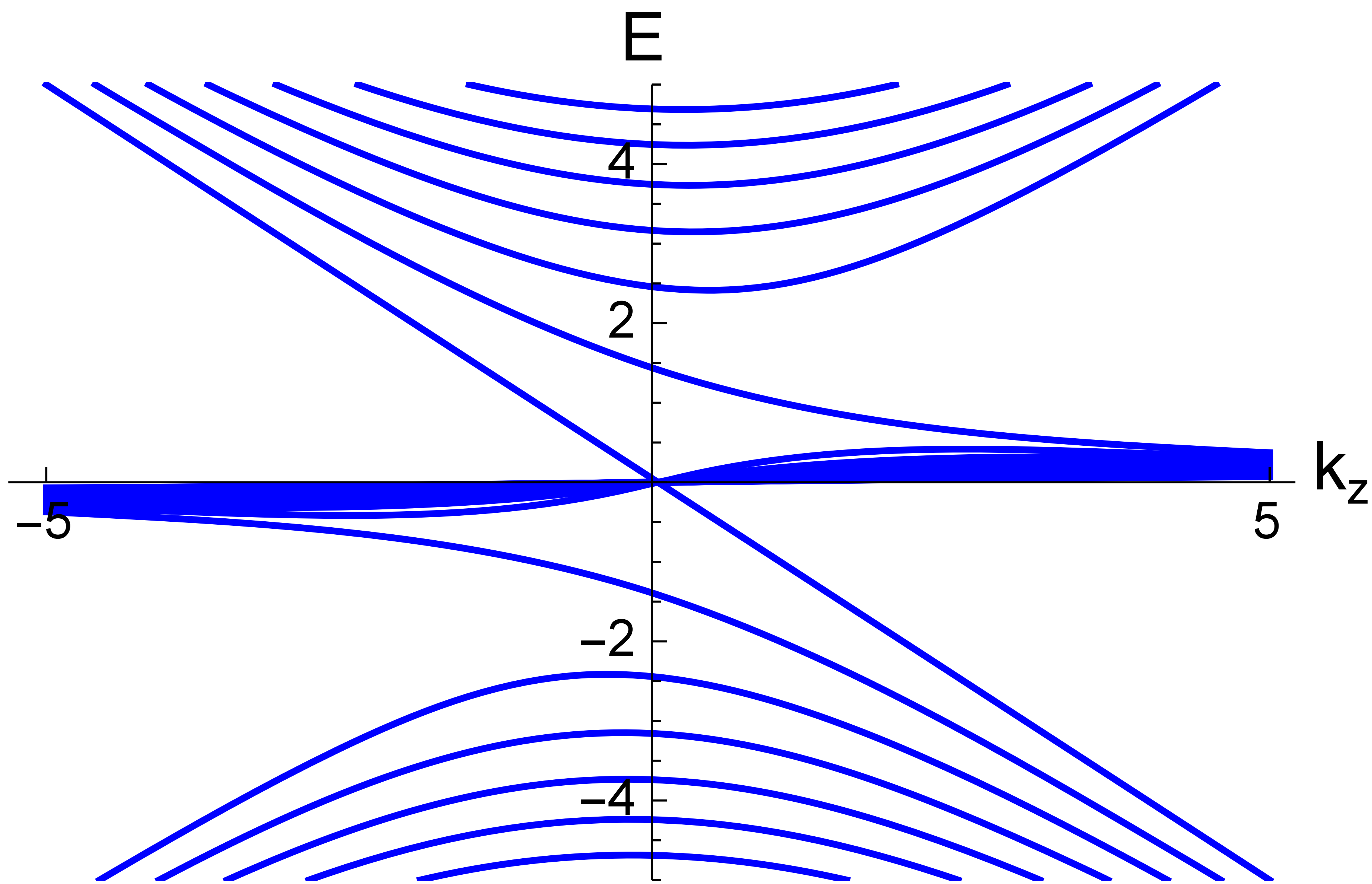
Surface spectral function:



“Spin-1 Weyl”

Experimental signature: Landau levels

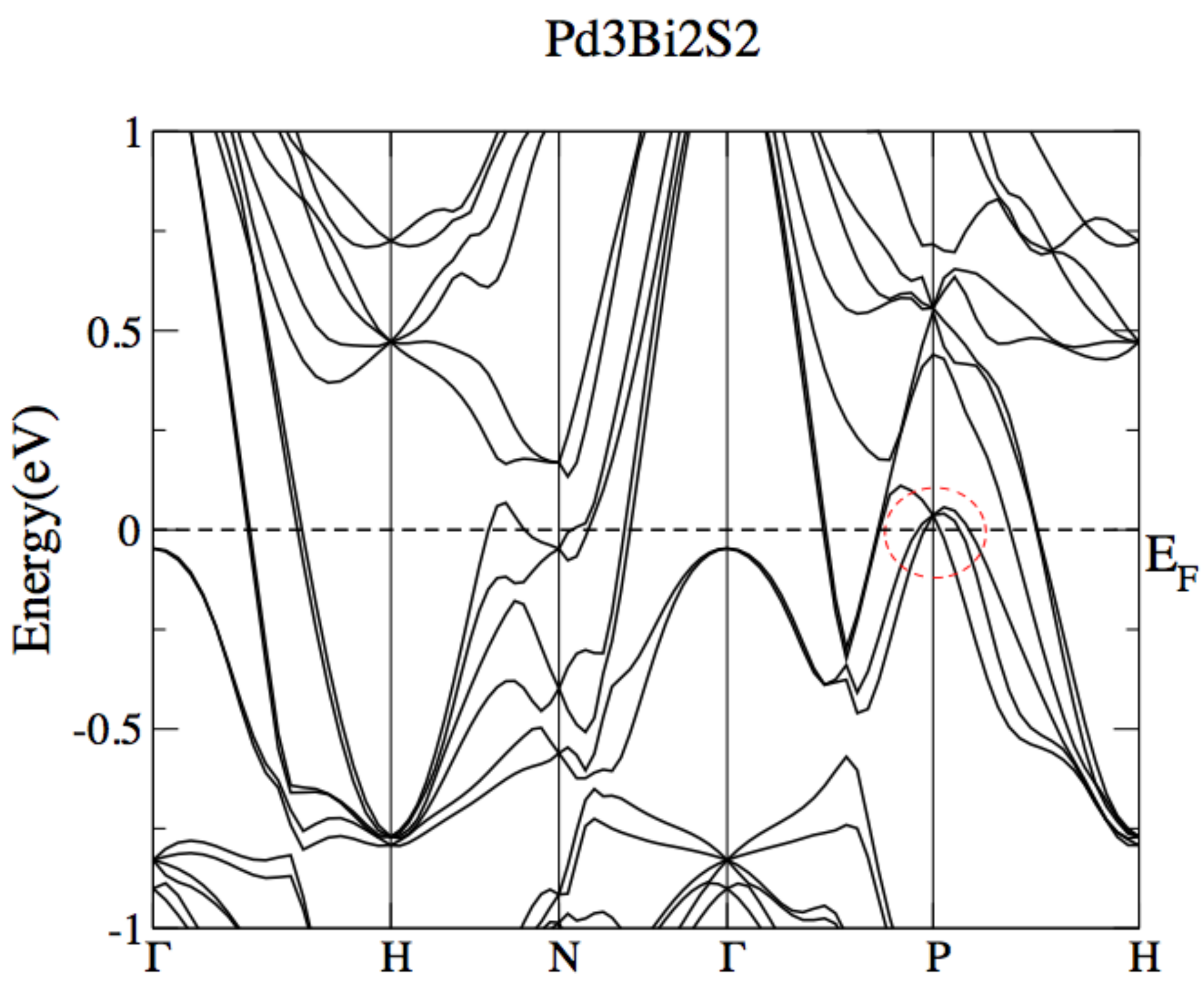
- Two chiral modes
  (like double Weyl)
- Level spacing ~$n^{1/2}$
  (like single Weyl)
- High d.o.s. at E=0

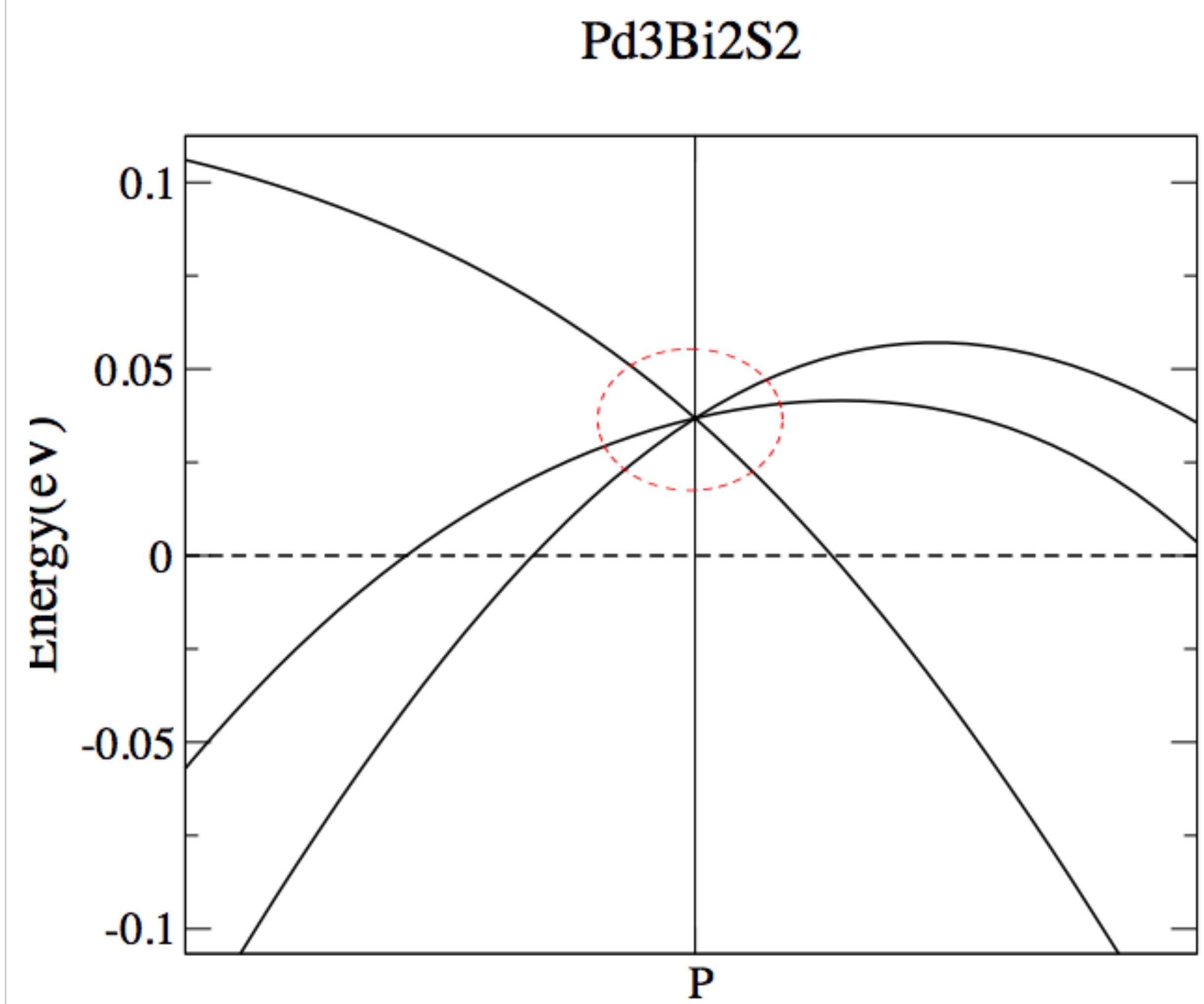


Exact spectrum when H=k.S

“Spin-1 Weyl”

Candidate materials

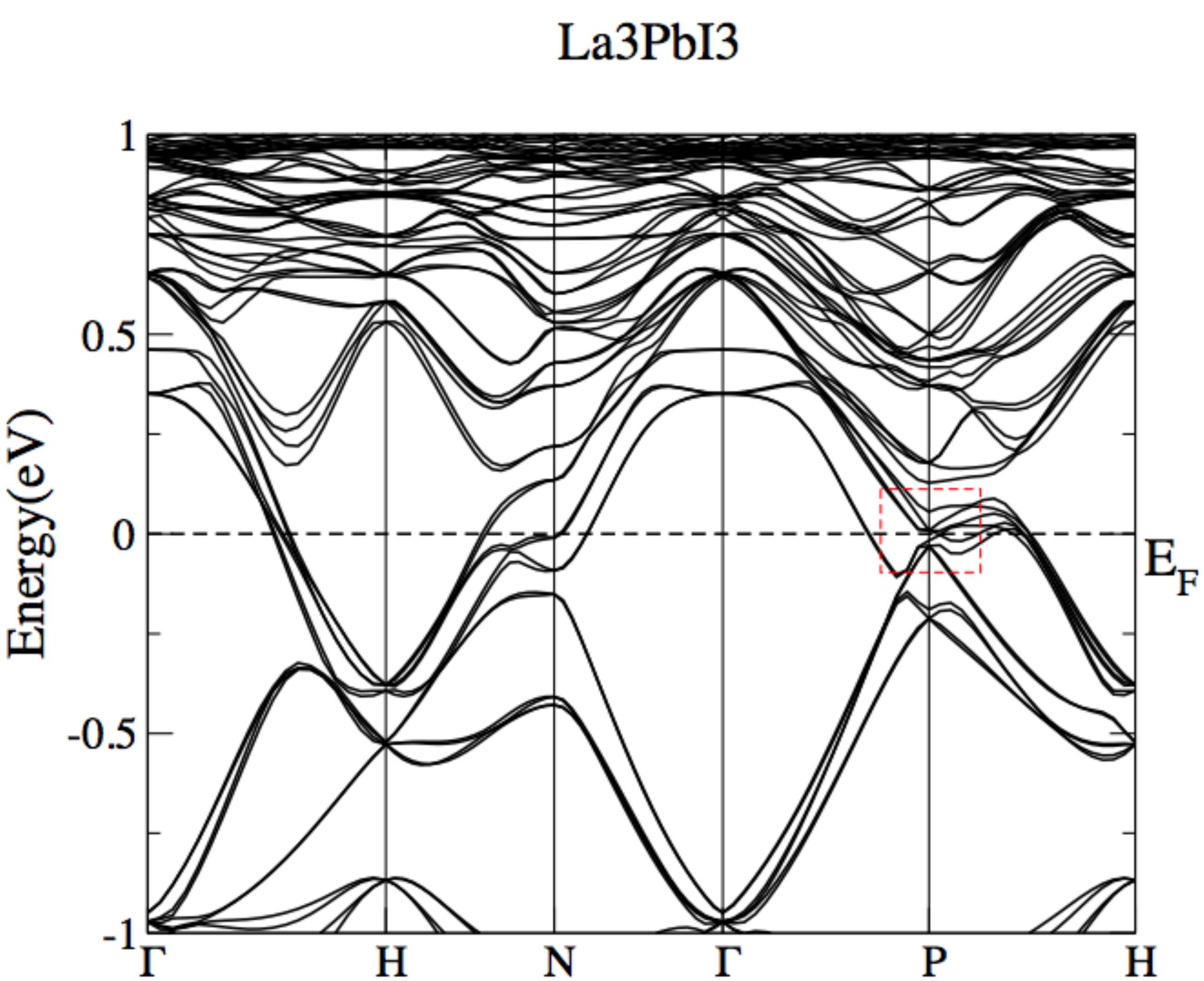


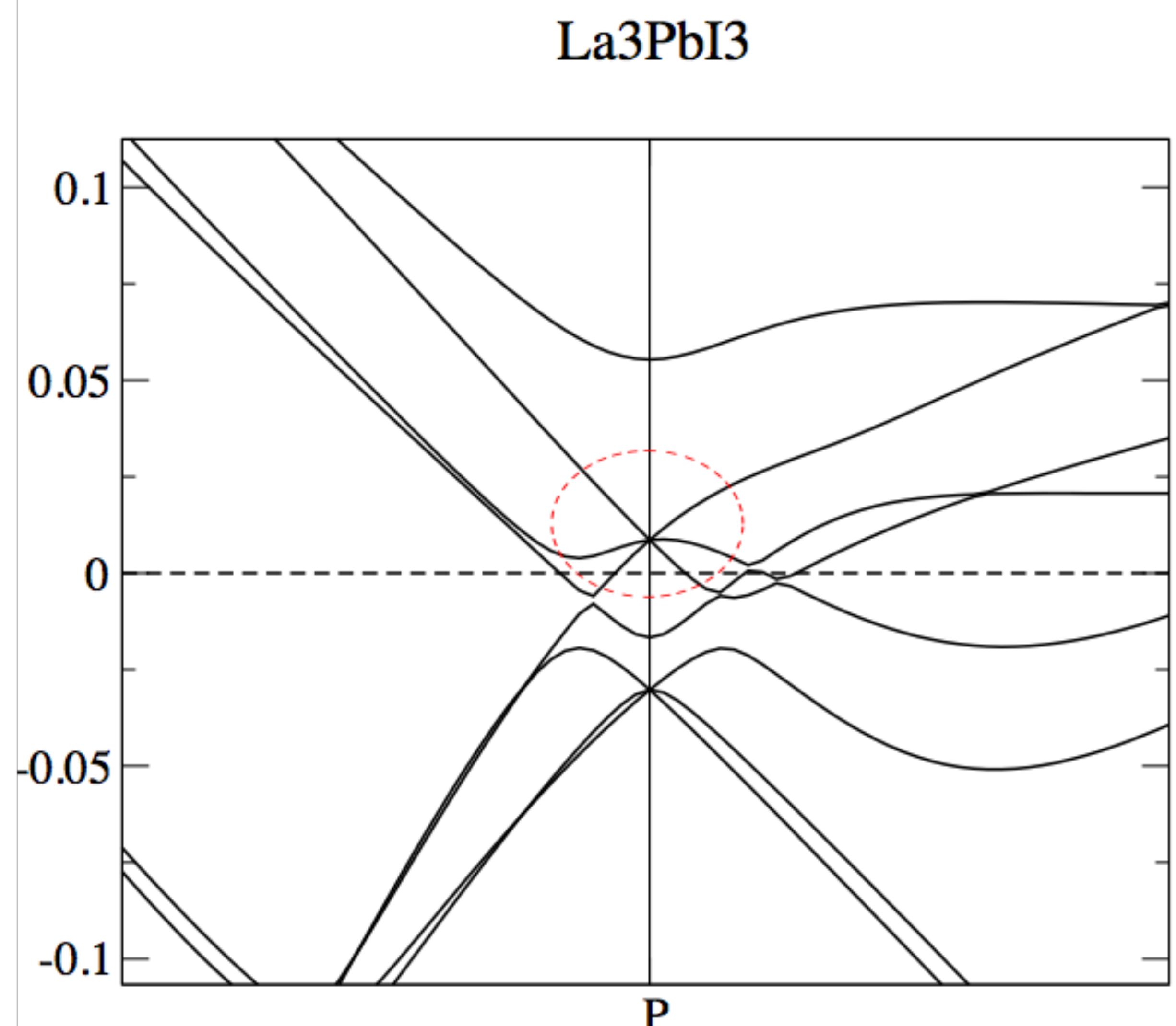


SG 199

"Spin-1 Weyl"

Candidate materials





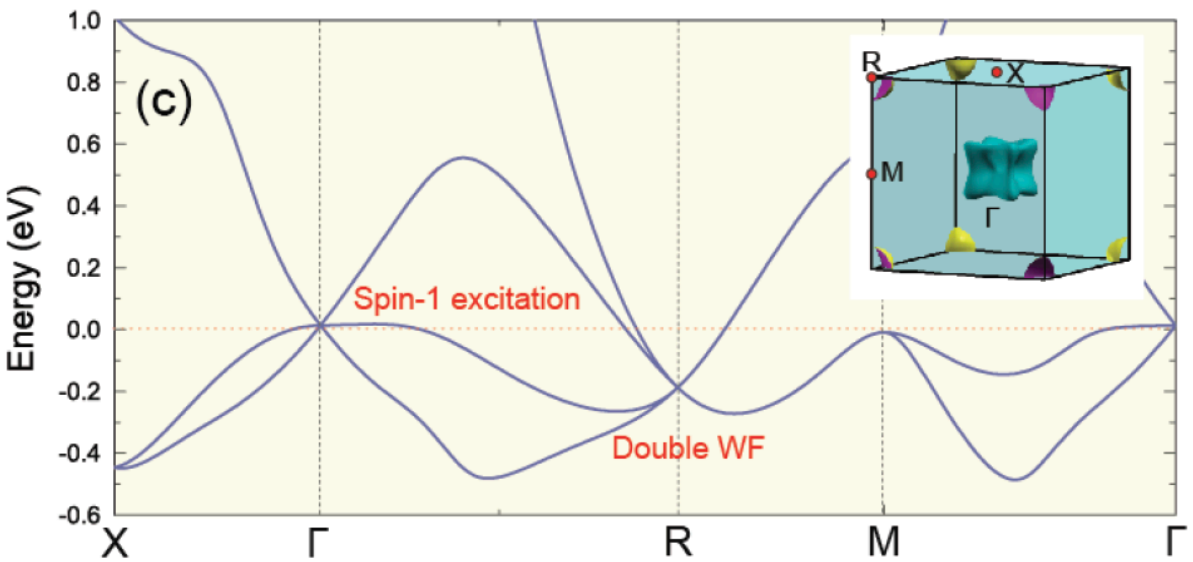
SG 214

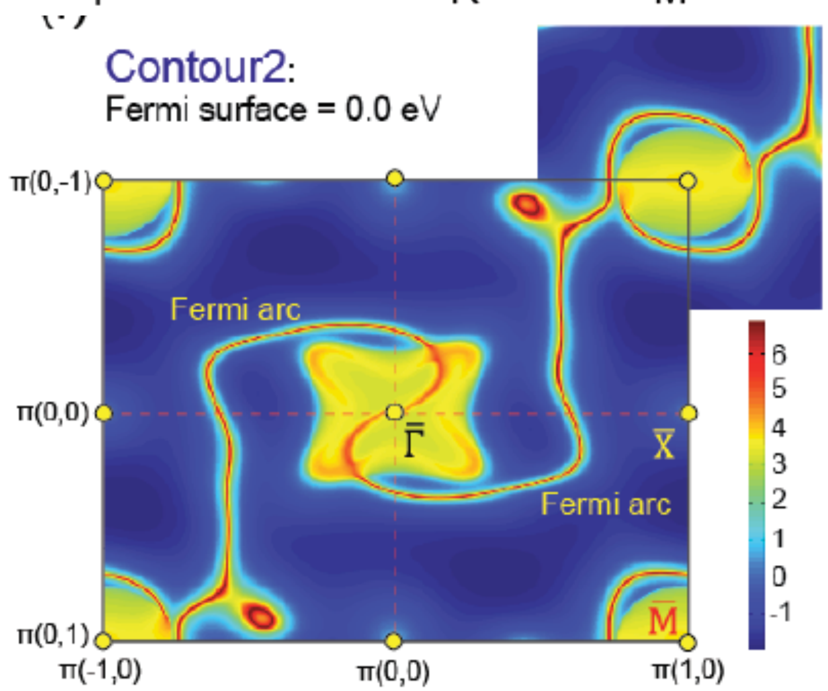
Observation of spin-1 Weyl in CoSi

Hong Ding group: Nature 567, 496-499 (2019)

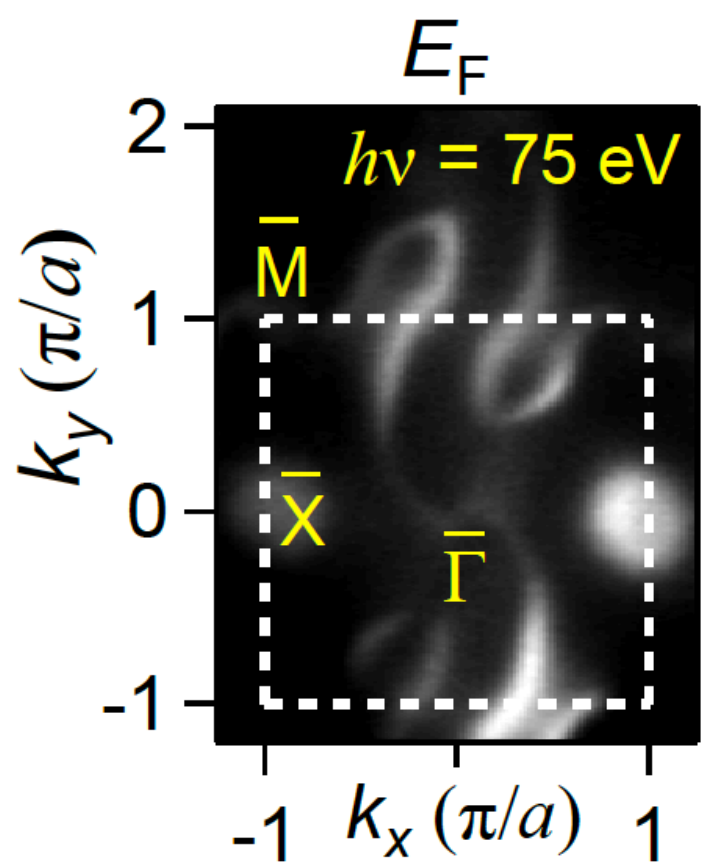
Theory: Tang, et al PRL 119, 206402 (2017); Chang, et al, PRL 119, 206401 (2017); Pshenay-Severin et al, J.Phys. Cond. Mat. 30 135501 (2018)

Theory

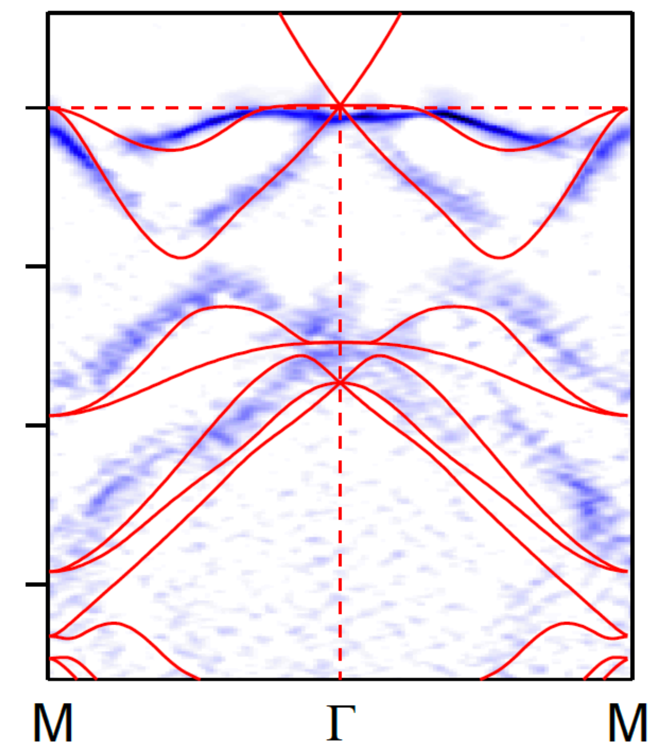




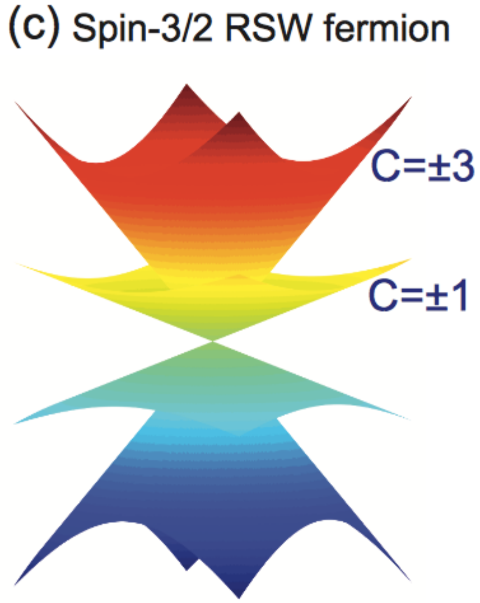
Experiment



ARPES



X-rays



"Spin-3/2 Weyl"

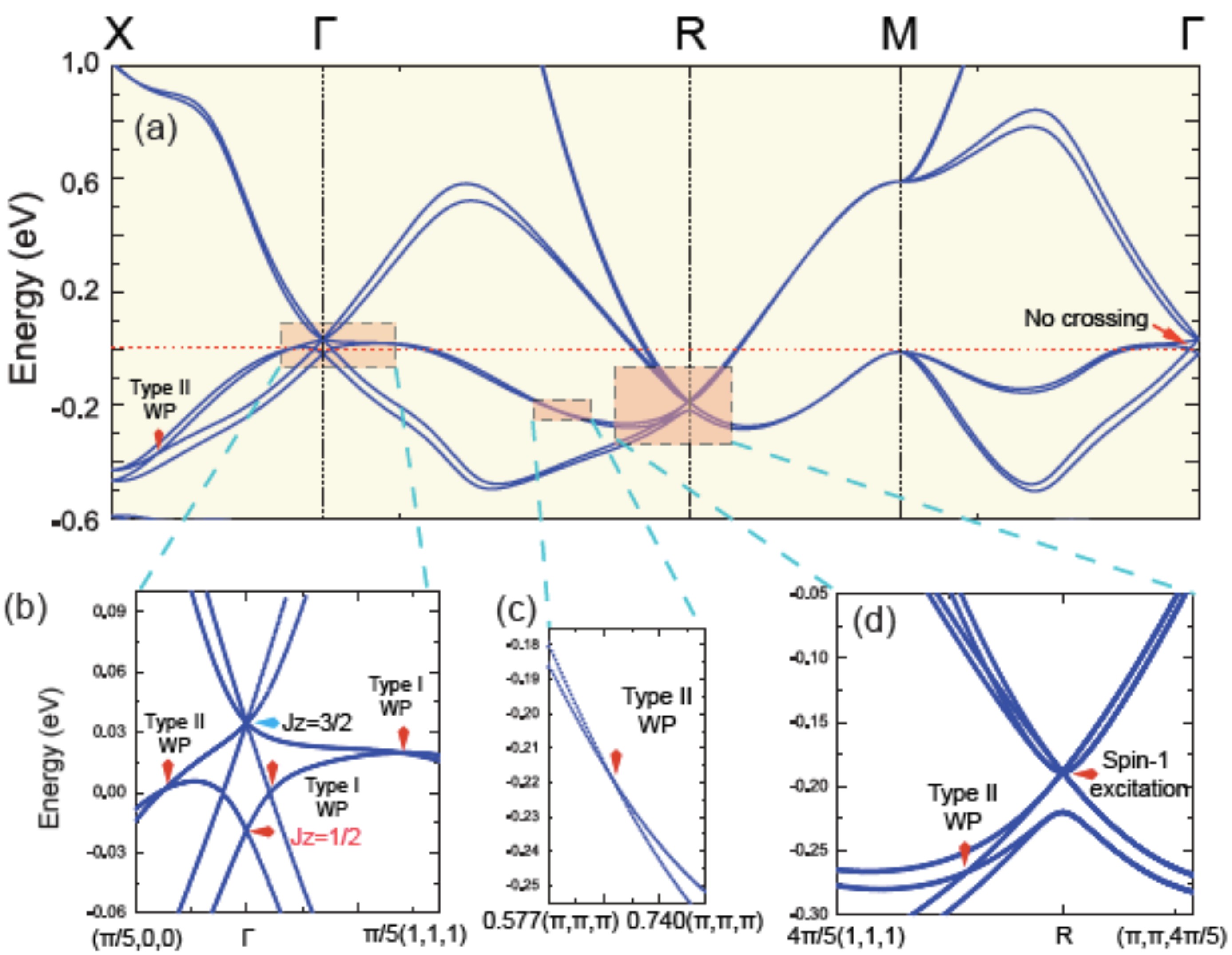
$$H = \mathbf{k} \cdot \mathbf{S}$$

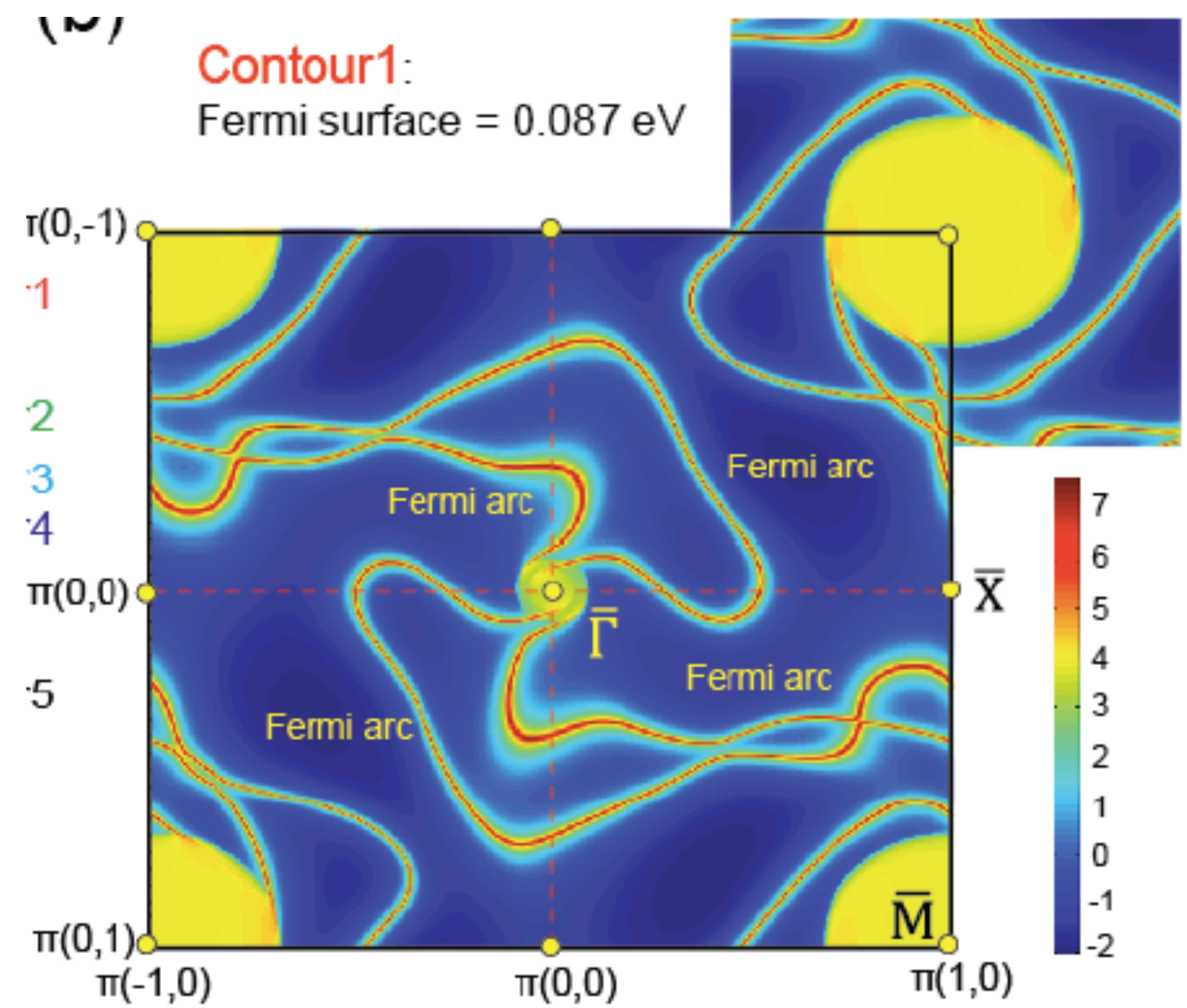
S_i are spin-3/2 matrices

Prediction in transition metal silicides:

Tang, Zhou, Zhang PRL 119, 206402 (2017); Chang, et al, (Hasan group) PRL 119, 206401 (2017)

CoSi





Only spin-1/2, -1, and -3/2 Weyl fermions protected by crystal symmetry

$$H = \mathbf{k} \cdot \mathbf{S}$$

S_i are spin-s matrices, s=1/2, 1, 3/2

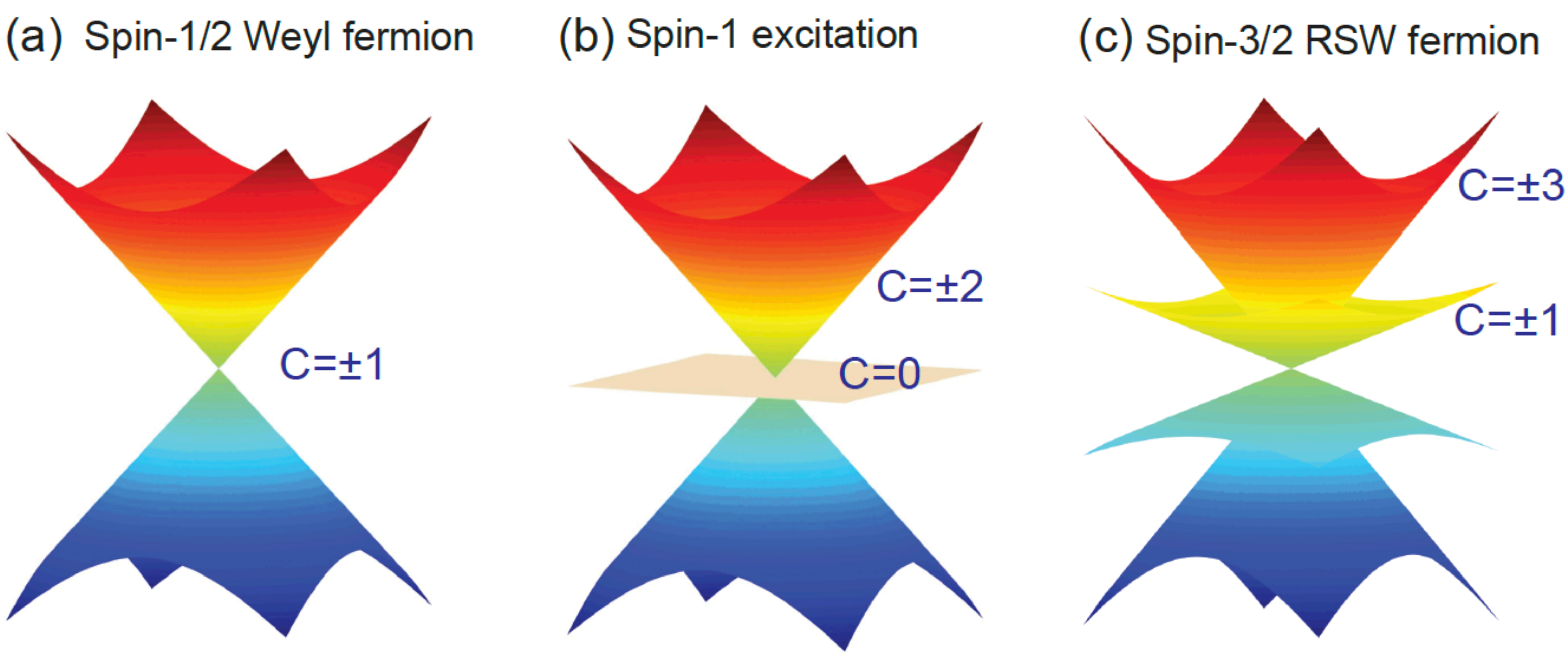


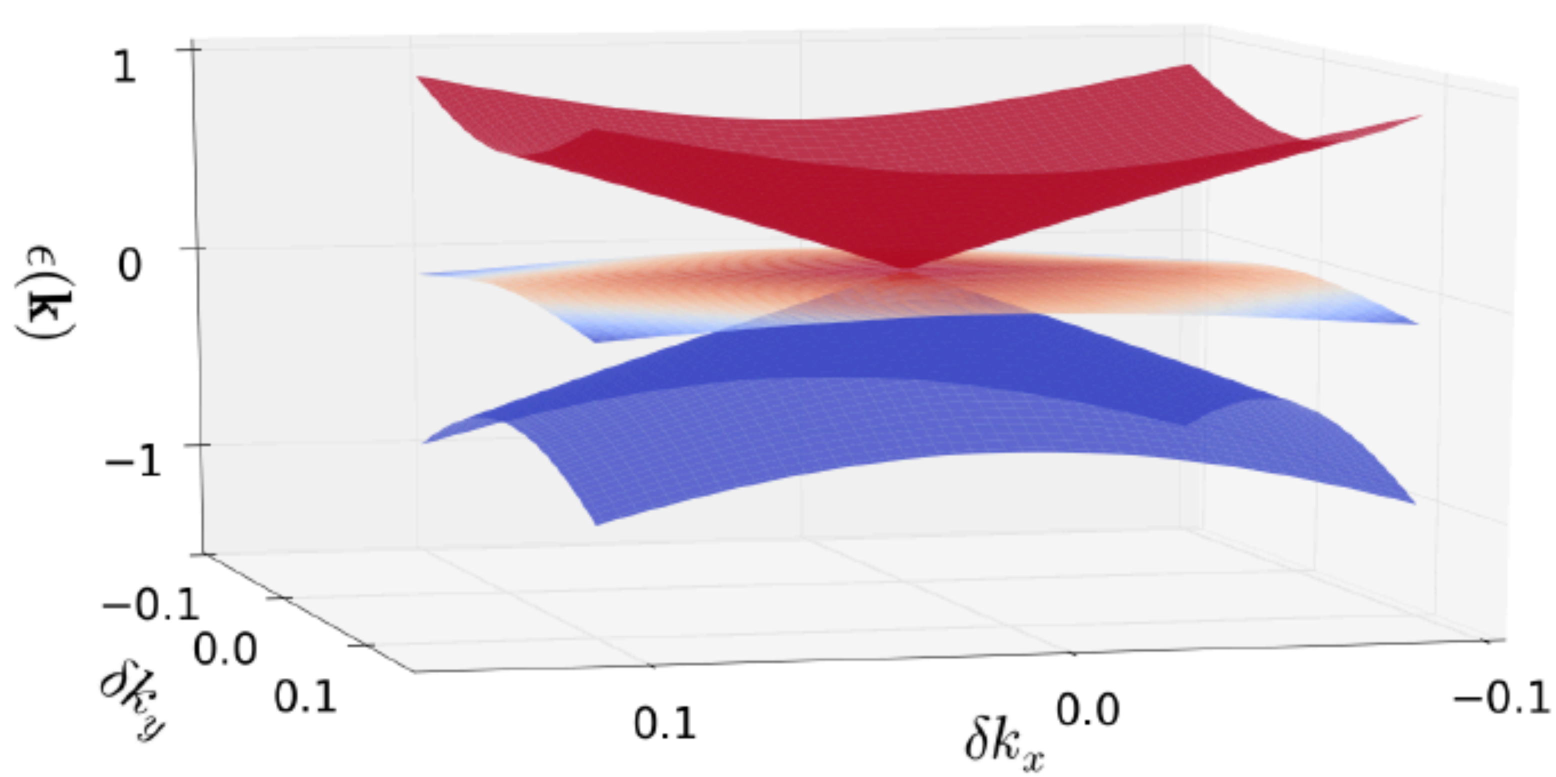
Figure: Tang, Zhou, Zhang PRL 119, 206402 (2017)

“Spin-1 Dirac”

Two copies of spin-1 Weyl with opposite chirality

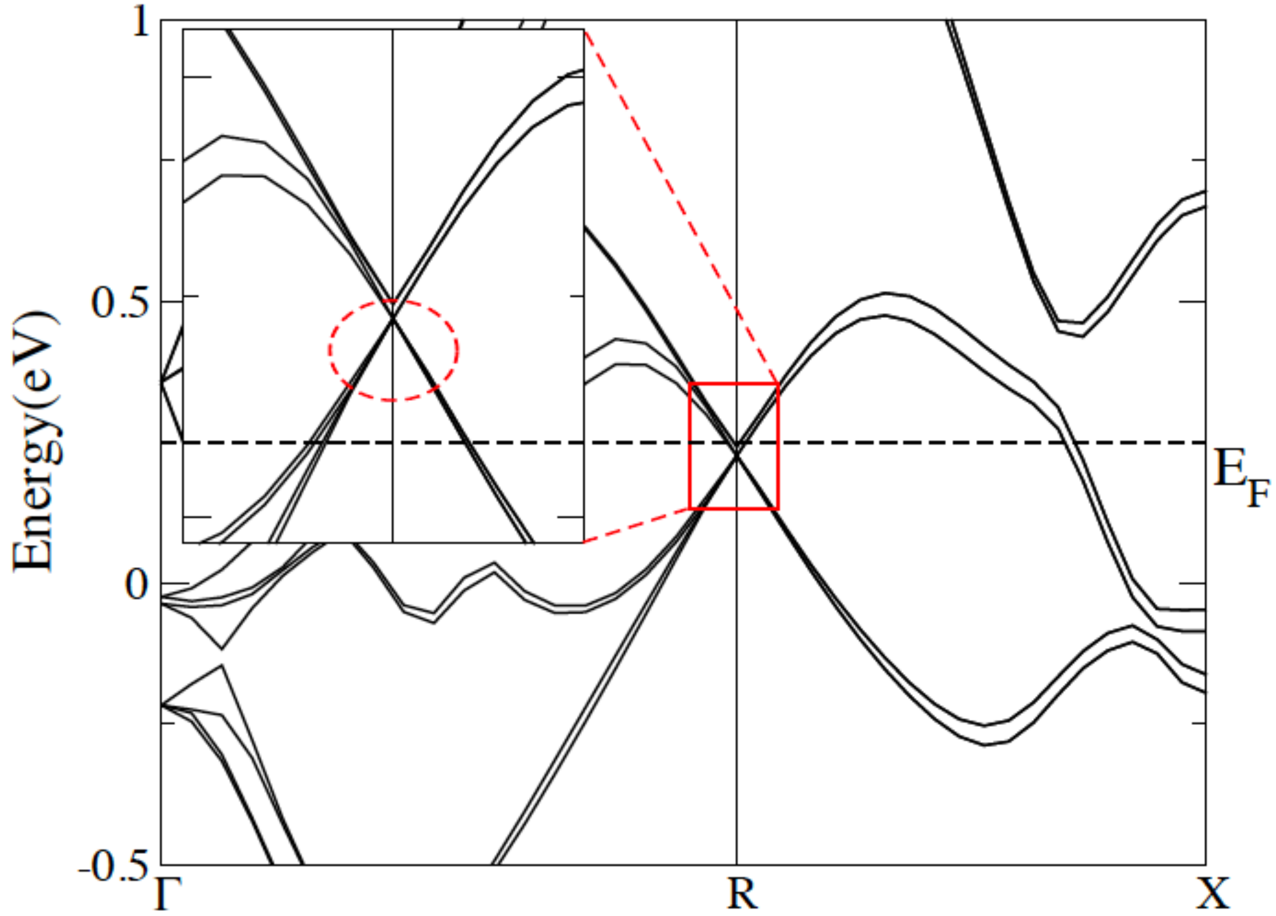
Protected by inversion symmetry

Occurs in SGs 206 and 230

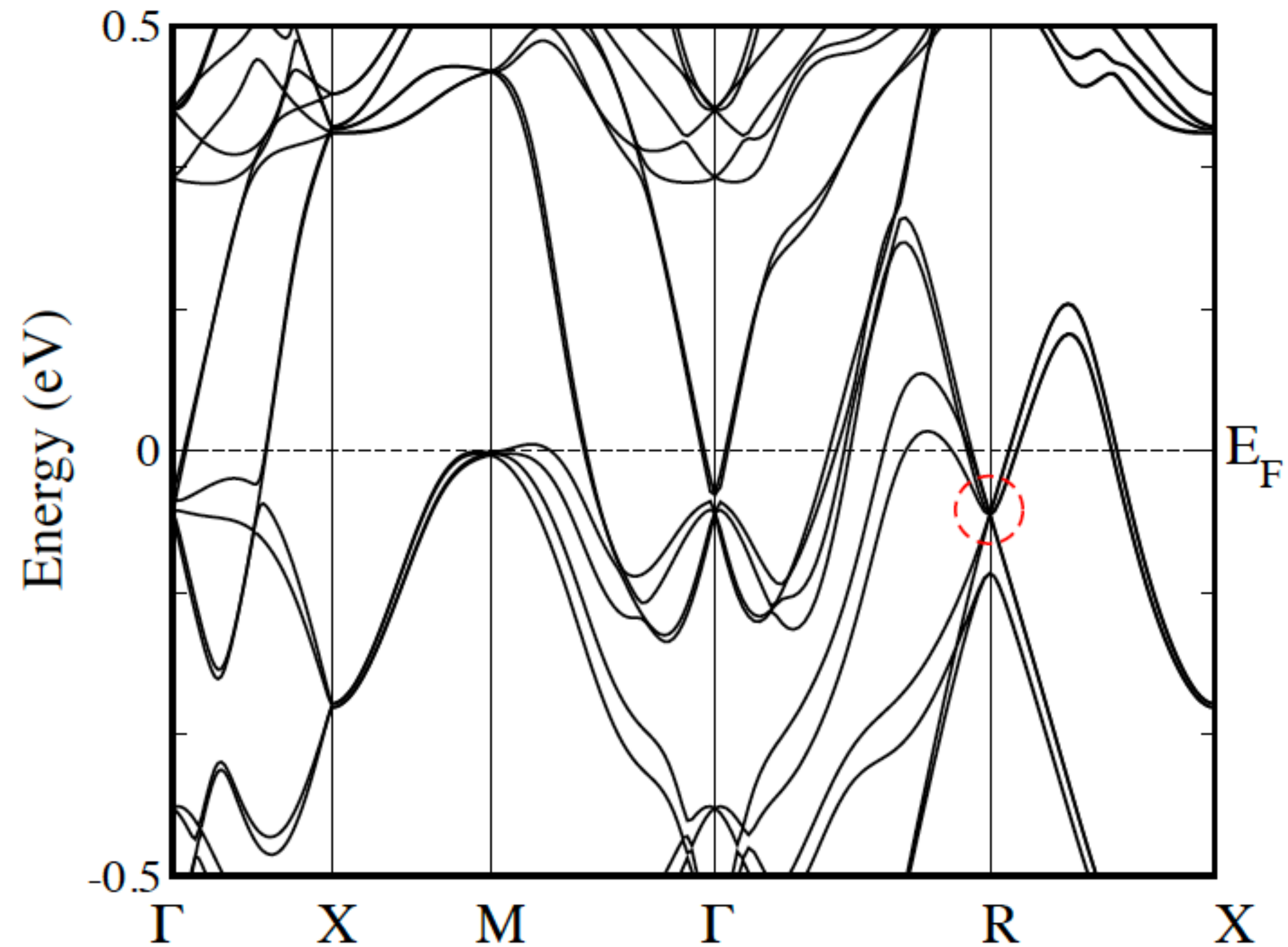


Experimental predictions for spin-1 Dirac

(d) Li_2Pd_3B (SG 212)

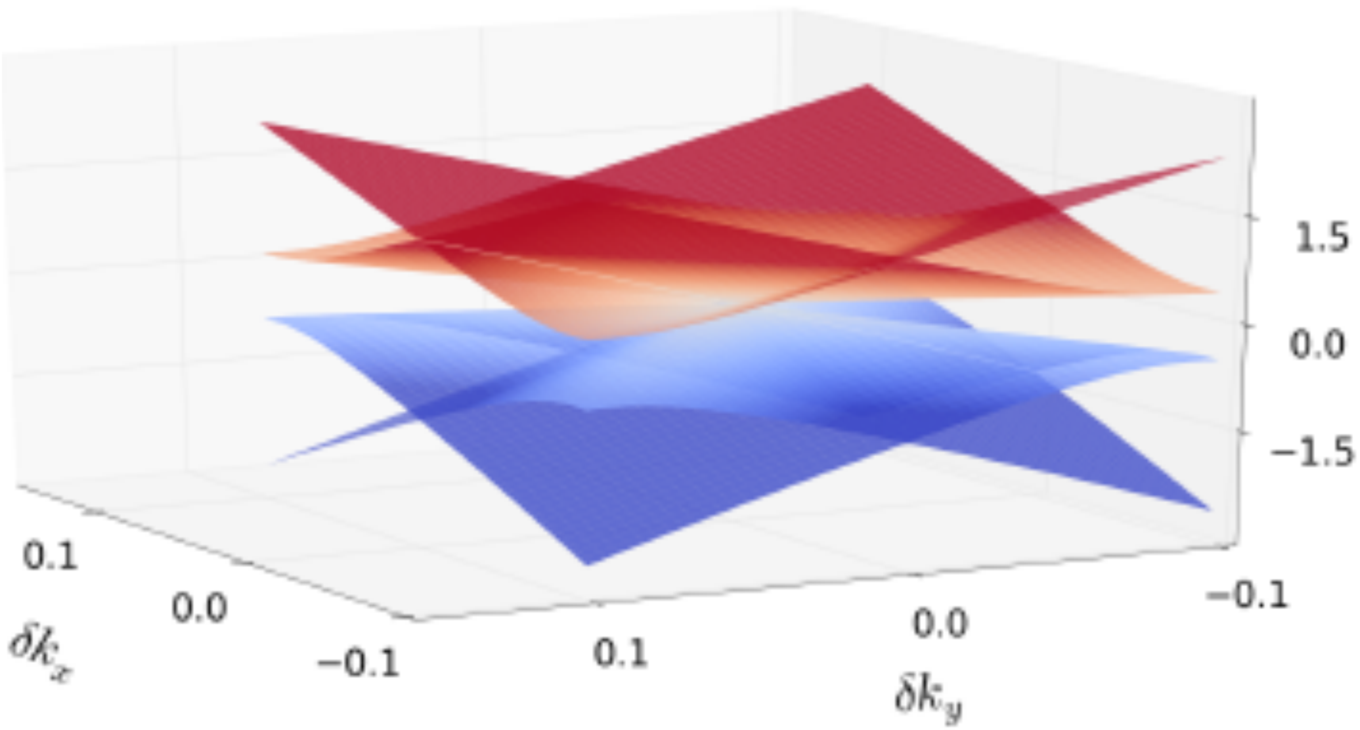


(e) Mg_3Ru_2 (SG 213)



A parent phase for topological semimetals: 8-fold band crossings

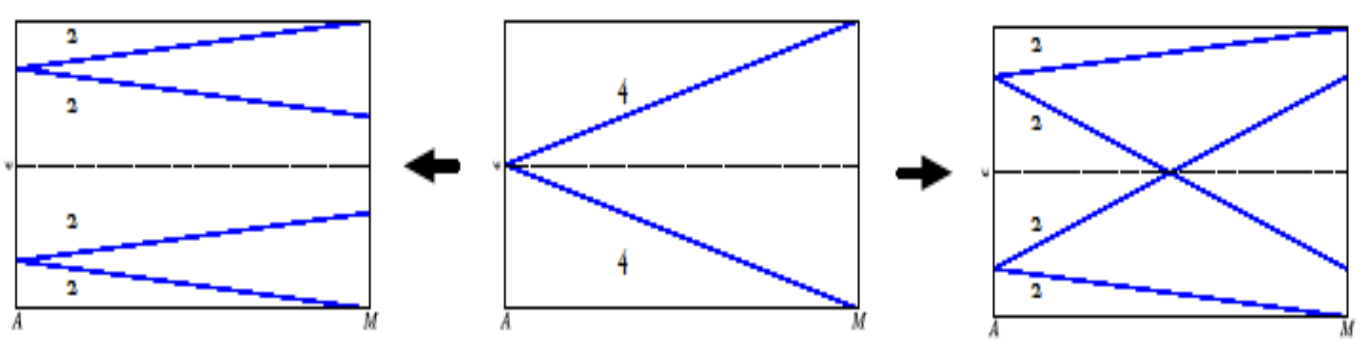
See also: Wieder, et al PRL 116, 186402 (2016)

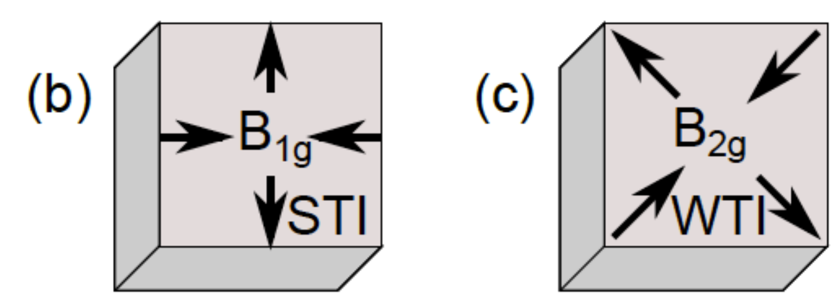


All bands doubly-degenerate

4x degenerate “Dirac line nodes”

Applied magnetic field: line node splits into Dirac point





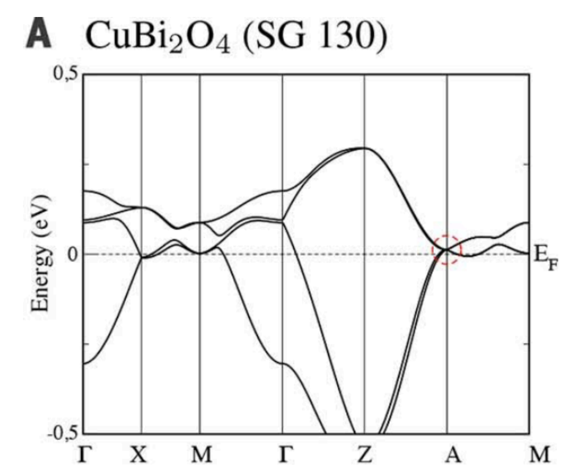
Wieder, et al: strain gaps into weak/strong TI

Topological band theory vs interactions

Ex: $CuBi_2O_4$

DFT predicts 8-fold "Double Dirac" at E=0

Experiment reveals large band gap



Rapid Communication

Realizing double Dirac particles in the presence of electronic interactions

Domenico Di Sante, Andreas Hausoel, Paolo Barone, Jan M. Tomczak, Giorgio Sangiovanni, and Ronny Thomale

Phys. Rev. B **96**, 121106(R) – Published 11 September 2017

How do interactions gap semimetals?

When are the resulting phases topological?

See also: Watanabe, Po, Vishwanath, Zaletel PNAS 112, 14551 (2015)

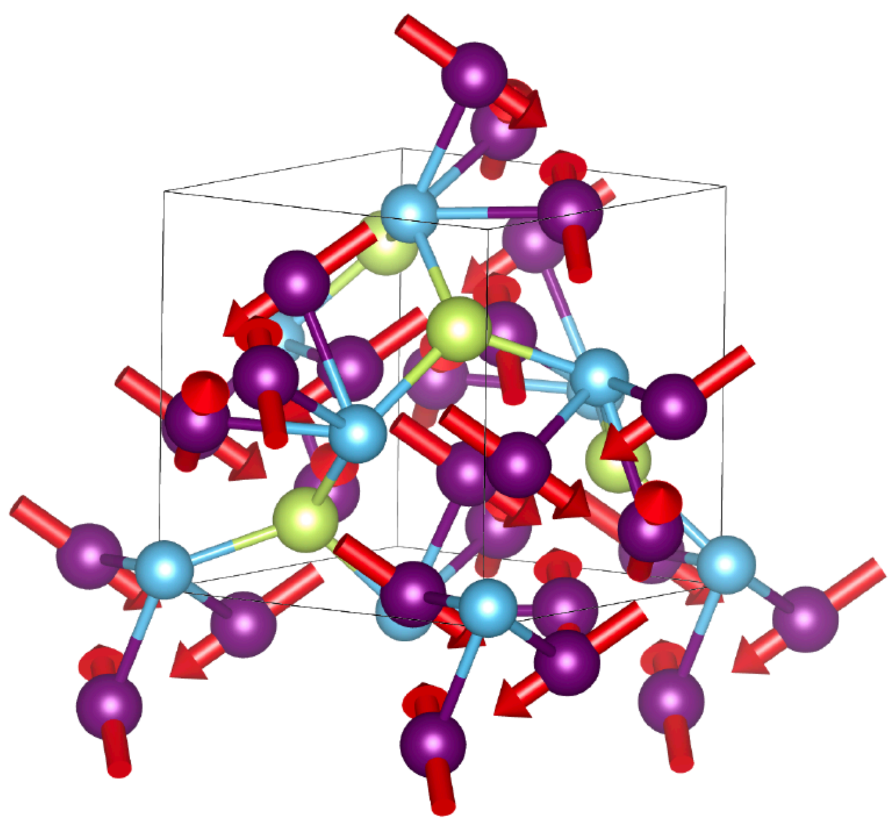
What’s new for magnetic semimetals?

JC, Bradlyn, Vergniory: ArXiv: 1904.12867

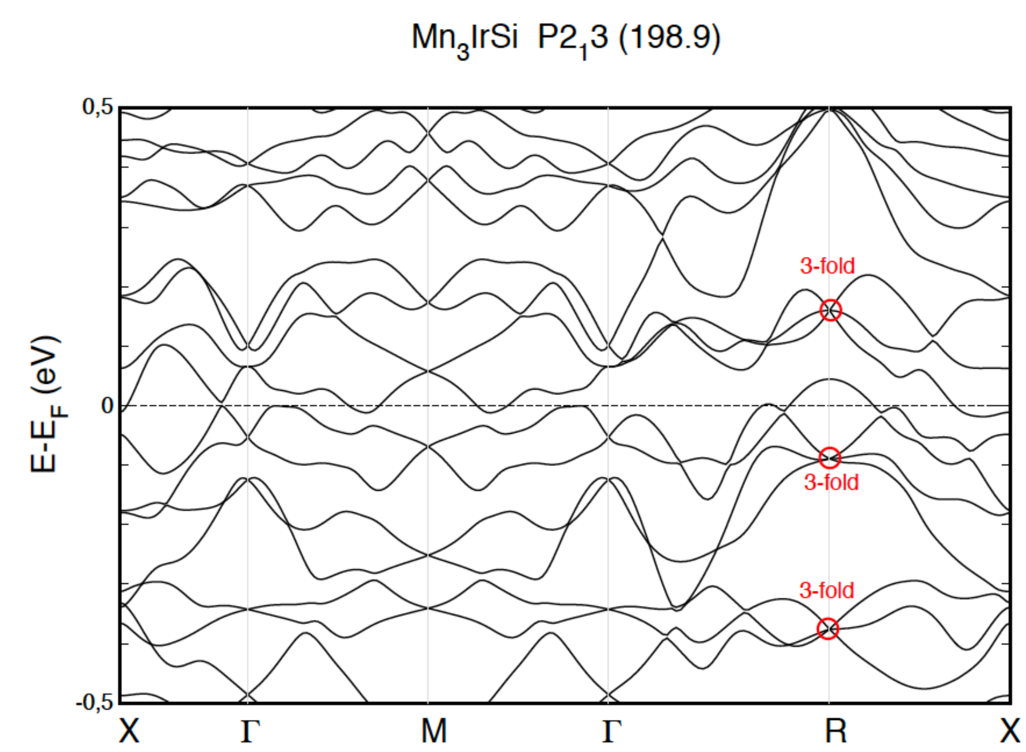
Making tables is a lot harder (recall: 1191 SGs)

Ab initio calculations are a lot harder

(a)



(b)



No new species of fermions appear,
but some are pinned to special exactly solvable points:
May be easier to observe and calculate properties

Collaborators

Theory

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(Princeton)

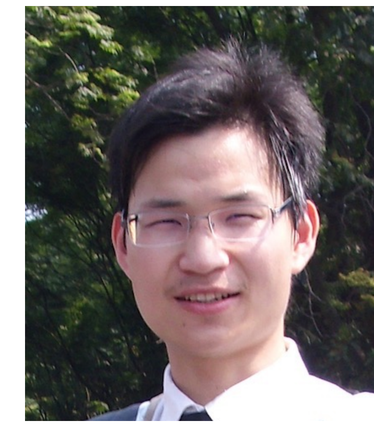
Barry Bradlyn
(UIUC)

Xi Dai
(Hong Kong)

Ben Wieder
(Princeton)

Ab initio

Maia Garcia
Vergniory
(DIPC, EHU)



Zhijun Wang
(Beijing National Lab, U.
Chinese Acad. of Sci.)

Experiment

Bob Cava
(Princeton)

Claudia Felser
(Max Planck)

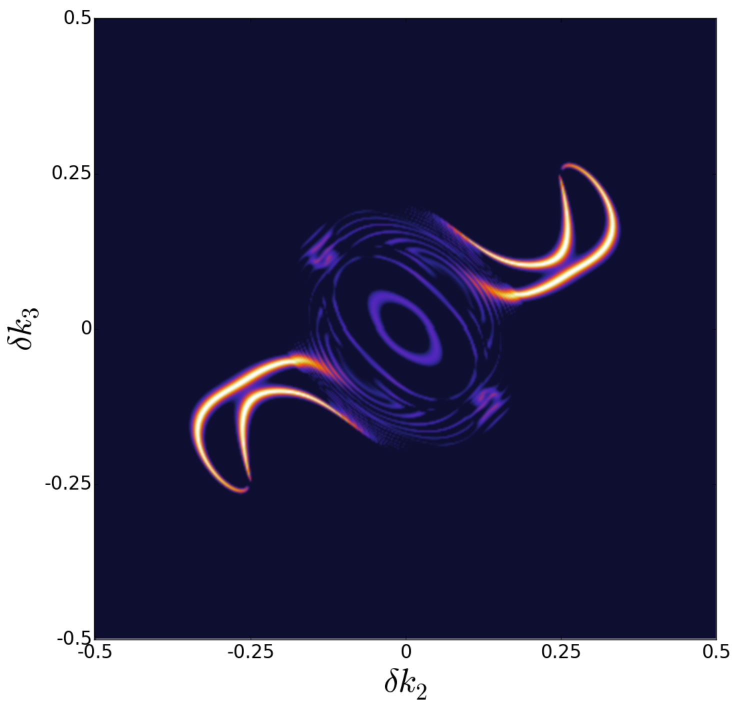
Leslie Schoop
(Princeton)

Crystallographic group theory

Mois Aroyo (EHU)

Luis Elcoro (EHU)

Conclusions



Topological semimetals exist beyond Dirac and Weyl fermions: 3-, 6-, 8-fold

Fermi arcs characterize *chiral* fermions

Non-chiral fermions: “parent phases”
Can display higher order Fermi arcs

Topological quantum chemistry: predict & classify topological materials

Effects of interactions largely unanswered:

1. When do interactions open gap?
2. When is resulting phase topological?