Symmetry Protected Topological Insulators and Semimetals

I. Introduction : Many examples of topological band phenomena

II. Recent developments :

- Line node semimetal

  Kim, Wieder, Kane, Rappe, PRL **115**, 036806 (2015).

- 2D Dirac semimetal

  Young, Kane PRL **115**, 126803 (2015).

- Double Dirac semimetal

  Wieder, Kim, Rappe, Kane, PRL **116**, 186402 (2016).

} Role of non-symmorphic space group symmetries

Thanks to:

Gene Mele, Ben Wieder — U. Penn. Physics Dept

Andrew Rappe, Youngkuk Kim — U. Penn. Chemistry Dept.

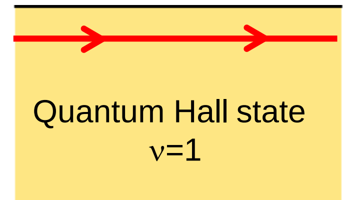
Steve Young — Naval Research Lab

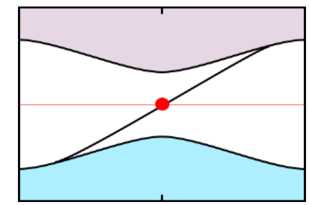
"Single Particle" Topological Phases

Bulk Topological Invariant ⟺ Boundary Topological Modes

2D Integer quantum Hall effect

Bulk: Integer Chern invariant
Boundary: Chiral edge states

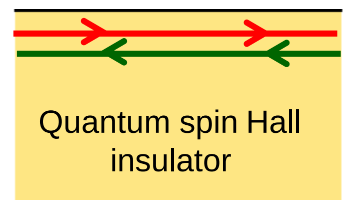


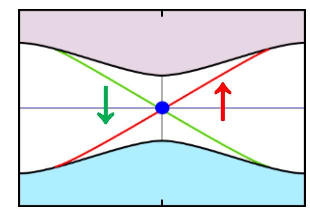


Topology + Time reversal symmetry

2D topological insulator

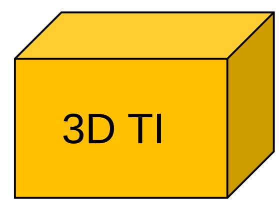
Bulk: Z_2 invariant
Boundary: Helical edge states

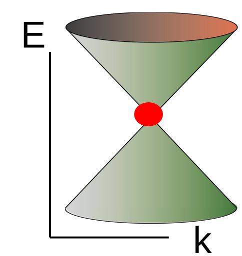




3D topological insulator

Bulk: Z_2 invariant
Boundary: Helical surface state

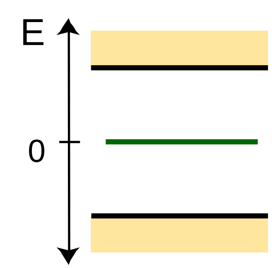




Topology + Particle-Hole symmetry

1D Topological Superconductor

Bulk: Z_2 invariant
Boundary: Majorana zero mode



Periodic Table of Topological Insulators and Superconductors

Kitaev, 2008
Schnyder, Ryu, Furusaki, Ludwig 2008

Anti-Unitary Symmetries :

- Time Reversal : $\Theta H(\mathbf{k})\Theta^{-1} = +H(-\mathbf{k})$; $\Theta^2 = \pm 1$
- Particle - Hole : $\Xi H(\mathbf{k})\Xi^{-1} = -H(-\mathbf{k})$; $\Xi^2 = \pm 1$

Unitary (chiral) symmetry : $\Pi H(\mathbf{k})\Pi^{-1} = -H(\mathbf{k})$; $\Pi = \Theta\Xi$

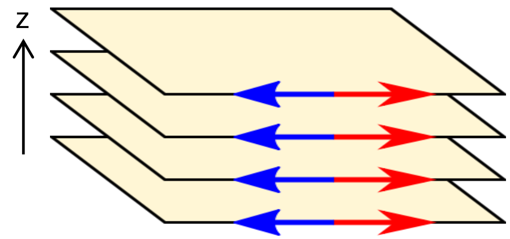
	Symmetry				d							
	AZ	Θ	Ξ	Π	1	2	3	4	5	6	7	8
T broken insulator →	A	0	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$
	AIII	0	0	1	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
	AI	1	0	0	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
	BDI	1	1	1	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
T broken superconductor →	D	0	1	0	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$
T invariant superconductor →	DIII	−1	1	1	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0
T invariant insulator →	AII	−1	0	0	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$
	CII	−1	−1	1	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0
	C	0	−1	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
	CI	1	−1	1	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0

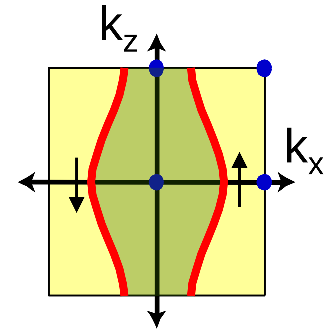
Topological Crystalline Phases

Crystal symmetry introduces new topological states

Weak Topological Insulator

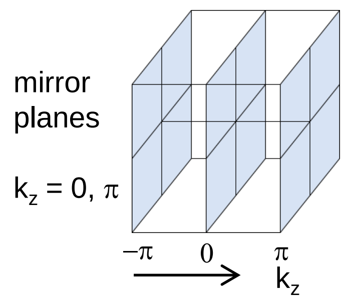
- Layered 2D topo. insulator
- Protected by translation symmetry T_z
- 3 Z_2 “Miller Indices”

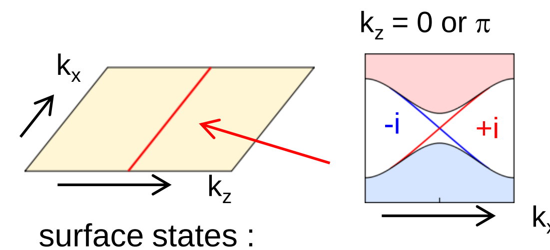




Topological Crystalline Insulator

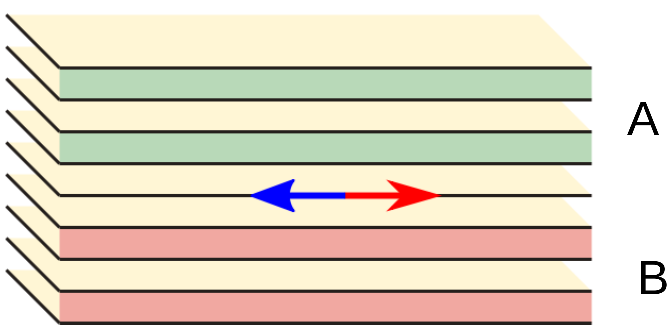
- Protected by Mirror symmetry M_z
- Mirror Chern Number defined in mirror invariant plane:
  $M_z = \pm i$: $n = n_{+i} - n_{-i}$



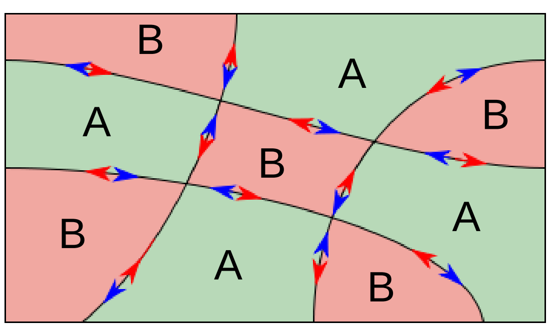


Surface states protected by crystal symmetry can remain even when symmetry is violated.

eg weak TI :



helical mode on domain wall



Average symmetry: absence of localization

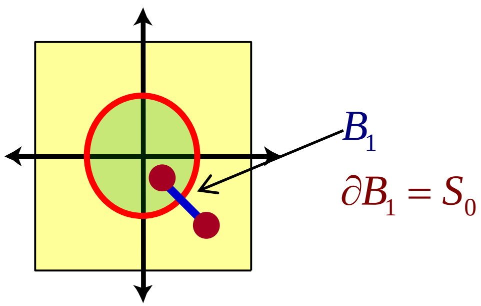
Topological (semi) metals

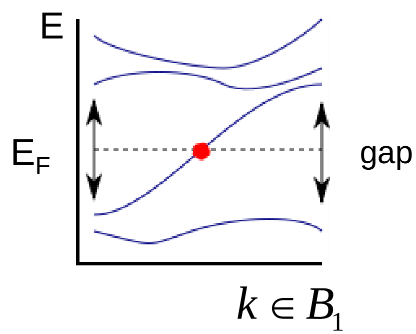
Topological band classification
without symmetries, for $k \in S_d = \partial B_{d+1}$

d	0	1	2	3	4
class A $n_d \in$	Z	0	Z	0	Z

Fermi Liquid :

The Fermi surface of a metal is “topological”



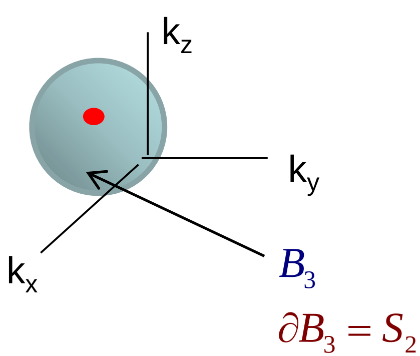


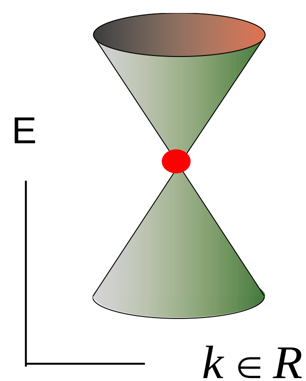
n_0 characterizes $k \in \partial B_1 = S_0$

= # Fermi crossings in B_1

$$H \sim \mathrm{v}\, k$$

Weyl semimetal :





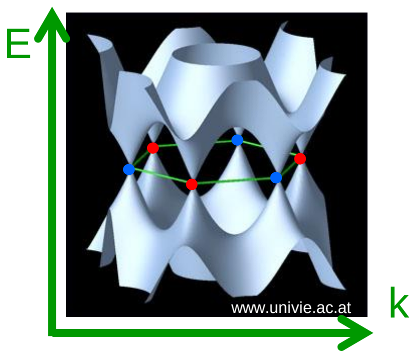
n_2 (Chern no.) characterizes $k \in \partial B_3 = S_2$

= # Weyl points in B_3

$$H \sim \mathrm{v}\,\vec{\sigma} \cdot \vec{k}$$

Symmetry Protected Topological Semimetal

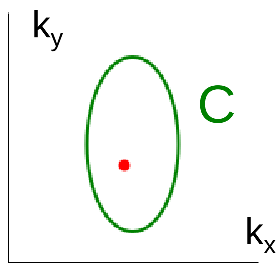
Prototype example: Graphene



Dirac points protected by

- Inversion symmetry (P)
- Time reversal symmetry (T)
- Absence of spin-orbit ($T^2 = +1$)

Z_2 topological invariant



Berry Phase : $\gamma_C = 0 \text{ or } \pi$

Loop C: 1 parameter family H(**k**) in class AI :

$$[H(\mathbf{k}), PT] = 0$$

d= 0 - 1 mod 8

d	-2	-1	0	1	2
Class AI	Z_2	Z_2	Z	0	0

3D Generalizations :

Weyl semimetal : topologically protected but “symmetry prevented”. Must break T or P.

3D Dirac line node semimetal

3D Dirac semimetal: 4 fold degnerate Dirac point protected by crystal symmetry

- “topological” Dirac semimetal
- “non – symmorphic Dirac semimetal”

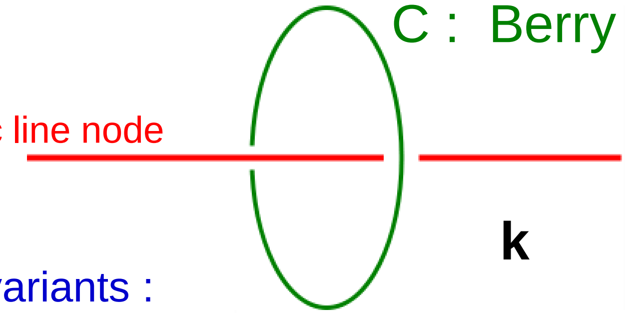
3D Dirac Line Node Semimetal

Kim, Wieder, Kane, Rappe, PRL 115, 036806 (2015)

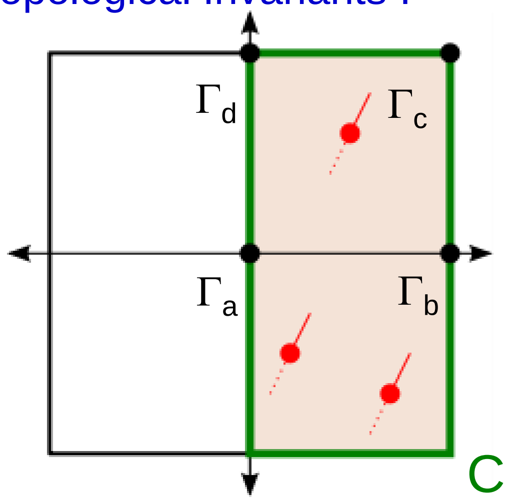
In absence of spin-orbit, P and T ($T^2 = +1$) allows symmetry protected line nodes.

C : Berry phase 0, π

dirac line node



Z_2 Topological Invariants :



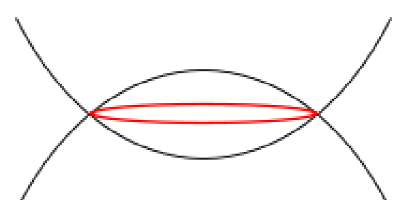
N_{abcd} = # DLN passing through P,T invariant plane spanned by $\Gamma_{a,b,c,d}$

$$(-1)^{N_{abcd}} = \xi_a \xi_b \xi_c \xi_d \qquad \xi_a = \prod_n \xi_n(\Gamma_a)$$ parity eigenvalues

Similar to invariants for TI and WTI with spin orbit

Band Inversion:

Inversion of opposite parity bands leads to a Dirac Circle



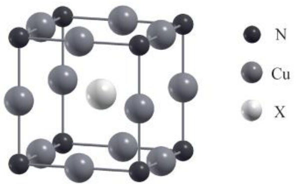
Realizations

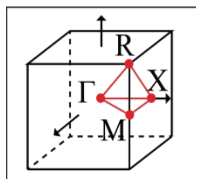
3D graphene networks Weng, Liang, Xu,Yu, Fang, Dai, Kawazoe, PRB 92, 045108 (2015).

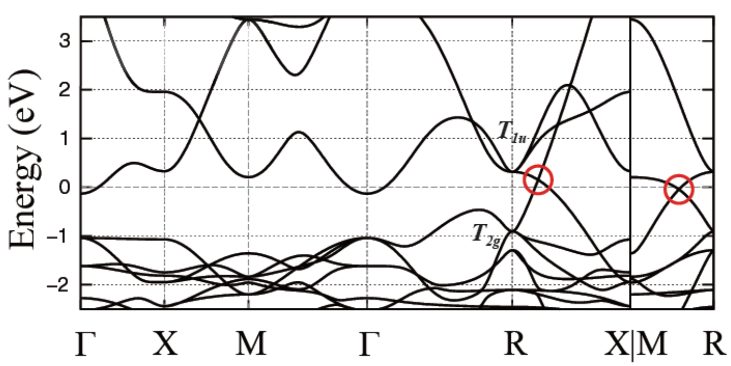
Ca_3P_2 Xie, Schoop, Seibel, Gibson, Xi, Cava, APL Mat. 3, 083602 (2015).

Cu_3N Kim, Wieder, Kane, Rappe, PRL 115, 036806 (2015).
Yu, Weng, Fang, Dai, Hu, PRL 115, 036807 (2015).

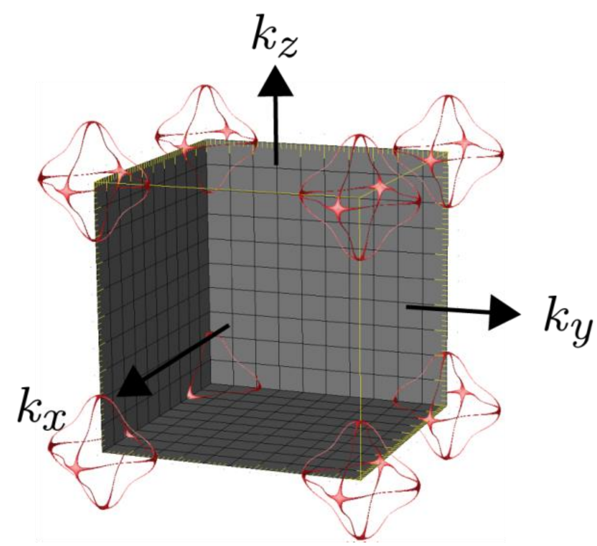
Cu_3N : Uninverted insulator
Band inversion can be controlled by doping with transition metal atoms X



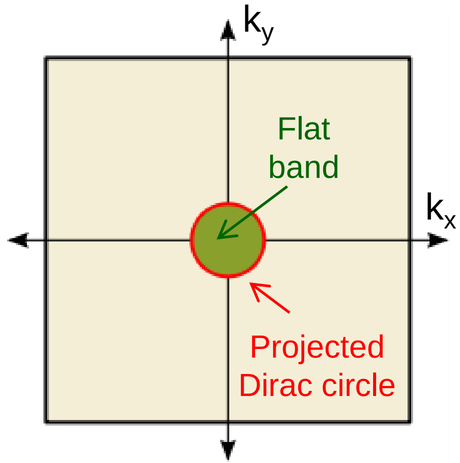




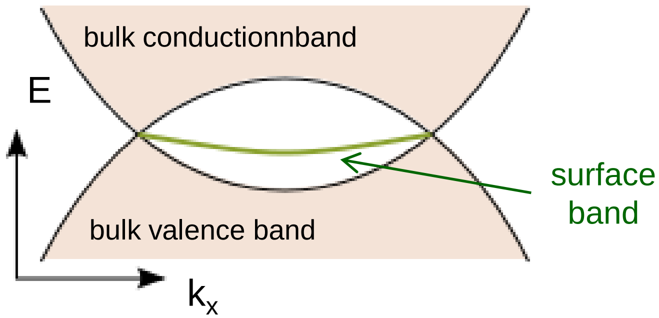
Cu_3N Pd



Nearly Flat Surface Bands



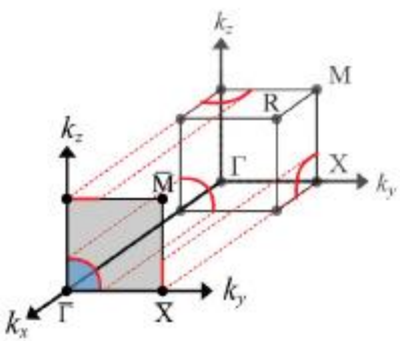
Surface Brillouin Zone

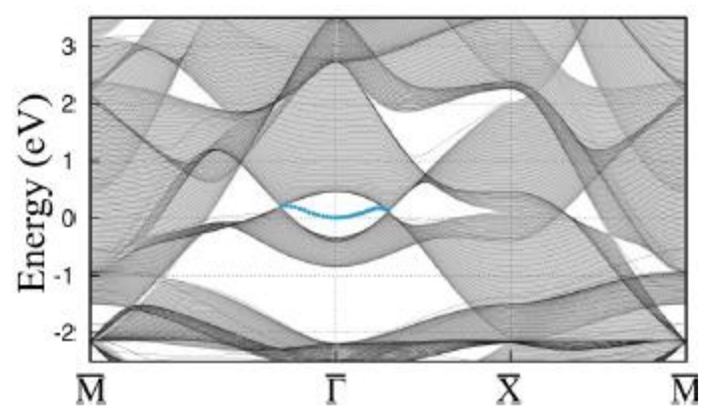


- Curvature of surface band depends on effective masses: $\frac{1}{m_{surf.}} = \frac{1}{m_c} - \frac{1}{m_v}$
- Surface is electrically neutral when surface band is half filled.
- Interesting platform for strong correlation physics.

Cu_3N Zn

slab calculation :





More classes of Line Node semimetals :

Nodal rings protected by P,T that can not be shrunk to zero
(weak spin orbit)

Fang, Chen, Kee and Fu, PRB 92, 081201 (2015).

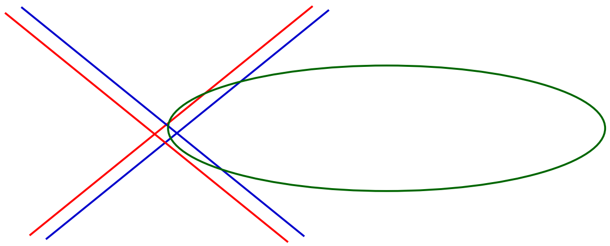
d	-2	-1	0	1	2
Class AI	Z_2	Z_2	Z	0	0

Line degeneracies connecting multiple bands are linked

Nodal rings protected by mirror symmetries
(weak spin orbit)

Weng, Fang, Fang, Bernevig, Dai, PRX 5, 011029 (2015)

Doubly degenerate line nodes
(strong spin orbit) Impossible to 'uninvert' : non-symmorphic symmetry

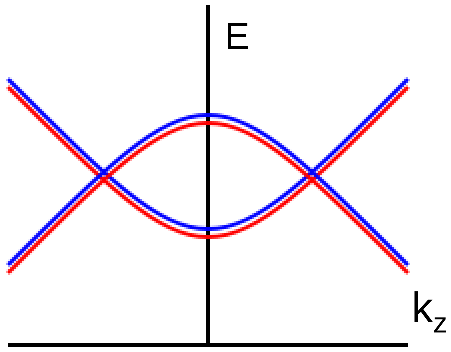


Kim, Chen, Kee, PRB 91, 235103 (2015).
Chen, Lu, Kee Nat. Comm. 6, 6593 (2015).
Fang, Chen, Kee and Fu, PRB 92, 081201 (2015).

“Topological” Dirac Semimetal

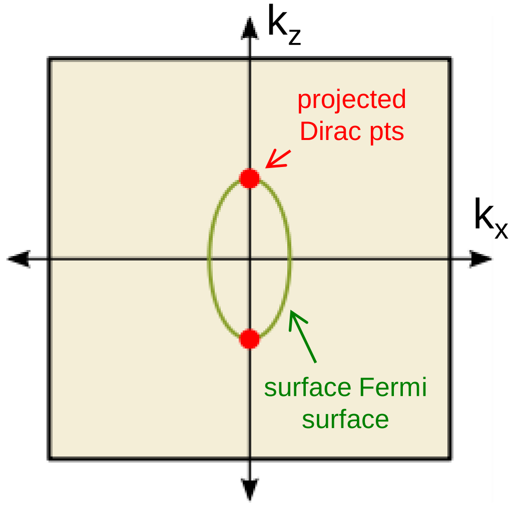
Dirac Points on a line via band inversion

- Consequence of band inversion in presence of spin orbit and C_3 rotational symmetry
- Located on C_3 rotation invariant line in Brillouin zone due to band inversion of opposite parity states in presence of spin orbit and C_3 rotational symmetry



Almost a topological insulator

- Opening a gap by lowering symmetry leads to TI
- Surface states similar to topological insulator



Realizations

- Predicted and observed in Na_3Bi and Cd_2As_3

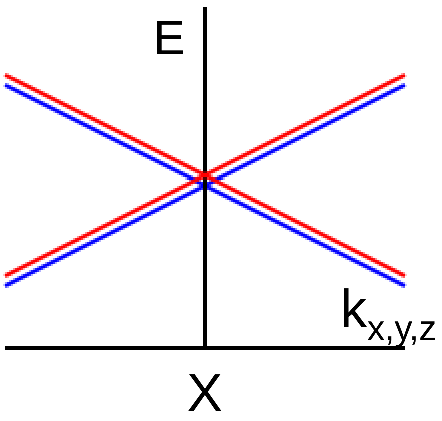
Wang, Sun, Chen, Franchini, Xu, Weng, PRB ‘12
Wang, Weng, Wu, Dai, and Fang, PRB ‘13

Liu, Zhou, Zhang,Wang, Weng, Prabhakaran, Mo, Shen, Fang, Dai, Science ‘14
Liu, Jiang, Zhou, Wang, Zhang, Weng, Prabhakaran, Mo,Peng, Dudin, Nat Mater ’14
Borisenko, Gibson, Evtushinsky, Zabolotnyy, Buchner, Cava, PRL 14

"Non-Symmorphic" Dirac Semimetal

Symmetry Protected Dirac Point

- Located at T invariant point X on Brillouin zone boundary
- Filling enforced semimetal
  - All states at X are fourfold degenerate.
  - Groups of 4 bands "stick together"
- Protected (and guaranteed) by non-symmorphic symmetry
- Symmetry tuned to transition between topological and trivial insulator : Lowering symmetry (e.g. by compressive or tensile strain) can lead to either TI or I



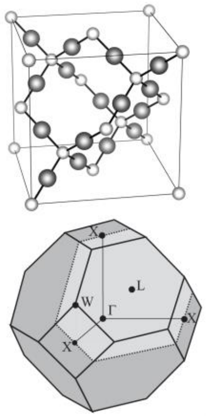
Realizations:

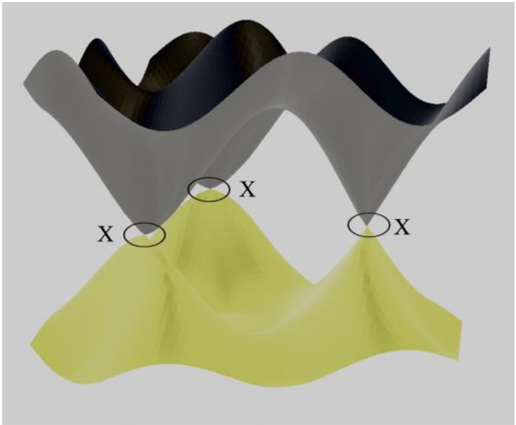
- Toy model: diamond lattice

  Fu, Kane, Mele, PRL '07

- Predicted (not yet observed) in BiO_2, $BiZnSiO_4$

  Young, Zaheer, Teo, Kane, Mele, Rappe PRL '12
  Steinberg, Young, Zaheer, Kane, Mele, Rappe PRL '14



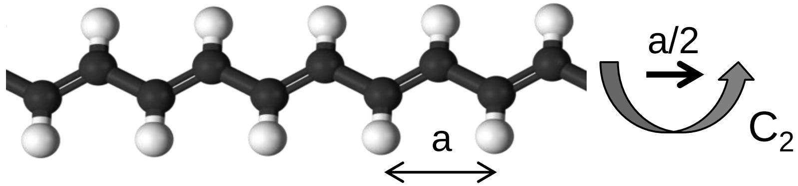


BiO_2

Non-Symmorphic Symmetry

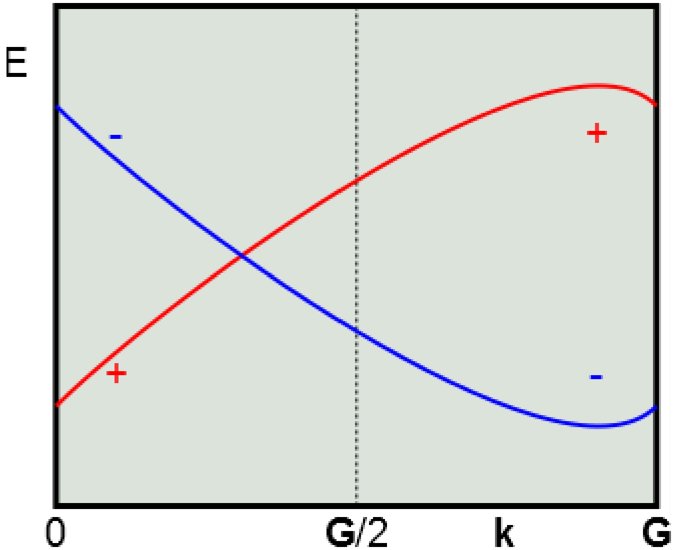
Simplest examples: Glide Plane, Screw Axis

- {g|**t**} : point group operation g + fractional translation **t**
- e.g. d=1 with screw symmetry { C_2 | a/2 }
- Guarantees bands "stick together"
- For k on g invariant line (plane), $\{g\,|\,\mathbf{t}\}\left|u_{\mathbf{k}}^{\pm}\right\rangle = \pm\lambda e^{i\mathbf{k}\cdot\mathbf{t}}$, with $e^{i\mathbf{G}\cdot\mathbf{t}} = -1$



No additional symmetries :

- Two bands cross between **k** and **k**+**G** (G=2π/a)



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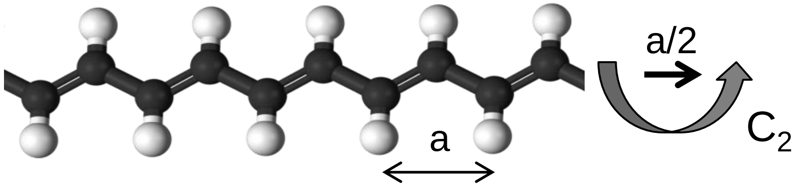

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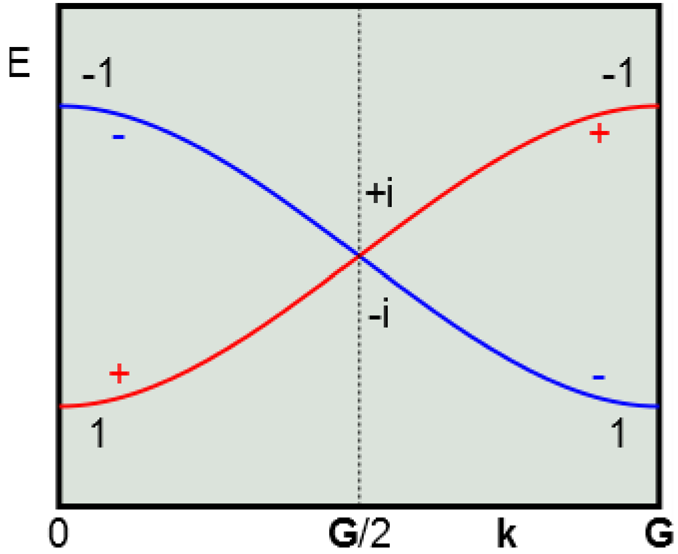
Time reversal (T^2=+1):

- Crossing at zone boundary **G**/2



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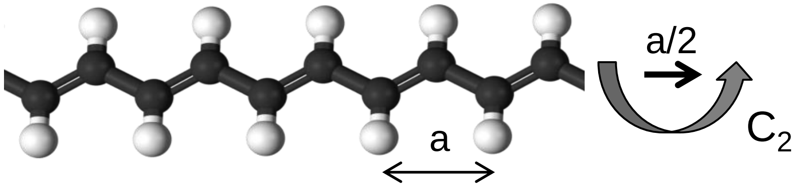

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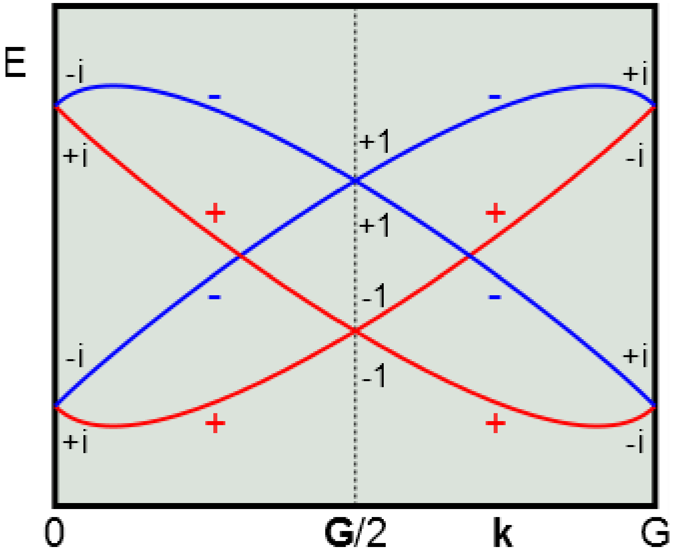
Time reversal (T^2=+1):

- Crossing at zone boundary **G**/2

Time reversal (T^2=-1):

- Kramers degeneracies split by spin-orbit
- Four bands cross between **k** and **k**+**G**



Non-Symmorphic Symmetry

Simplest examples: Glide Plane, Screw Axis

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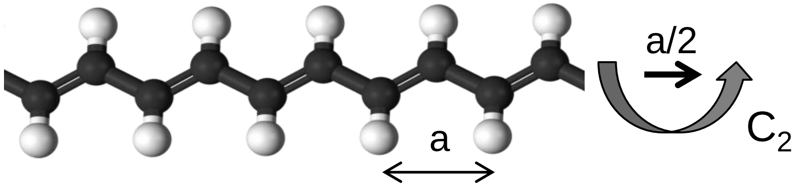

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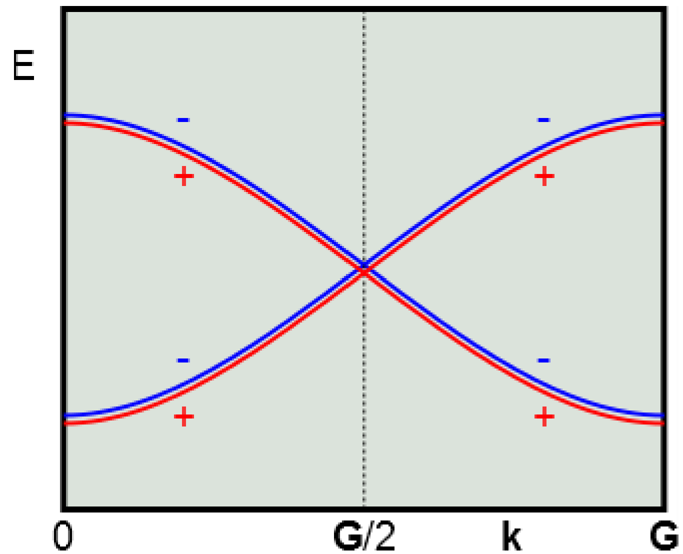
Inversion P and T (T^2=-1):

- Degenerate crossing at zone boundary **G**/2

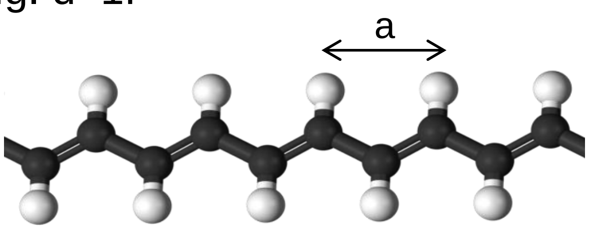


Filling Enforced Semimetals with Strong Interactions

Watanabe, Po, Vishwanath, Zaletel, PNAS '15

Treat crystal with twisted periodic boundary conditions.

e.g. d=1:



- # unit cells = N + ½
- band filling ν = #e/cell
- #e = 2 M   necessary for energy gap (Kramers' thm)
- 2M = ν (N + ½) ⇒ **band filling = multiple of 4 required for insulator**

Generalization to 3D :

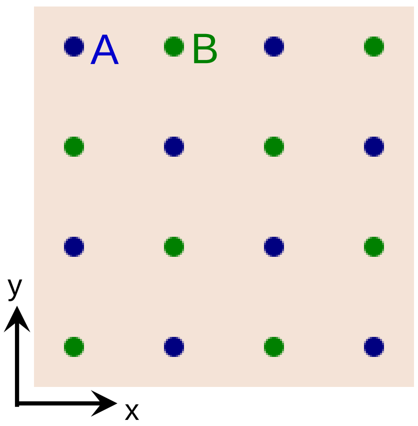
- Put crystal on one of 10 flat 3D "Bieberbach manifolds"
- Determines WPVZ bound on band filling for all 230 space groups

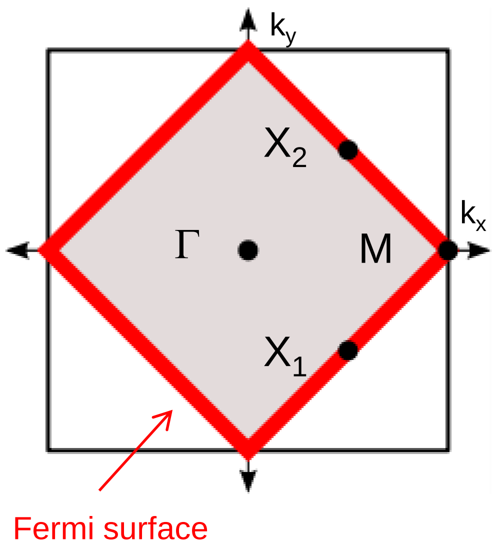
2D Dirac Semimetal

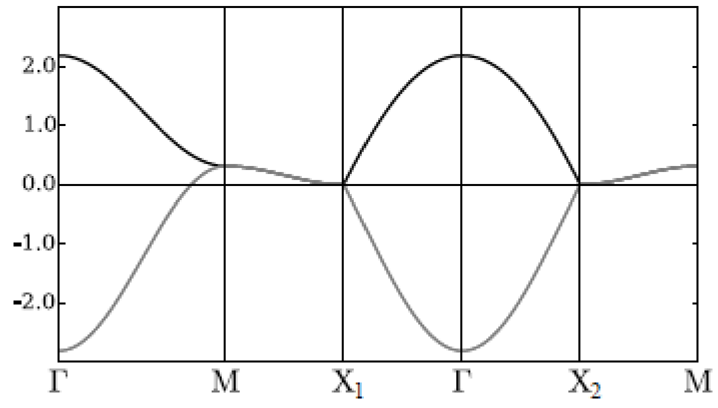
SM Young and CL Kane, Phys. Rev. Lett. **115**, 126803 (2015).

- 2D Dirac points with strong spin orbit interaction
- Symmetry tuned to transition between 2D Topological and Trivial Insulator
- Toy model : Deformed Square lattice

Undeformed square lattice (doubled unit cell)







2D Dirac Semimetal

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- 2D Dirac points with strong spin orbit interaction
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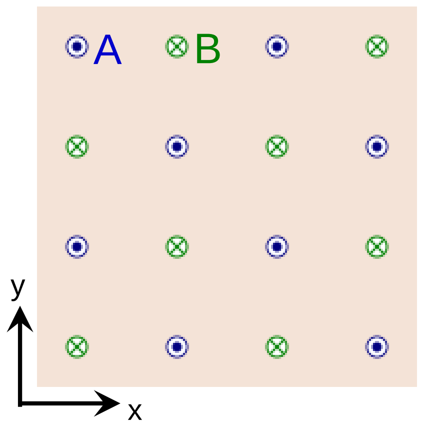
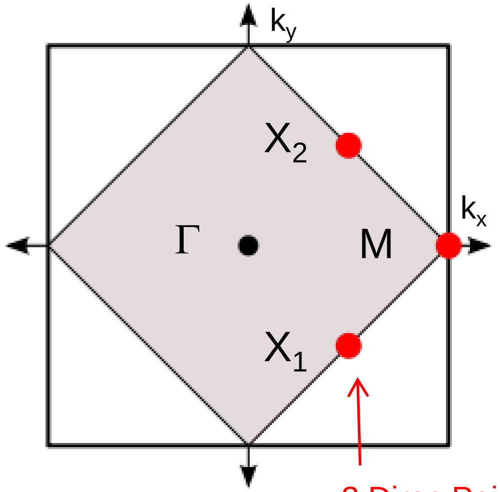
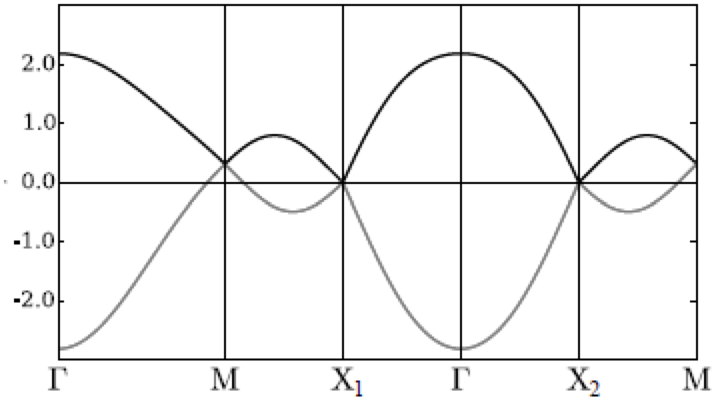
Out of plane deformation: allows 2nd neighbor spin-orbit $i\lambda_{so}\vec{\sigma}\cdot(\mathbf{d}_1\times\mathbf{d}_2)$

Non-symmorphic screw and glide symmetries







3 Dirac Points
Symmetry Inequivalent

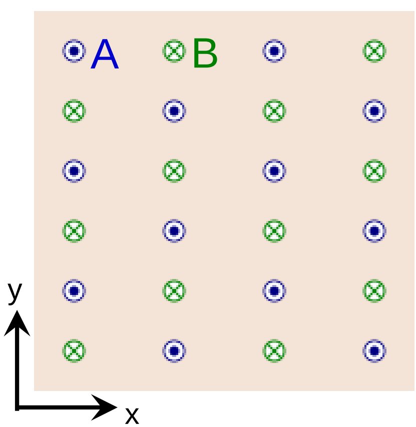
2D Dirac Semimetal

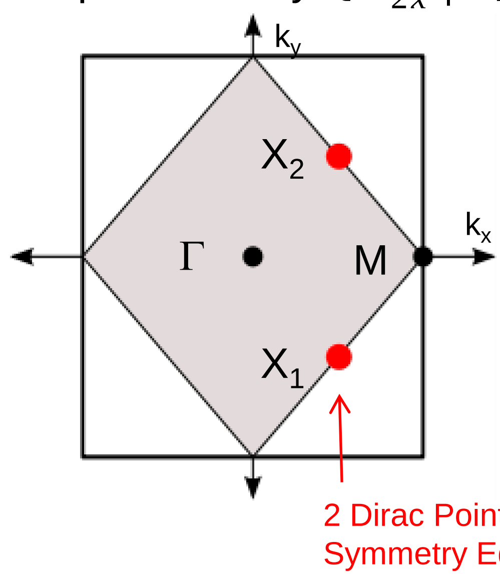
SM Young and CL Kane, Phys. Rev. Lett. **115**, 126803 (2015).

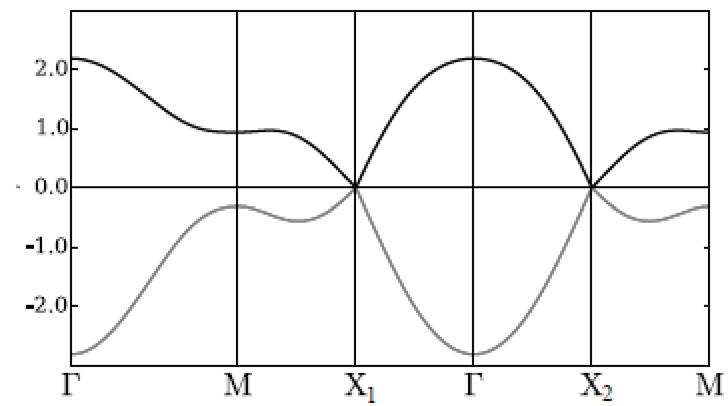
- 2D Dirac points with strong spin orbit interaction
- Symmetry tuned to transition between 2D Topological and Trivial Insulator
- Toy model : Deformed Square lattice

Lower symmetry further:

Two equivalent Dirac points protected by $\{C_{2x} \mid \hat{x}\}$







Possible Realization

PHYSICAL REVIEW B **90**, 195145 (2014)

Topological phases in iridium oxide superlattices: Quantized anomalous charge or valley Hall insulators

Yige Chen[1] and Hae-Young Kee[1,2,*]
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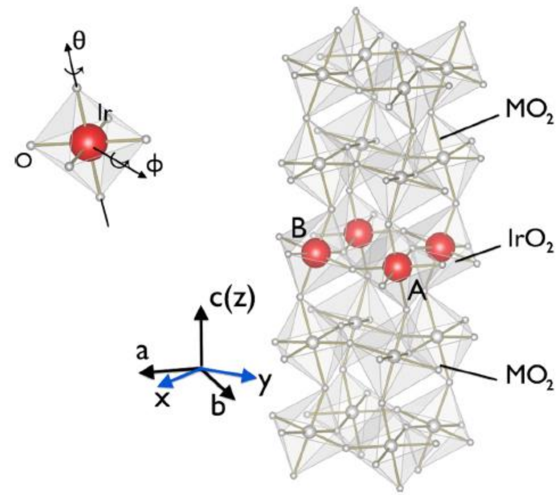
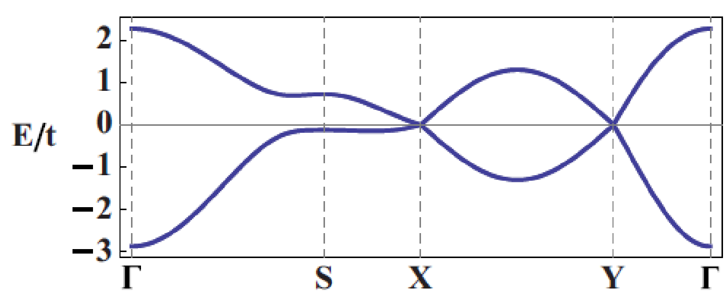
(Received 23 June 2014; revised manuscript received 4 October 2014; published 24 November 2014)

Iridium oxide superlattice grown along [001] with certain rotations of IrO_6 octahedra.





(b) Finite ϕ with b-glide symmetry

Double Dirac Semimetal

3D Semimetal with 8-fold degenerate double Dirac point

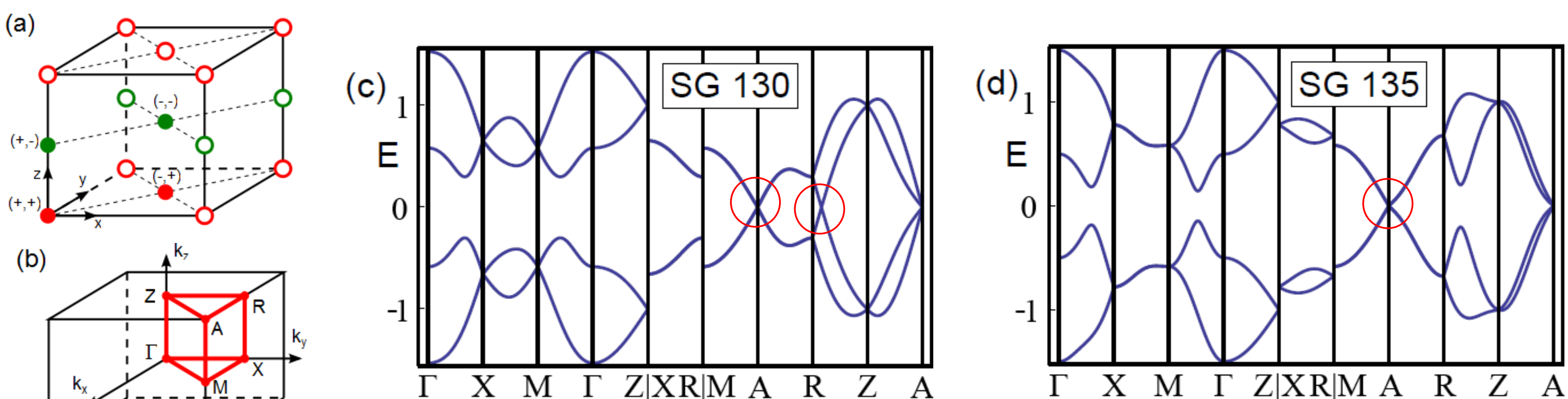
Wieder, Kim, Rappe, Kane, PRL **116**, 186402 (2016).

7 of the 230 space groups host double Dirac points

Space groups 130, 135* :
filling enforced semimetal.

Tight binding models :

Space Group			K	Reps at K
130	$P4/ncc$	$\Gamma_q D_{4h}^8$	A	$\Gamma_5^{\oplus 2}(8)$
135	$P4_2/mbc$	$\Gamma_q D_{4h}^{13}$	A	$\Gamma_5^{\oplus 2}(8)$
218	$P\bar{4}3m$	$\Gamma_c T_d^4$	R	$\Gamma_6 \oplus \Gamma_7(4)$, $\Gamma_8^{\oplus 2}(8)$
220	$P\bar{4}3d$	$\Gamma_c^v T_d^6$	H	$\Gamma_6 \oplus \Gamma_7(4)$, $\Gamma_8^{\oplus 2}(8)$
222	$Pn3n$	$\Gamma_c O_h^2$	R	$\Gamma_5(4)$, $\Gamma_6 \oplus \Gamma_7(8)$
223	$Pm3n$	$\Gamma_c O_h^3$	R	$\Gamma_5(4)$, $\Gamma_6 \oplus \Gamma_7(8)$
230	$Ia3d$	$\Gamma_c^v O_h^{10}$	H	$\Gamma_5(4)$, $\Gamma_6 \oplus \Gamma_7(8)$

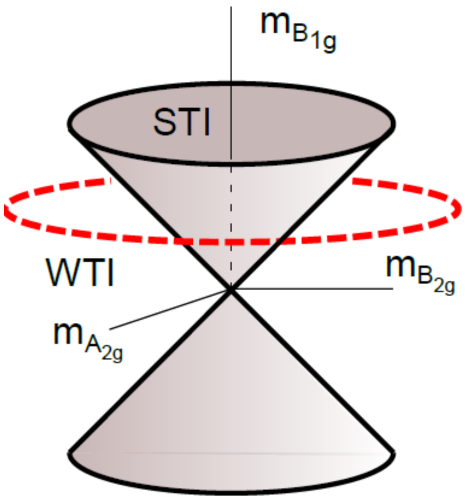


Intrinsic double Dirac semimetal

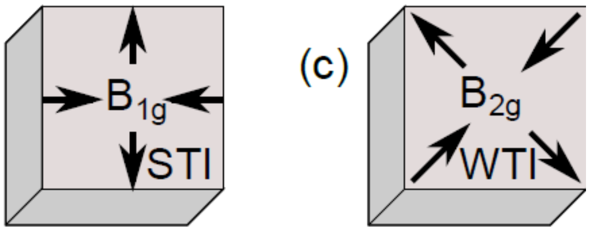
Features of the Double Dirac Point

Multiple T – invariant mass terms
introduced by lowering symmetry

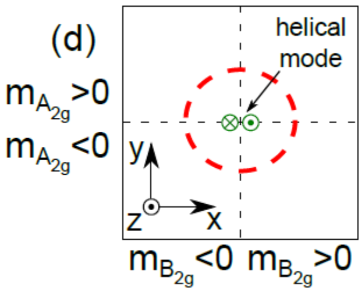
$$H = \gamma_x k_x + \gamma_y k_y + \gamma_z k_z + m_{B_{1g}} \Gamma_1 + m_{B_{2g}} \Gamma_2 + m_{A_{2g}} \Gamma_3$$



Both topological and trivial Insulators can be
created with uniaxial compression



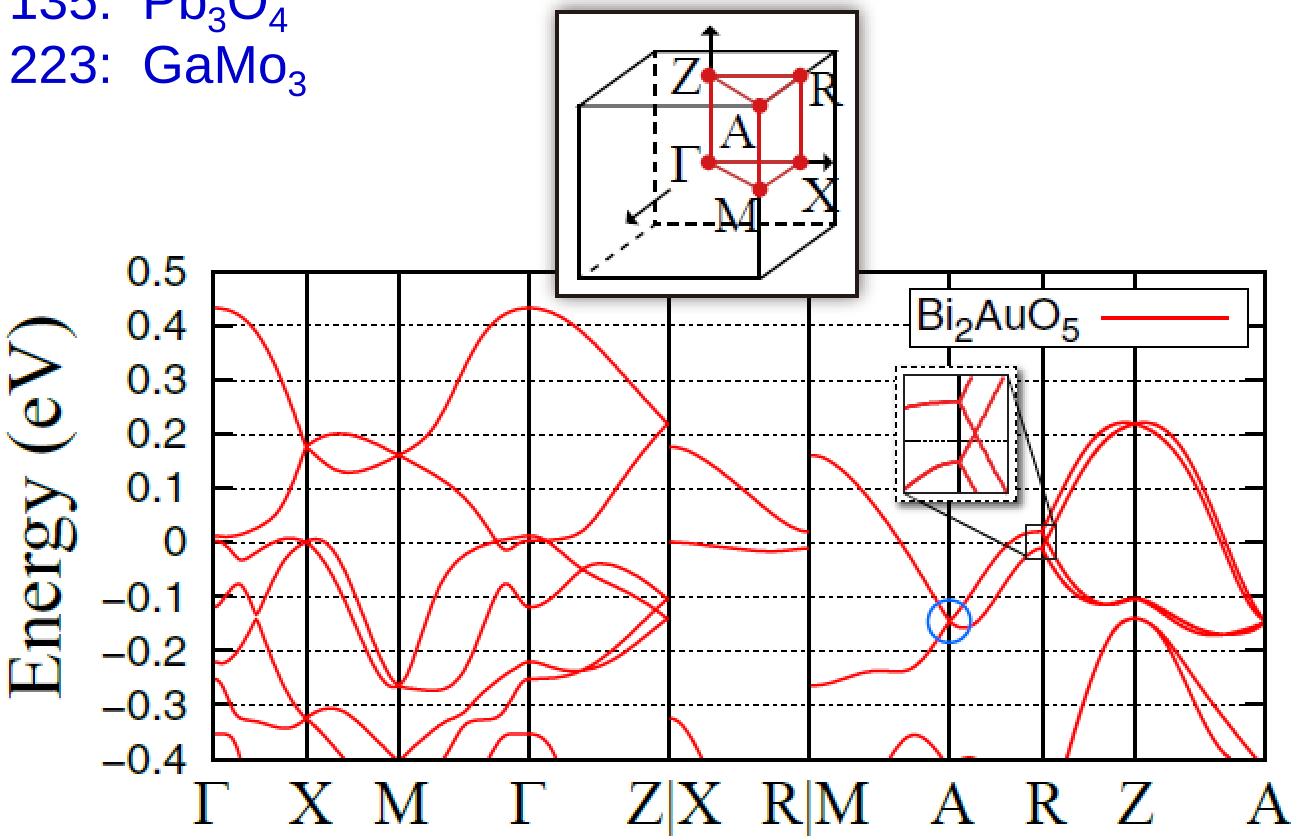
Topological line defects host 1D helical modes



Towards Materials Realization:

Known materials hosting double Dirac points:

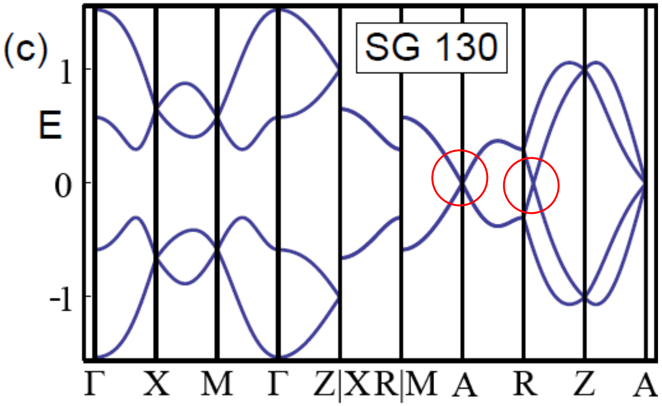
130: Bi_2AuO_5
135: Pb_3O_4
223: $GaMo_3$



Strong Interactions

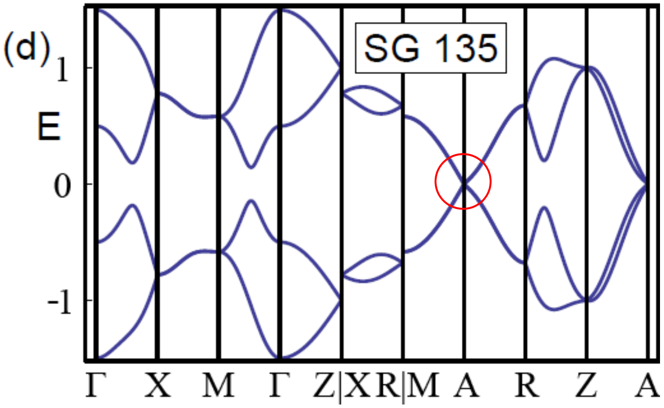
Space group 130:

- WPVZ bound = 8
- Filling enforced semimetal even for strong interactions
- Single DPs along RZ in addition to double DP at A.



Space group 135:

- WPVZ bound = 4
- Band Theory and WPVZ bound disagree
- Could there be an insulator for strong interactions?



Conclusion

Topological Band Phenomana are both Rich and Feasible

Dirac Semimetals come in two varieties

- “topological” vs non-symmorphic Dirac semimetals

2D Dirac Semimetal

- Protected by non-symmorphic symmetry
- At intersection between topological and trivial insulator

3D Dirac line node semimetal

- Driven by band inversion in absence of spin-orbit
- Dirac Circle
- Many variants

Double Dirac semimetal

- Hosted by certain space groups
- Multiple mass terms give new handle for topological states
- Target for band structure engineering
- Interesting question for strong interactions