

Topological crystalline insulator: from symmetry indicators to material discovery



Department of physics, National Cheng Kung University, Taiwan

(國立成功大學 物理系)

Tay-Rong Chang (張泰榕)

2018/Dec./6

Outline

2

↑
slides
number

1. Topology in condensed matter physics

Basic concepts and properties of topological band structure

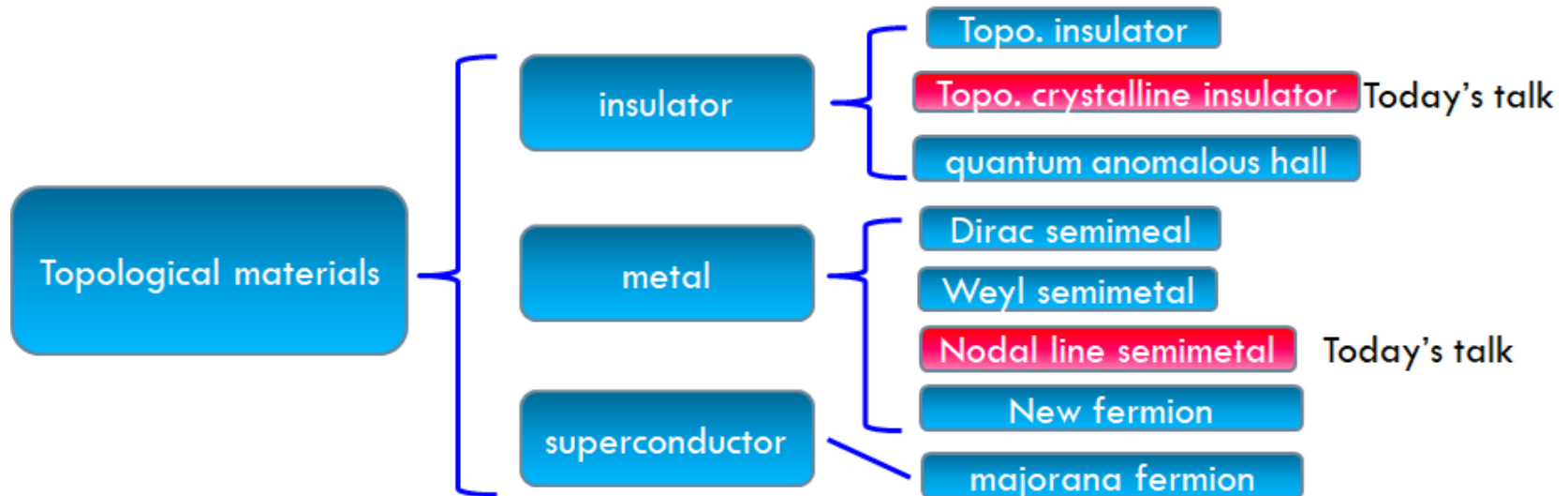
Example: Bi_2Se_3

2. Topological crystalline insulator

Recent prediction: Ca_2As family

3. Type-II nodal line semimetal

Recent prediction: Mg_3Bi_2



Topology in condensed matter physics

3

Math => real space



genus $g = 0$

$g = 1$

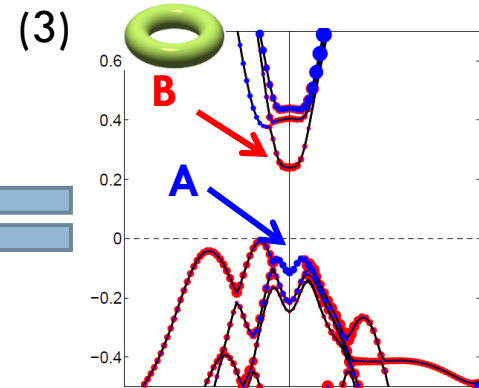
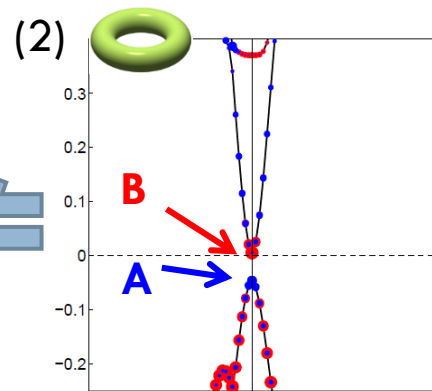
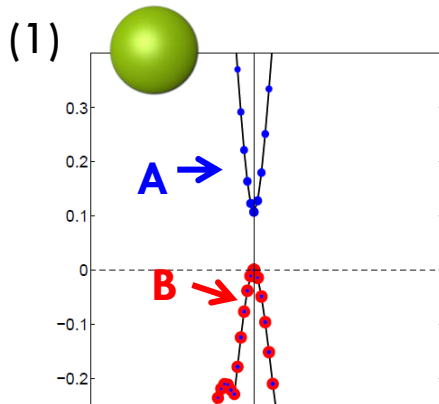
$g = 1$

Gauss-Bonnet Theorem:

$$\int_S K_{Gauss} ds = 2(1 - g)$$

↑ Gauss curvature
 ↑ genus

Phys => momentum space



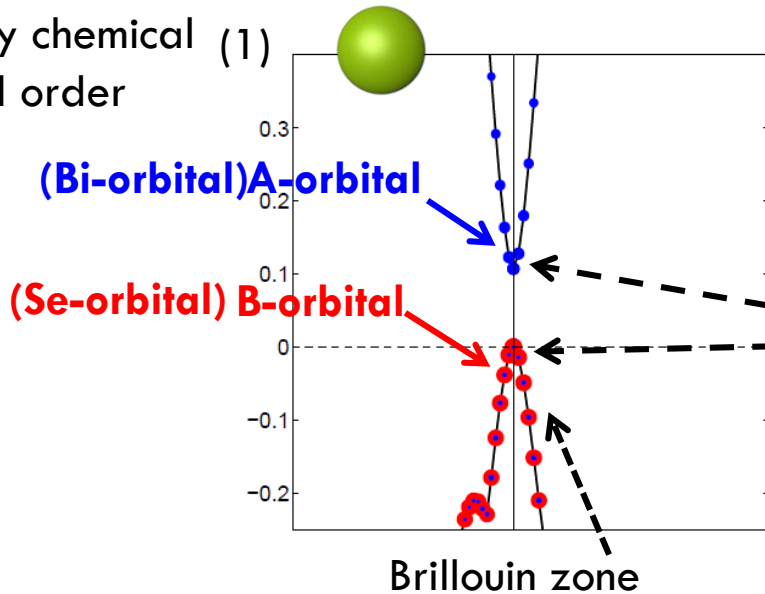
物理雙月刊 藏在邊緣的物理：拓樸材料與拓樸能帶理論

http://pb.ps-taiwan.org/catalog/ins.php?index_ml_id=5&index_id=235

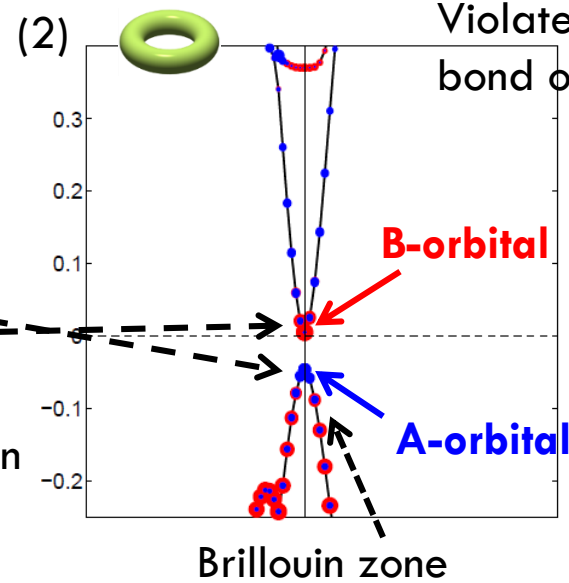
Topology in condensed matter physics

4

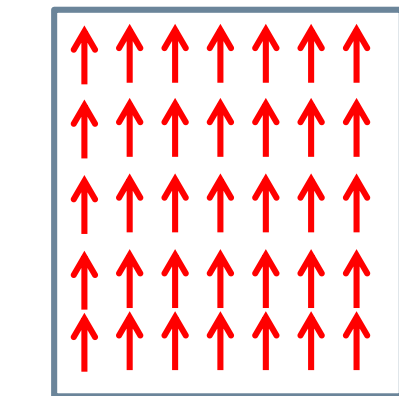
Obey chemical bond order



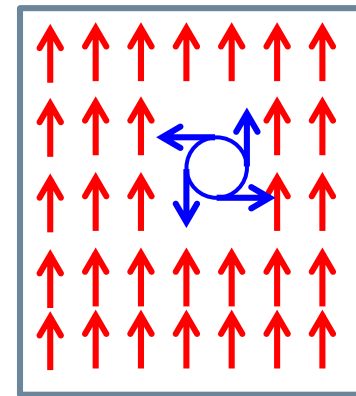
Violate chemical bond order



band inversion



wavefunction is smoothly



wavefunction is NOT smoothly

Topology in condensed matter physics

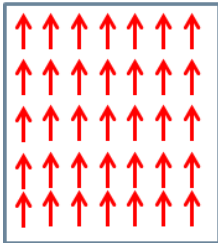
5

Math => real space

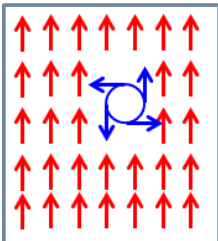
Gauss-Bonnet Theorem:

$$\int_S K_{Gauss} ds = 2(1 - g)$$

↑
↑
 Gauss curvature genus



wavefunction is smoothly : $n = 0 \Rightarrow$ Topological trivial (normal insulator)



wavefunction is NOT smoothly : $n = \text{integer} \Rightarrow$ Topological nontrivial (topological insulator)

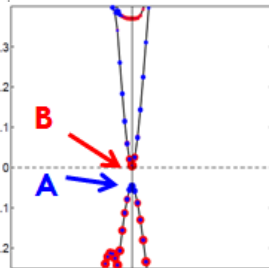
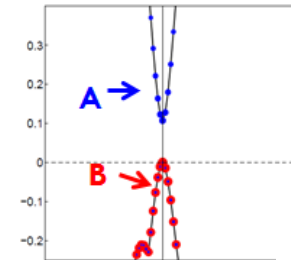
Phys => momentum space

TKNN theory:

$$\sum_m \frac{1}{2\pi} \int_{BZ} d^2k \nabla \times i \langle u_m | \nabla | u_m \rangle = n$$

↑
↑
 Berry curvature Bloch wavefun

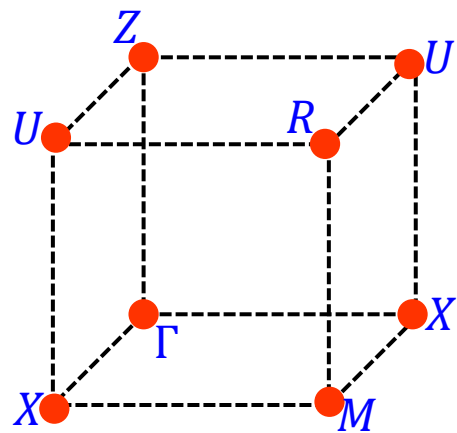
Topological invariant number



Calculating invariant number

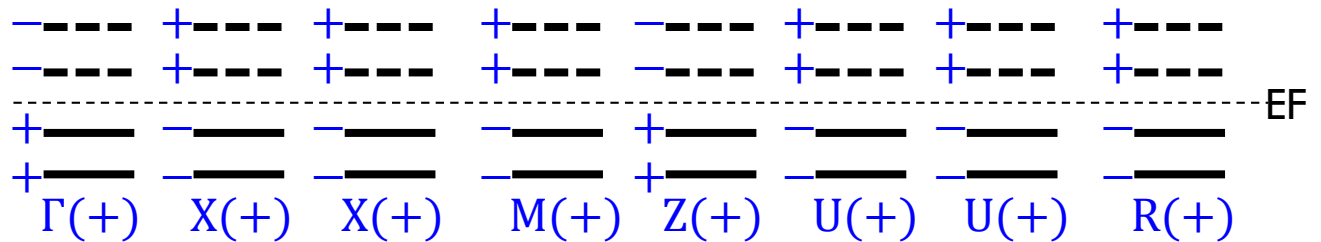
6

L. Fu, PRB **76**, 045302 (2007)

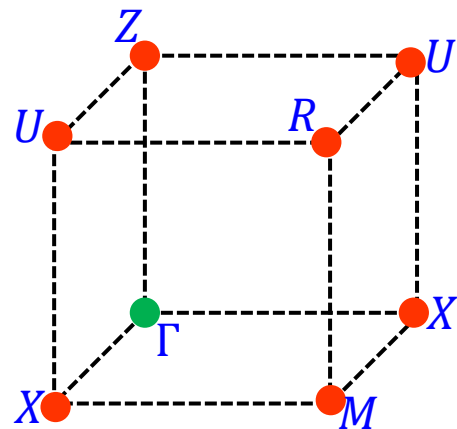


$$\delta_{\Gamma}\delta_X\delta_M\delta_Y\delta_Z\delta_U\delta_T\delta_R = (-1)^{Z_2}$$

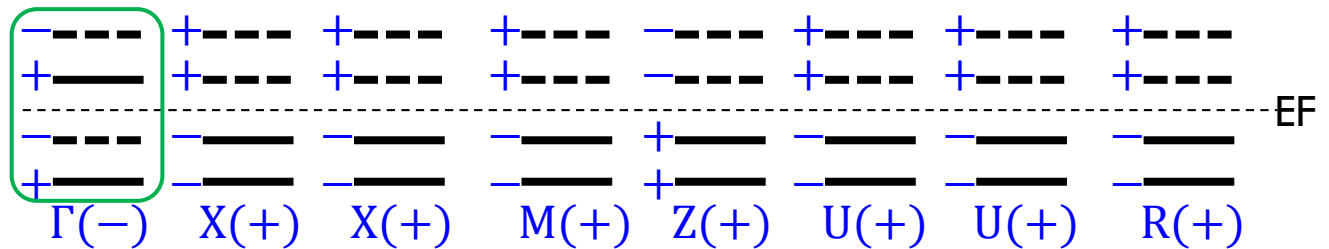
Normal insulator ($Z_2=0$)



Band inversion at Γ

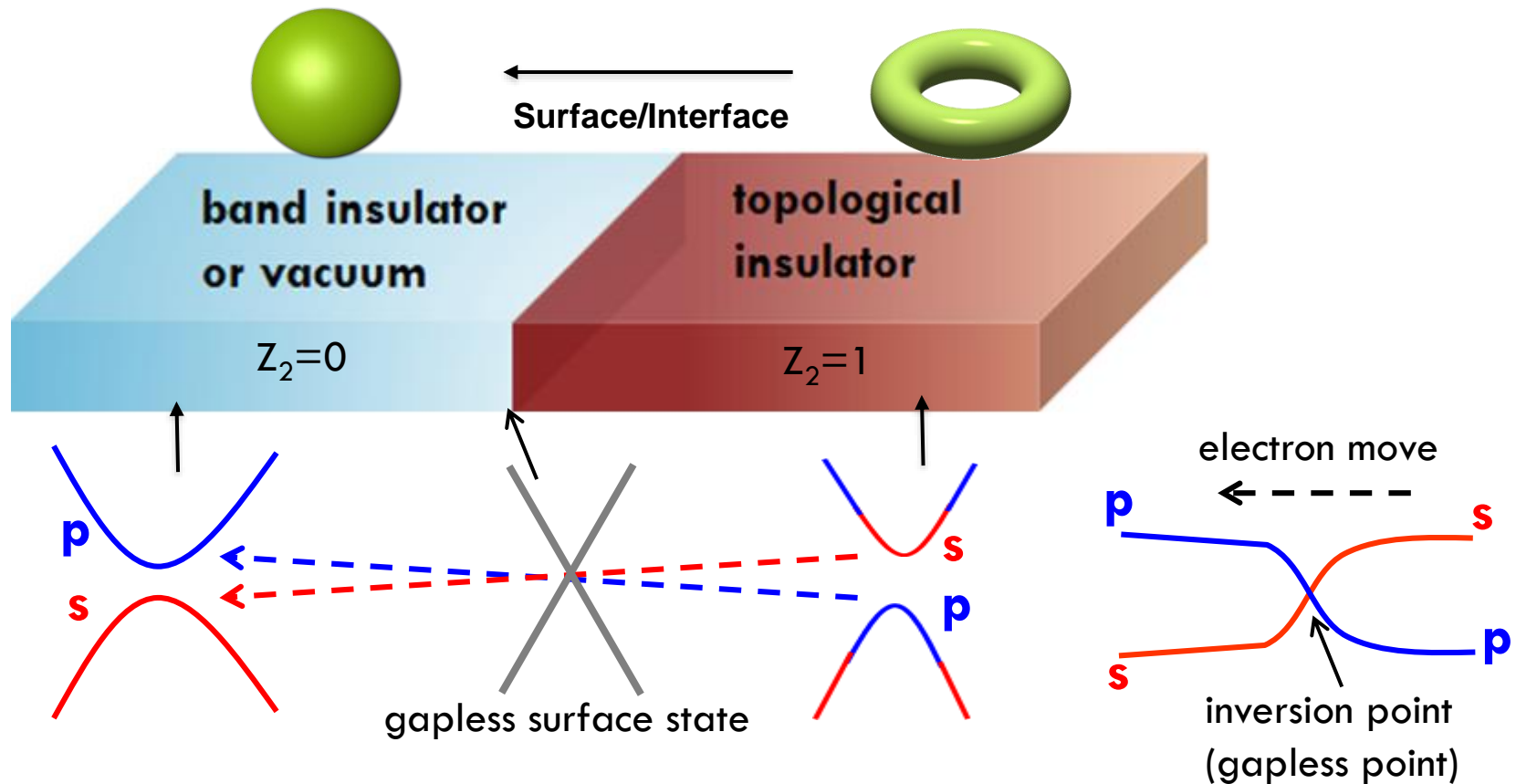


Topological insulator ($Z_2=1$)



Topology in condensed matter physics (bulk-edge correspondence)

7



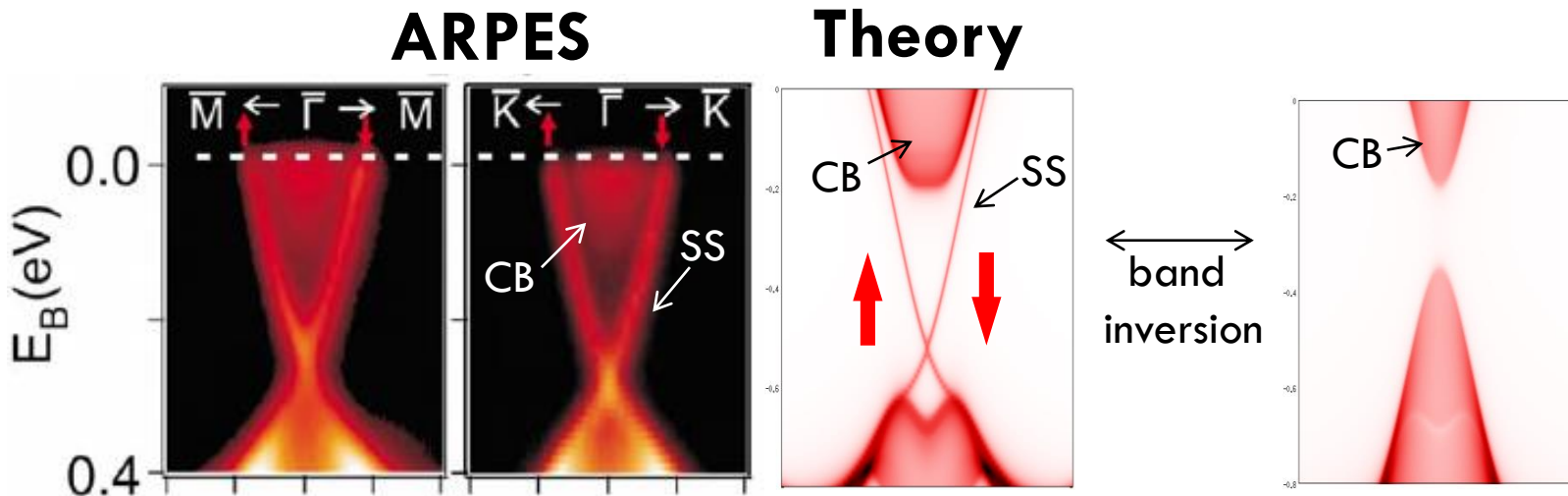
The gapless surface state is the hallmark of topological phase.

M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. **82**, 3045 (2010)

X.-L. Qi and S.-C. Zhang, Rev. Mod. Phys. **83**, 1057 (2011)

Topological insulator: Bi_2Se_3

8



Bulk: insulating gap
topological Z_2 invariant



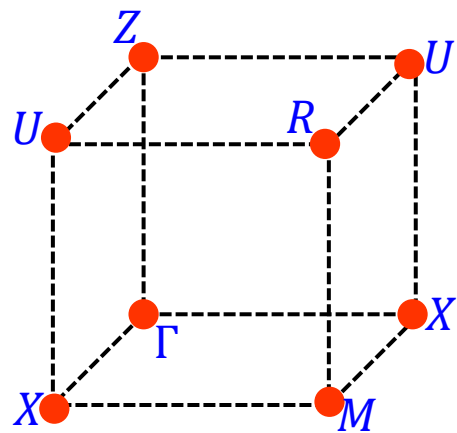
odd/even number
surface states

Surface: gapless surface states
spin-momentum locked

Y. Xia et al. Nature Physics **5**, 398 (2009)
D. Hsieh et al. Nature **460**, 1101 (2009)

Topological crystalline insulator

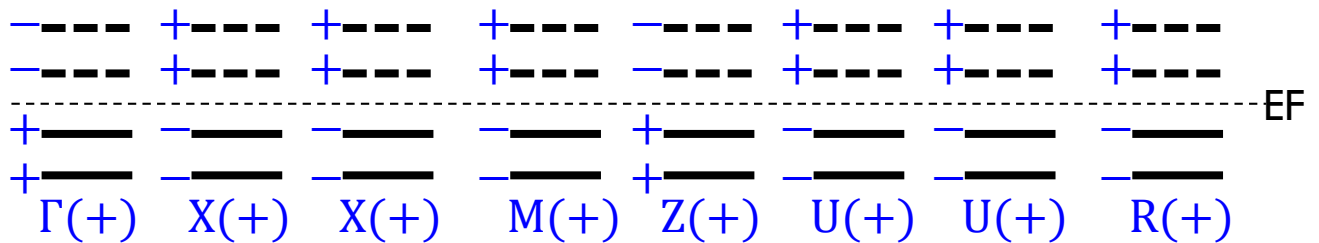
9



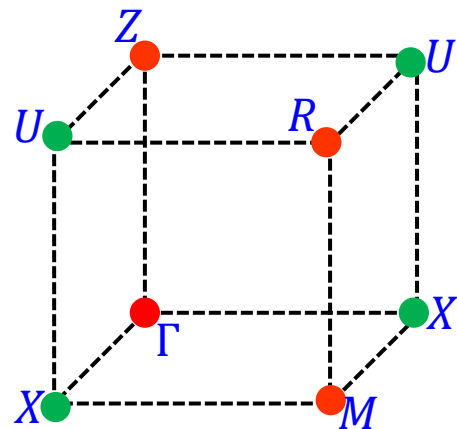
$$\delta_{\Gamma}\delta_X\delta_M\delta_Y\delta_Z\delta_U\delta_T\delta_R = (-1)^{Z_2}$$

Normal insulator ($Z_2=0$)

L. Fu, PRB **76**, 045302 (2007)

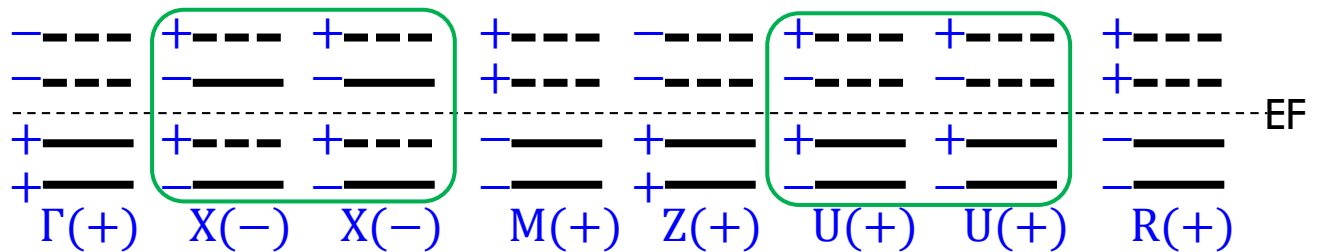


Band inversion at X and U



$$??? (Z_2=0)$$

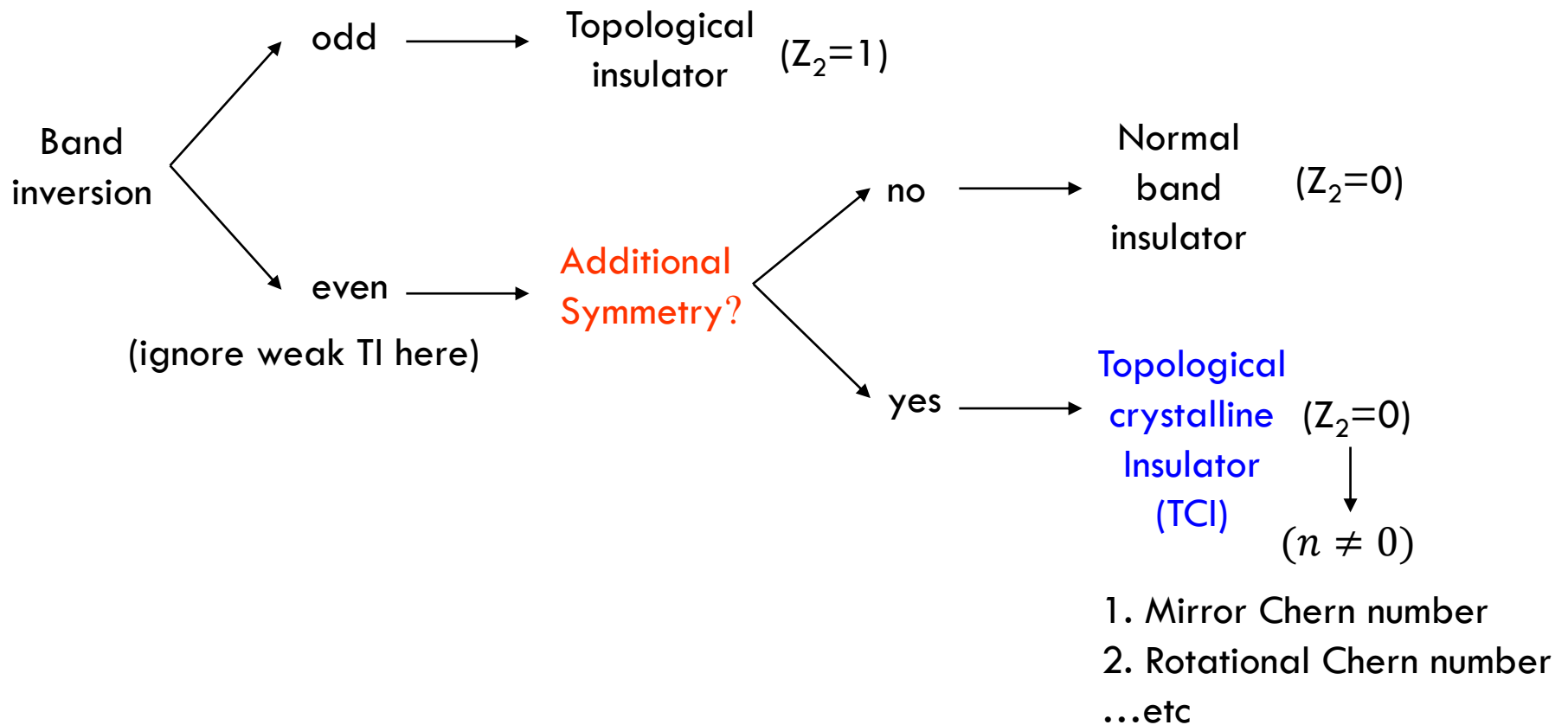
L. Fu, PRL **106**, 106802 (2011)



Normal band insulator?

Topological crystalline insulator

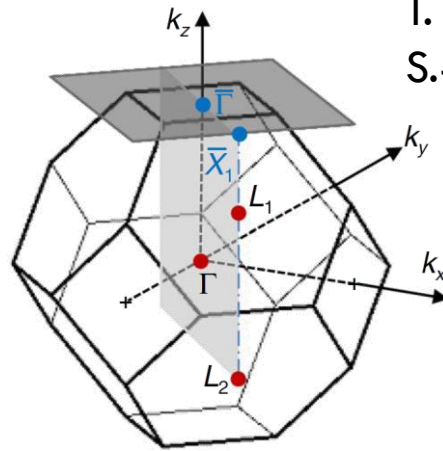
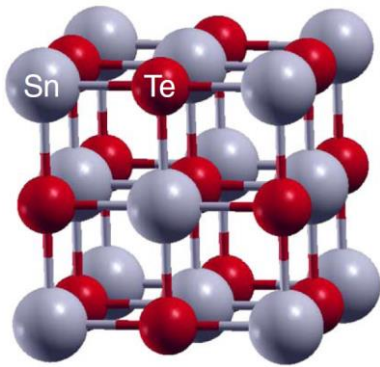
10



SnTe: mirror symmetry

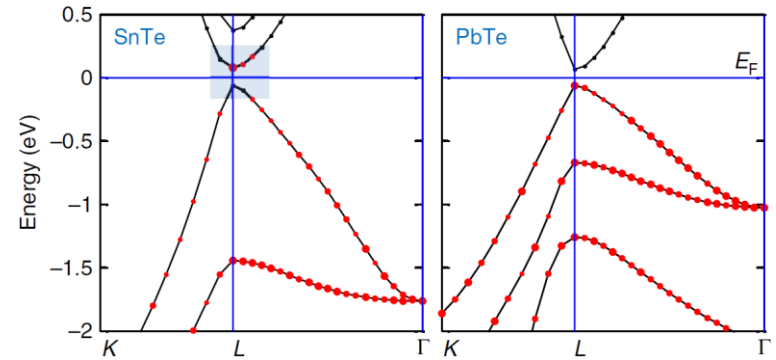
11

SnTe

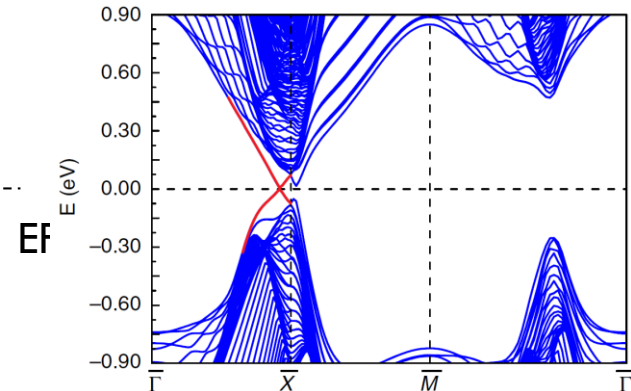
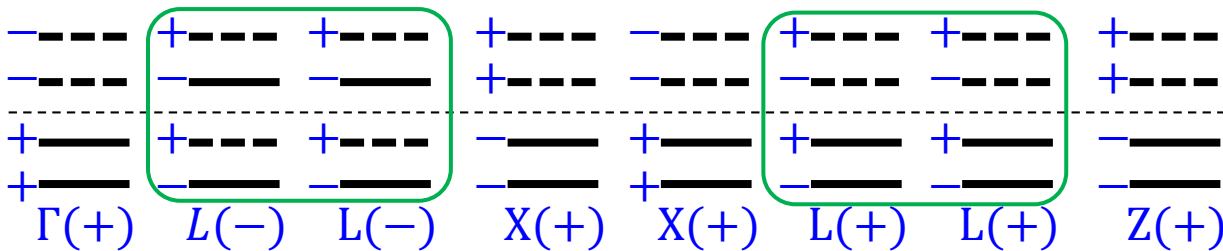


T. H. Hsieh et al., Nature Commun. **3**, 1192 (2012)

S.-Y. Xu et al., Nature Commun. **3**, 982 (2012)



$Z_2=0$



Even number of times band inversion + additional crystalline symmetry

$$\text{Mirror Chern number } n_M = (n_{+i} - n_{-i})/2$$

where $n_{\mp i}$ = mirror eigenvalue

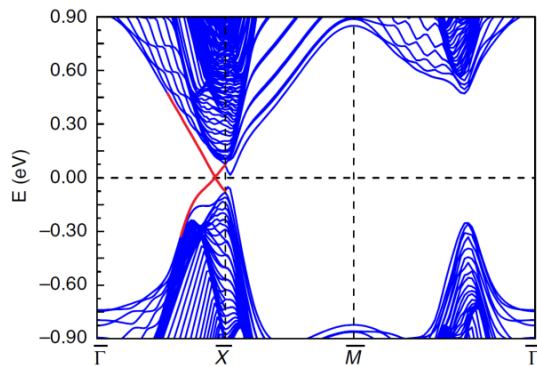
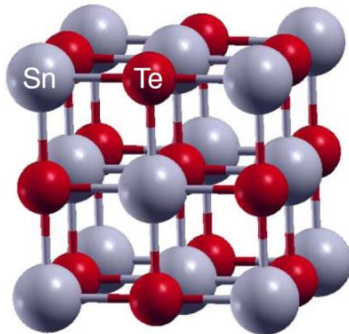
TCl: mirror and glide mirror

12

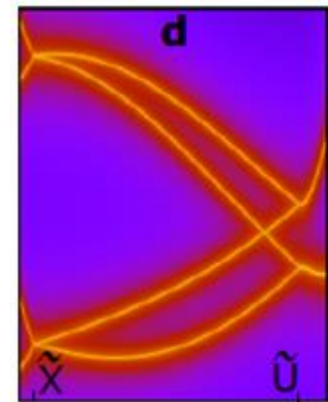
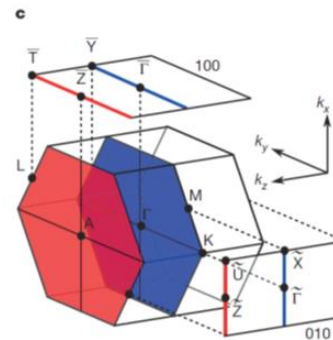
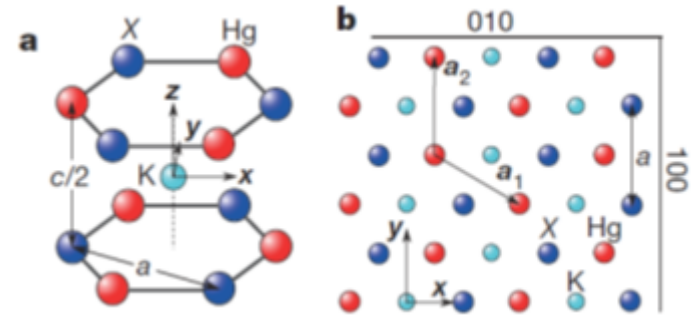
T. H. Hsieh et al., Nature Commun. **3**, 1192 (2012)
S.-Y. Xu et al., Nature Commun. **3**, 982 (2012)

Z. Wang et al., Nature **532**, 189 (2016)
J. Ma et al., Science Advances **3**, e1602415 (2017)

SnTe => mirror



KHgX (X=As,Sb,Bi) => glide mirror



TCl beyond (glide) mirror symmetry ?

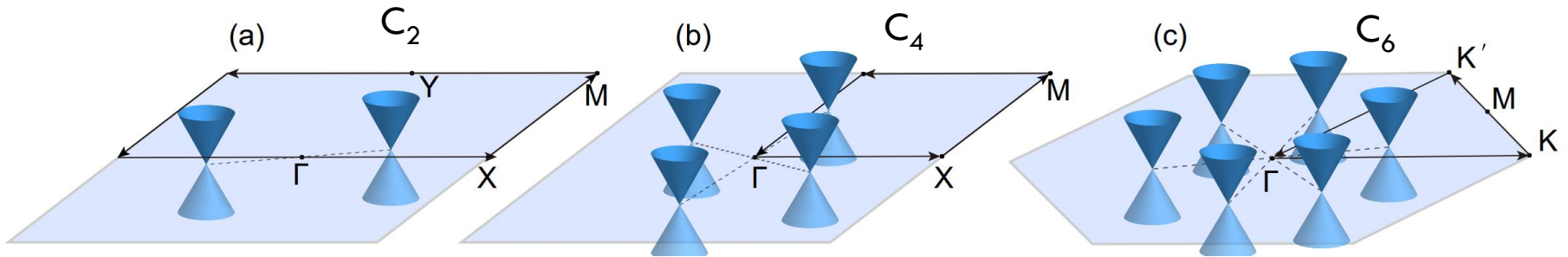
TCI: rotational symmetry

13

New TCI: protected by the N-fold rotational symmetries

Chen Fang and Liang Fu, arXiv:1709.01929 (2017).

$C_n = n$ Dirac points on one surface



Topological invariant number is not convenient to calculate from DFT.

Real material ???

TCl: symmetry indicator

14

ARTICLE

DOI: [10.1038/s41467-017-00133-2](https://doi.org/10.1038/s41467-017-00133-2)

OPEN

Symmetry-based indicators of band topology in the 230 space groups (symmetry indicator)

Hoi Chun Po^{1,2}, Ashvin Vishwanath^{1,2} & Haruki Watanabe³

How to implement on first-principle?

TCl: symmetry indicator

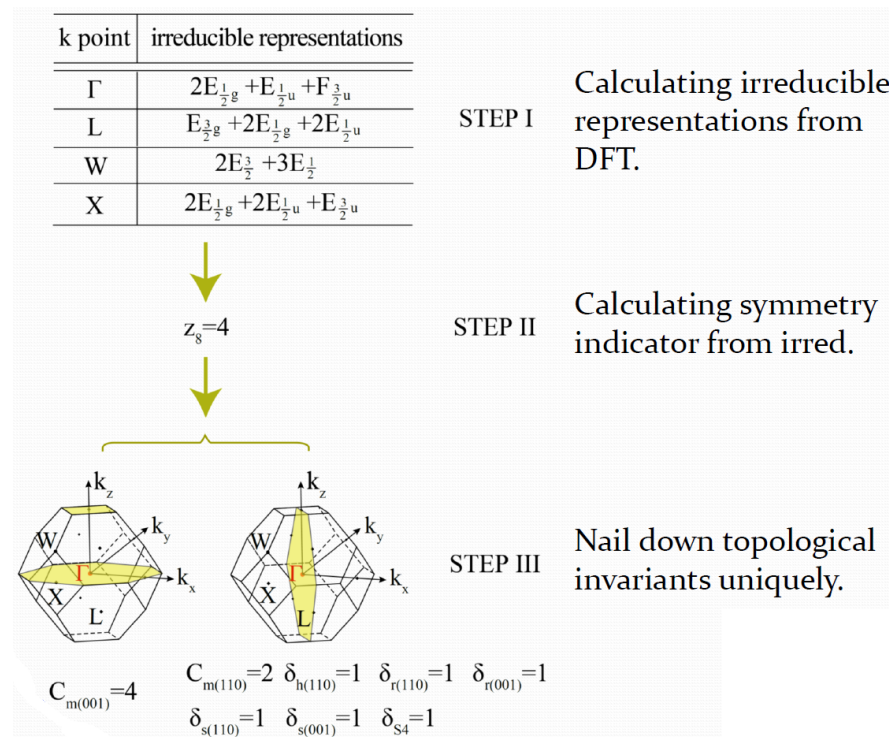
15

Systematic method (Fu-Kane-like formula) for searching TCI based on symmetry indicator

Zhida Song, Tiantian Zhang, Zhong Fang, Chen Fang:

Nature Communications **9**, 3530 (2018)

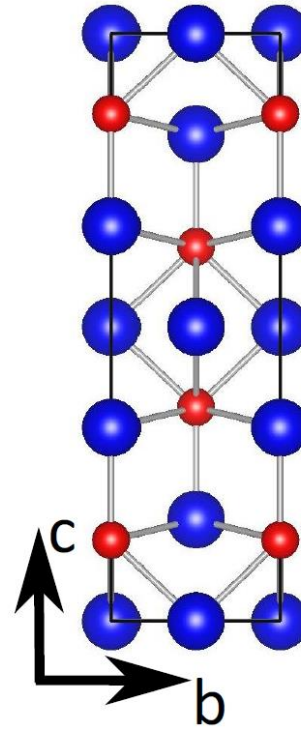
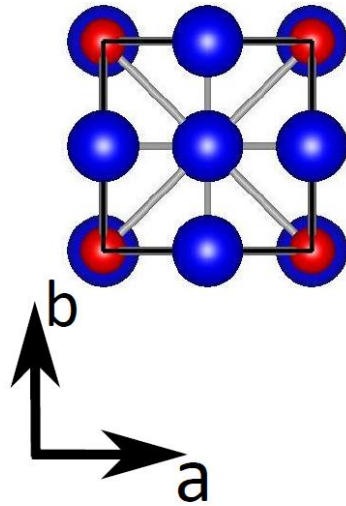
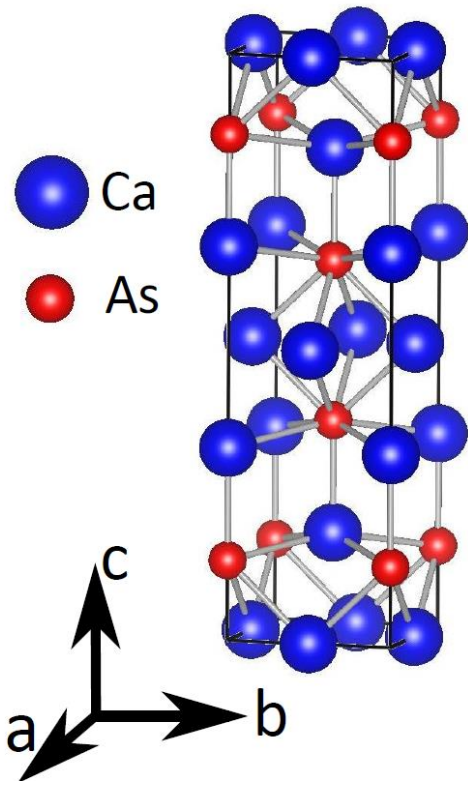
when certain additional symmetry Y is present, topological invariants of TCIs protected by symmetry X can be inferred by the Y -symmetry eigenvalues of energy band.



TCl: candidate material Ca_2As

16

Ca_2As : body-centered tetragonal lattice



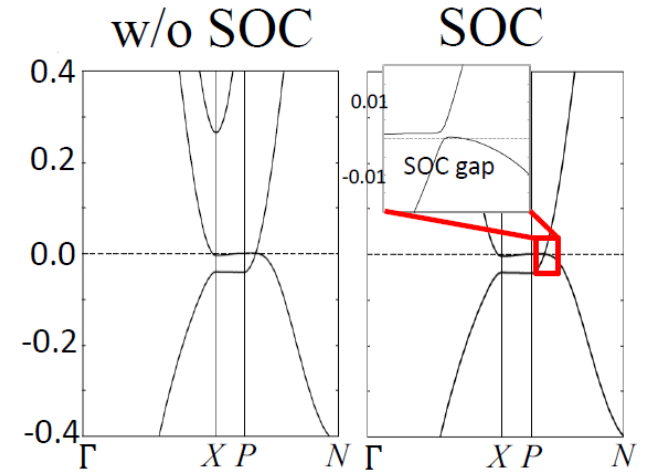
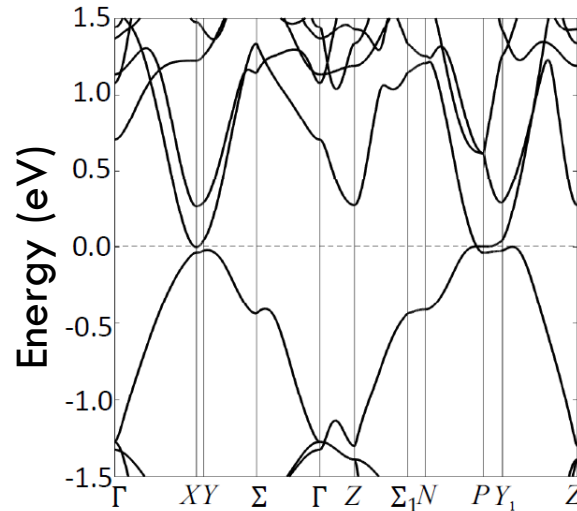
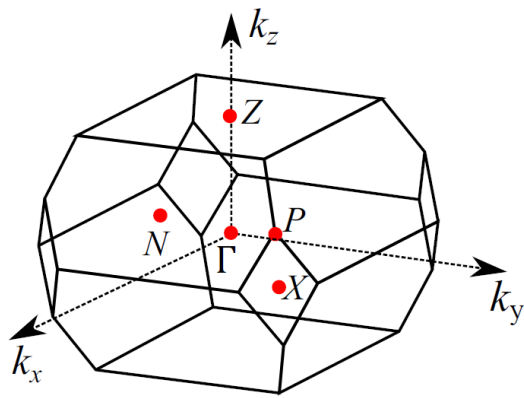
$I4/mmm$ (#139)

Symmetry operation

- Time-reversal
- Inversion
- $M(100)$
- $M(010)$
- $M(001)$
- $M(110)$
- $M(1-10)$
- $C_4(001)$
- $C_2(100)$
- $C_2(010)$
- $C_2(001)$
- $C_2(110)$
- $C_2(1-10)$

Ca₂As: symmetry indicator

17



Step-1

Counting the irred. rep. number of each band

Tetragonal body-centred	87 (139, 140) ^a	$n_{\frac{1}{2}}^+$	$n(E_{\frac{1}{2}g}^{\Gamma}) + n(E_{\frac{1}{2}g}^M) + n(E_{\frac{1}{2}g}^X) + 2n(E_{\frac{1}{2}g}^N) + n(E_{\frac{1}{2}g}^P)^b$
		$n_{\frac{1}{2}}^-$	$n(E_{\frac{1}{2}u}^{\Gamma}) + n(E_{\frac{1}{2}u}^M) + n(E_{\frac{1}{2}u}^X) + 2n(E_{\frac{1}{2}u}^N) + n(E_{\frac{1}{2}u}^P)$
		$n_{\frac{3}{2}}^+$	$n(E_{\frac{3}{2}g}^{\Gamma}) + n(E_{\frac{3}{2}g}^M) + n(E_{\frac{3}{2}g}^X) + 2n(E_{\frac{3}{2}g}^N) + n(E_{\frac{3}{2}g}^P)$
		$n_{\frac{3}{2}}^-$	$n(E_{\frac{3}{2}u}^{\Gamma}) + n(E_{\frac{3}{2}u}^M) + n(E_{\frac{3}{2}u}^X) + 2n(E_{\frac{3}{2}u}^N) + n(E_{\frac{3}{2}u}^P)$

The symmetry indicator of # 139 is (Z_2, Z_8)

z_2	All SGs with S_4	$\sum_{\mathbf{K}} \frac{1}{2} n_{\mathbf{K}}^{\frac{3}{2}} - \frac{1}{2} n_{\mathbf{K}}^{\frac{1}{2}} \pmod{2}^b$
z_8	83, 87, 123, 124, 127, 128, 139, 140, 221, 225, 226, 229	$\frac{3}{2} n_{\frac{3}{2}}^+ - \frac{3}{2} n_{\frac{3}{2}}^- - \frac{1}{2} n_{\frac{1}{2}}^+ + \frac{1}{2} n_{\frac{1}{2}}^- \pmod{8}^d$ $(Z_2, Z_8) = (0, 4)$ for Ca ₂ As

Ca₂As: symmetry indicator

18

	$(Z_2 Z_8)$
Ca ₂ As and Ca ₂ Sb	(04)

Step-2

$Z_{2,8}$	weak	mirror			glide mirror			rotation				I4/mmm (#139)						
		$m_{(4)}^{001}$	$m_{(2)}^{1\bar{1}0}$	$m_{(2)}^{100}$	$g_{\frac{1}{2}\frac{1}{2}0}^{001}$	$g_{\frac{1}{2}\frac{1}{2}0}^{1\bar{1}0}$	$g_{0\frac{1}{2}\frac{1}{2}}^{100}$	2^{001}	2^{100}	2^{110}	4^{001}	i	2_1^{001}	2_1^{100}	2_1^{110}	4_2^{001}	$\bar{4}^{001}$	
00	000	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
00	000	0	2	2	0	1	1	0	1	1	0	0	0	1	1	0	0	0
00	000	4	0	2	0	0	1	0	1	0	1	0	0	1	0	1	1	1
00	000	4	2	0	0	1	0	0	0	1	1	0	0	0	1	1	1	1
04	000	0	0	2	0	0	1	0	1	0	1	0	0	1	0	1	1	1
04	000	0	2	0	0	1	0	0	0	1	1	0	0	0	1	1	1	1
04	000	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
04	000	4	2	2	0	1	1	0	1	1	0	0	0	1	1	0	0	0
12	111	2	0	0	0	0	1	0	1	1	0	1	1	0	0	1	1	1
12	111	2	2	2	0	1	0	0	0	0	0	1	1	1	1	1	1	1
12	111	$\bar{2}$	0	2	0	0	0	0	0	1	1	1	1	1	0	0	0	0
12	111	$\bar{2}$	2	0	0	1	1	0	1	0	1	1	1	0	1	0	0	0

Ca₂As: symmetry indicator

19

	($Z_2 Z_8$)
Ca ₂ As and Ca ₂ Sb	(04)

Step-3

14/mmm (#139)

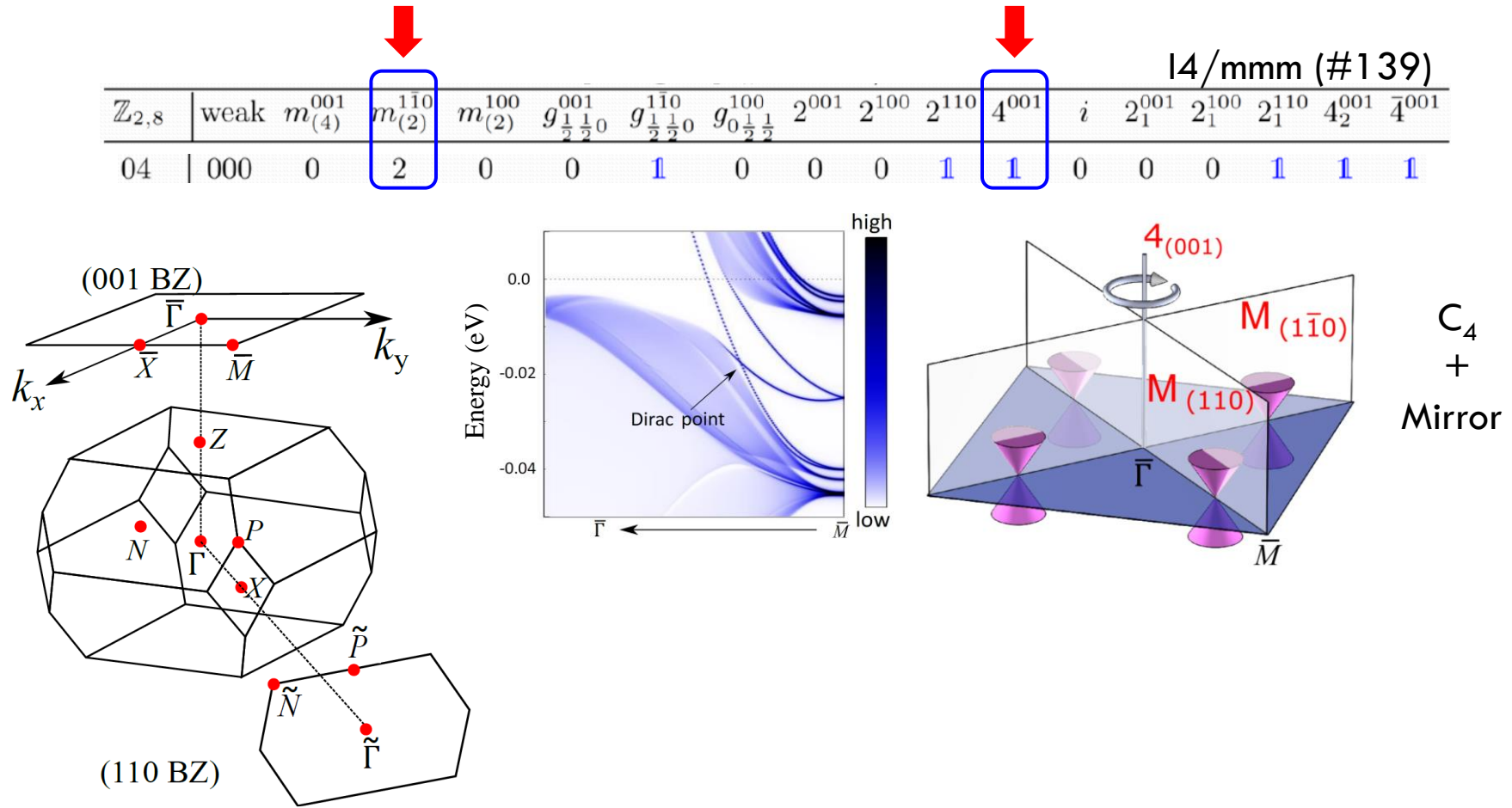
$Z_{2,8}$	weak	$m_{(4)}^{001}$	$m_{(2)}^{\bar{1}\bar{1}0}$	$m_{(2)}^{100}$	$g_{\frac{1}{2}\frac{1}{2}0}^{001}$	$g_{\frac{1}{2}\frac{1}{2}0}^{\bar{1}\bar{1}0}$	$g_{0\frac{1}{2}\frac{1}{2}}^{100}$	2^{001}	2^{100}	2^{110}	4^{001}	i	2_1^{001}	2_1^{100}	2_1^{110}	4_2^{001}	$\bar{4}^{001}$
00	000	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
00	000	0	2	2	0	1	1	0	1	1	0	0	0	1	1	0	0
00	000	4	0	2	0	0	1	0	1	0	1	0	0	1	0	1	1
00	000	4	2	0	0	1	0	0	0	1	1	0	0	0	1	1	1
04	000	0	0	2	0	0	1	0	1	0	1	0	0	1	0	1	1
04	000	0	2	0	0	1	0	0	0	1	1	0	0	0	1	1	1
04	000	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
04	000	4	2	2	0	1	1	0	1	1	0	0	0	1	1	0	0
12	111	2	0	0	0	0	1	0	1	1	0	1	1	0	0	1	1
12	111	2	2	2	0	1	0	0	0	0	0	1	1	1	1	1	1
12	111	$\bar{2}$	0	2	0	0	0	0	0	1	1	1	1	1	0	0	0
12	111	$\bar{2}$	2	0	0	1	1	0	1	0	1	1	1	0	1	0	0

	$(\nu_0; \nu_1 \nu_2 \nu_3)$	$n_{4(001)}$	$n_{2(100)}$	$n_{2(001)}$	$n_{2(110)}$	$n_{\mathcal{M}_{(1\bar{1}0)}}$	$n_{\mathcal{M}_{(001)}}$	$n_{\mathcal{M}_{(100)}}$	\mathcal{I}
Ca ₂ As	(0;000)	1	0	0	1	2	0	0	1

↑ ↑ ↑
mirror Chern number

Topological surface states

20

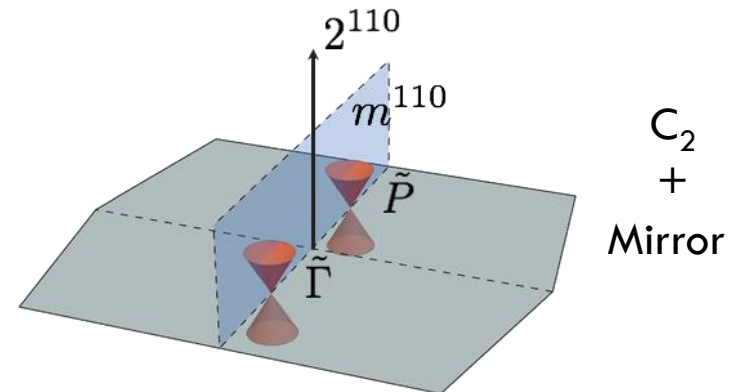
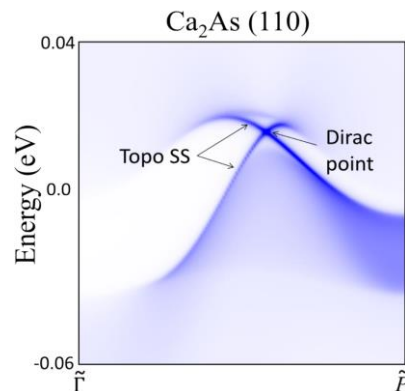
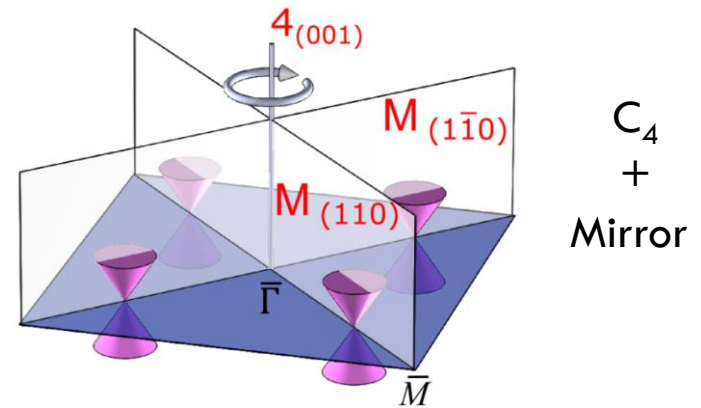
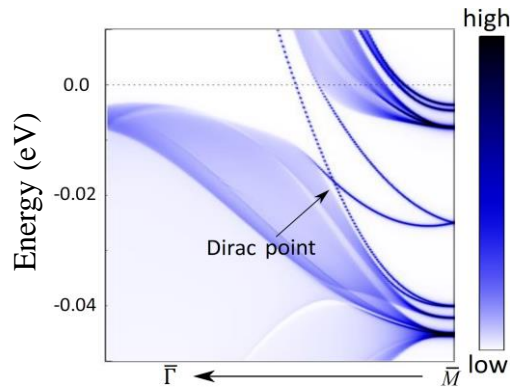
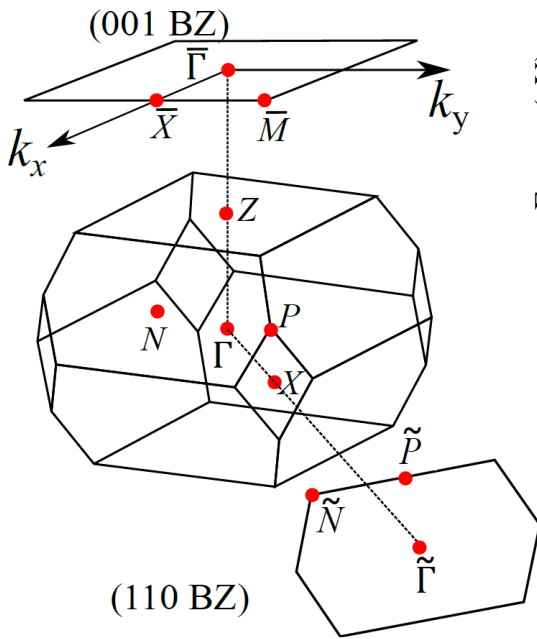


Topological surface states

21

14/mmm (#139)

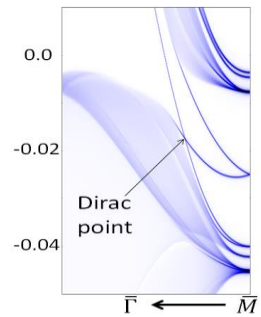
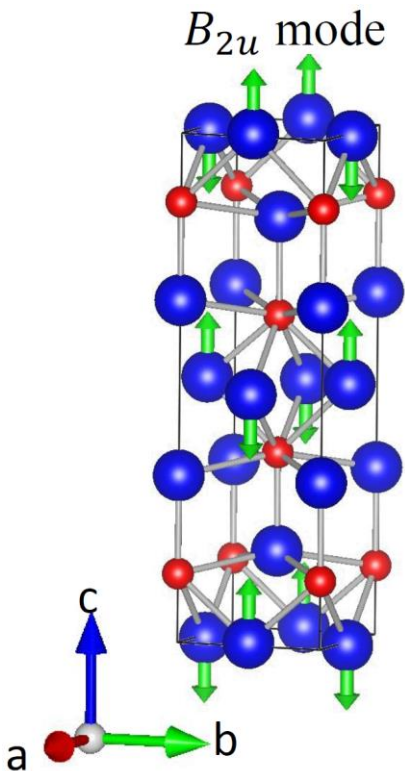
$\mathbb{Z}_{2,8}$	weak	$m_{(4)}^{001}$	$m_{(2)}^{110}$	$m_{(2)}^{100}$	$g_{\frac{1}{2}\frac{1}{2}0}^{001}$	$g_{\frac{1}{2}\frac{1}{2}0}^{110}$	$g_{0\frac{1}{2}\frac{1}{2}}^{100}$	2^{001}	2^{100}	2^{110}	4^{001}	i	2_1^{001}	2_1^{100}	2_1^{110}	4_2^{001}	$\bar{4}^{001}$
04	000	0	2	0	0	1	0	0	0	1	1	0	0	0	1	1	1



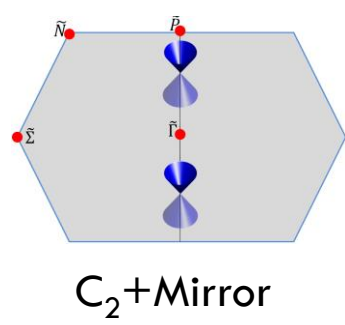
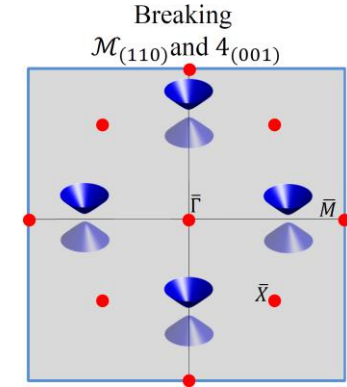
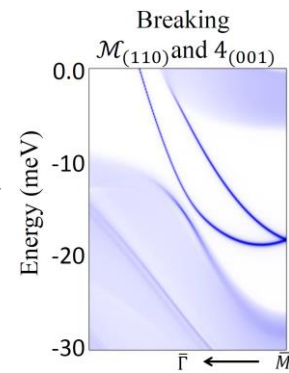
TCl: rotational symmetry protected

22

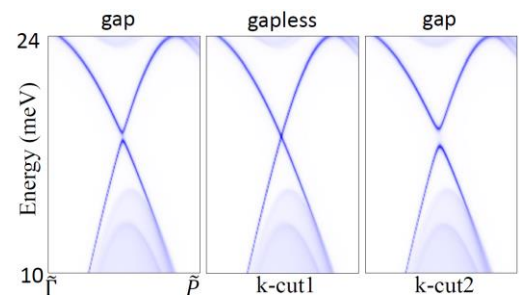
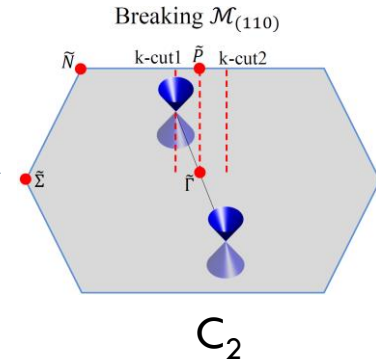
$\mathbb{Z}_{2,8}$	weak	$m_{(4)}^{001}$	$m_{(2)}^{10}$	$m_{(2)}^{100}$	$g_{\frac{1}{2}\frac{1}{2}0}^{001}$	$g_{\frac{1}{2}\frac{1}{2}0}^{110}$	$g_{0\frac{1}{2}\frac{1}{2}}^{100}$	2^{001}	2^{100}	2^{110}	4^{001}	i	2_1^{001}	2_1^{100}	2_1^{110}	4_2^{001}	$\bar{4}^{001}$
04	000	0	2	0	0	1	0	0	0	1	1	0	0	0	1	1	1



Breaking mirror & C_4

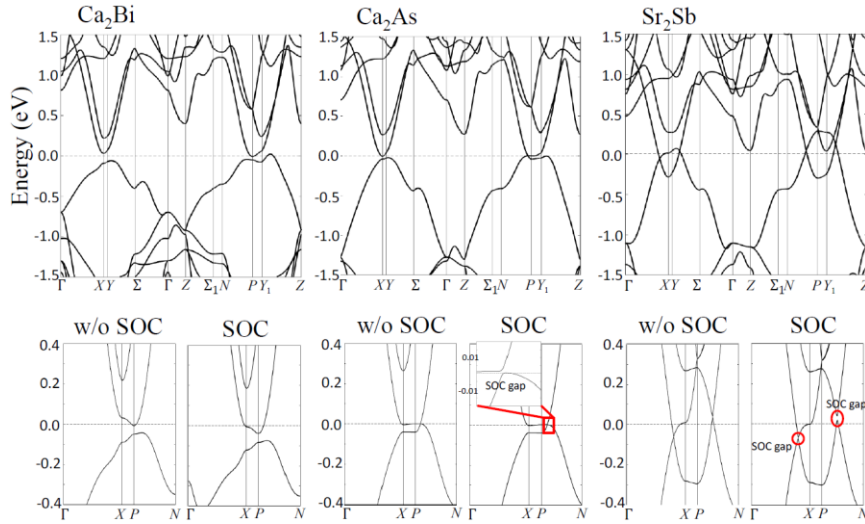


Breaking mirror

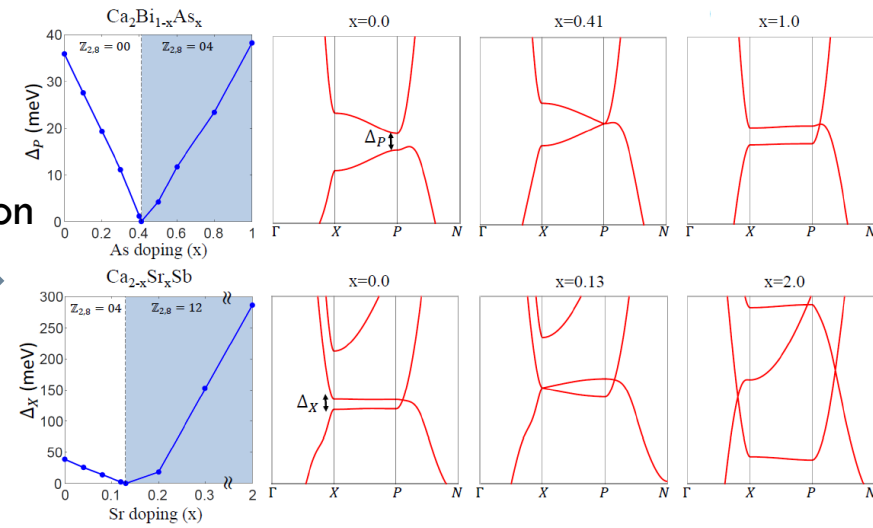
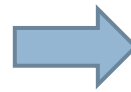


Topological phase transition

23



Phase transition

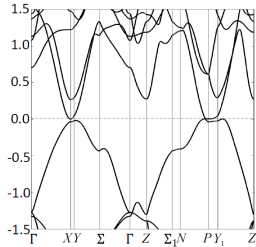


	$Z_{2,8}$	weak	$m_{(4)}^{001}$	$m_{(2)}^{110}$	$m_{(2)}^{100}$	$g_{\frac{1}{2}\frac{1}{2}0}^{001}$	$g_{\frac{1}{2}\frac{1}{2}0}^{110}$	$g_{\frac{1}{2}\frac{1}{2}}^{100}$	2^{001}	2^{100}	2^{110}	4^{001}	i	2_1^{001}	2_1^{100}	2_1^{110}	4_2^{001}	$\bar{4}^{001}$	
Ca_2Bi	00	000	0	2	2	0	1	1	0	1	1	0	0	0	1	1	0	0	Normal insulator
	00	000	4	0	2	0	0	1	0	1	0	1	0	0	1	0	1	1	
	00	000	4	2	0	0	1	0	0	0	1	1	0	0	0	1	1	1	
	04	000	0	0	2	0	0	1	0	1	0	1	0	0	1	0	1	1	
Ca_2As	04	000	0	2	0	0	1	0	0	0	1	1	0	0	0	1	1	1	TCI
	04	000	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
	04	000	4	2	2	0	1	1	0	1	1	0	0	0	1	1	0	0	
Sr_2Sb	12	111	2	0	0	0	0	1	0	1	1	0	1	1	0	0	1	1	TCI+Weak TI
	12	111	2	2	2	0	1	0	0	0	0	0	1	1	1	1	1	1	
	12	111	$\bar{2}$	0	2	0	0	0	0	0	1	1	1	1	1	0	0	0	
	12	111	$\bar{2}$	2	0	0	1	1	0	1	0	1	1	0	1	0	0	0	

Conclusion (TCI)

24

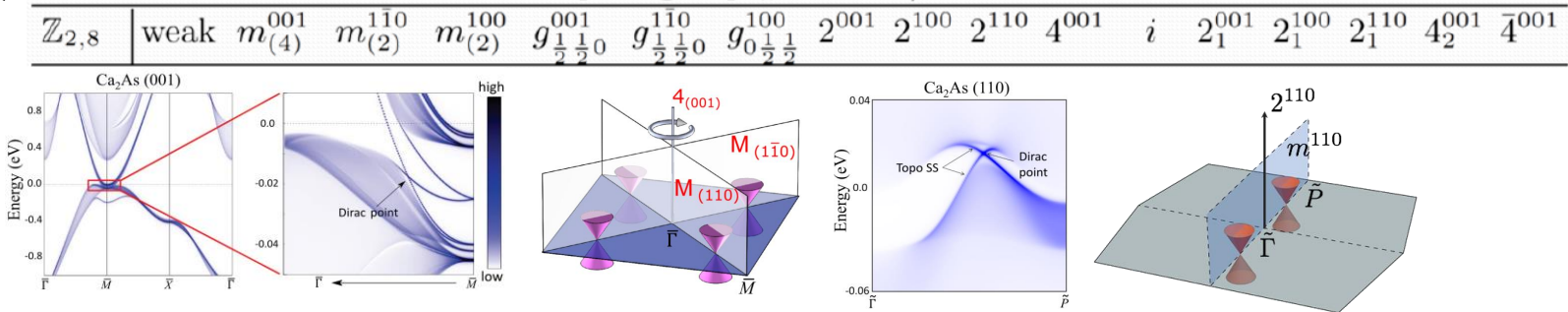
(1) Searching TCI by using symmetry indicator for the first time



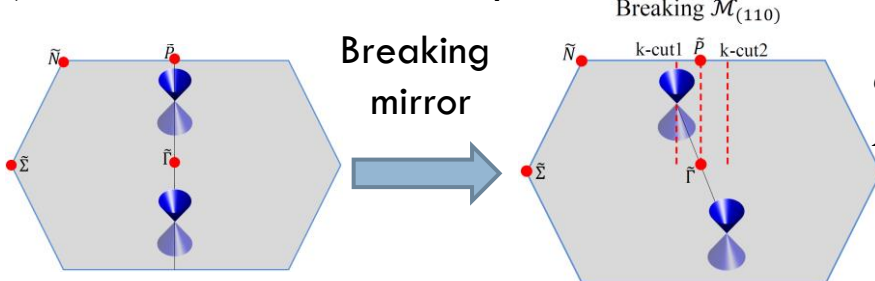
Ca_2As (Z_2, Z_8) = (0, 4)

Tetragonal body-centred	87 (139, 140) ^a	$n_{\frac{1}{2}}^+$	$n(E_{\frac{1}{2}g}^{\Gamma}) + n(E_{\frac{1}{2}g}^M) + n(E_{\frac{1}{2}g}^X) + 2n(E_{\frac{1}{2}g}^N) + n(E_{\frac{1}{2}g}^P)^b$
		$n_{\frac{1}{2}}^-$	$n(E_{\frac{1}{2}u}^{\Gamma}) + n(E_{\frac{1}{2}u}^M) + n(E_{\frac{1}{2}u}^X) + 2n(E_{\frac{1}{2}u}^N) + n(E_{\frac{1}{2}u}^P)$
		$n_{\frac{3}{2}}^+$	$n(E_{\frac{3}{2}g}^{\Gamma}) + n(E_{\frac{3}{2}g}^M) + n(E_{\frac{3}{2}g}^X) + 2n(E_{\frac{3}{2}g}^N) + n(E_{\frac{3}{2}g}^P)$
		$n_{\frac{3}{2}}^-$	$n(E_{\frac{3}{2}u}^{\Gamma}) + n(E_{\frac{3}{2}u}^M) + n(E_{\frac{3}{2}u}^X) + 2n(E_{\frac{3}{2}u}^N) + n(E_{\frac{3}{2}u}^P)$

(2) Topological surface states are protected by multi topological invariant numbers



(3) It is first time that the Topological surface states are protected by rotational symmetry



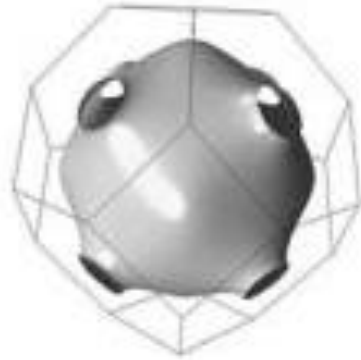
arXiv:1805.05215 (2018)

X. Zhou et al., Phys. Rev. B 98, 241104(R) (2018)

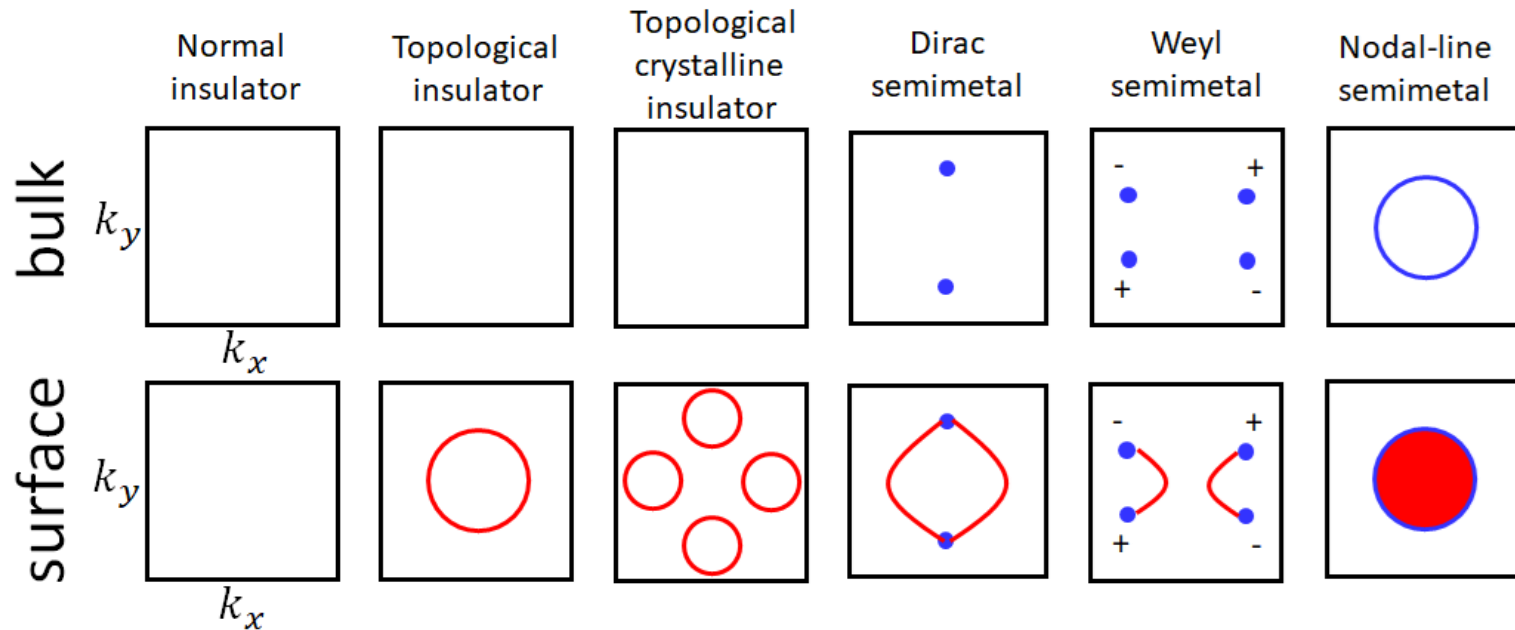
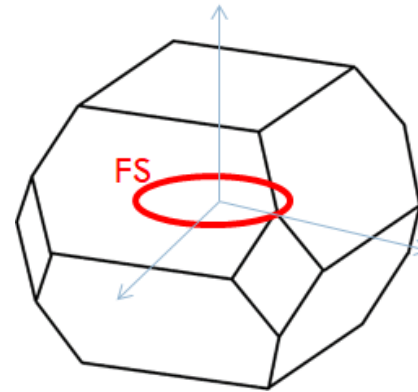
Nodal-line semimetal (節線半金屬)

25

Normal metal: 2D Fermi surface



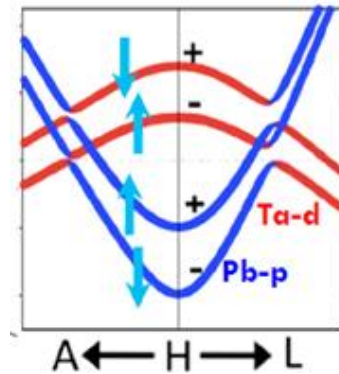
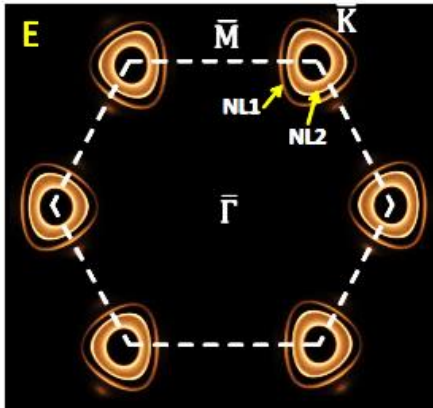
Topological metal: 1D Nodal-line



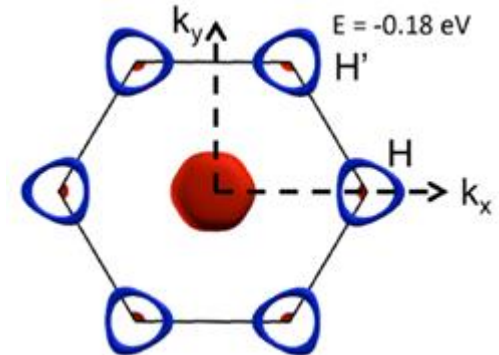
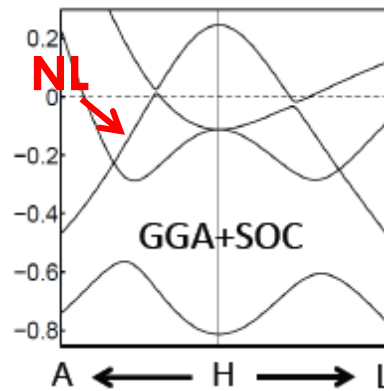
Nodal-line semimetal

26

PbTaSe₂



TlTaSe₂



G. Bian et al., Nature Commun. 7, 10556 (2016)

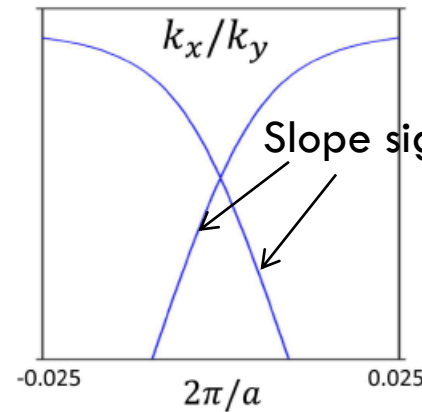
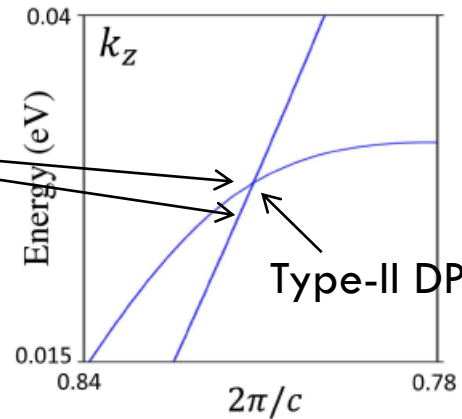
G. Bian et al., Phys. Rev. B 93, 12113(R) (2016)

Type-I vs Type-II

27

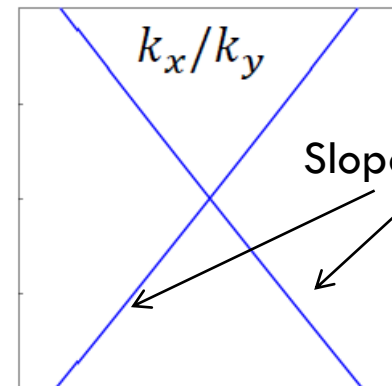
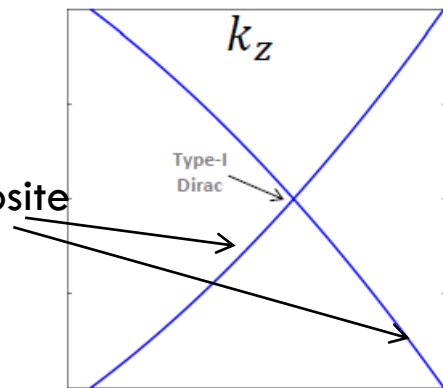
Type-II

Slope sign:
the same



Type-I

Slope sign: opposite



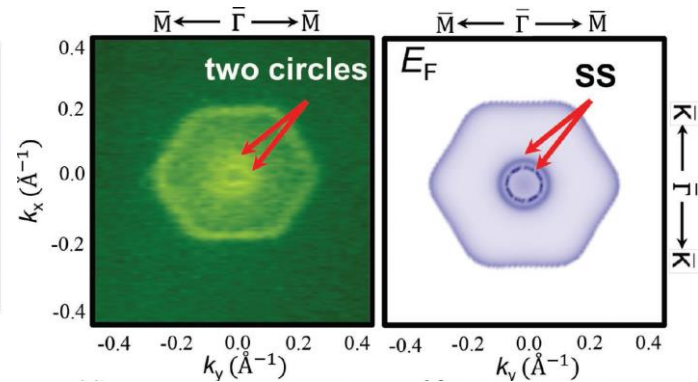
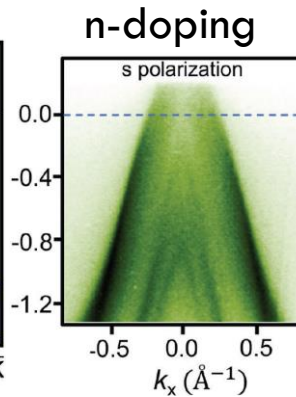
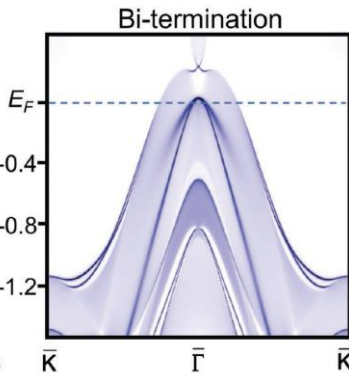
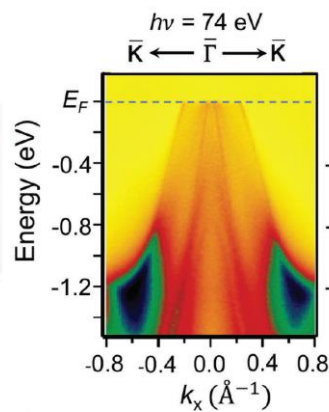
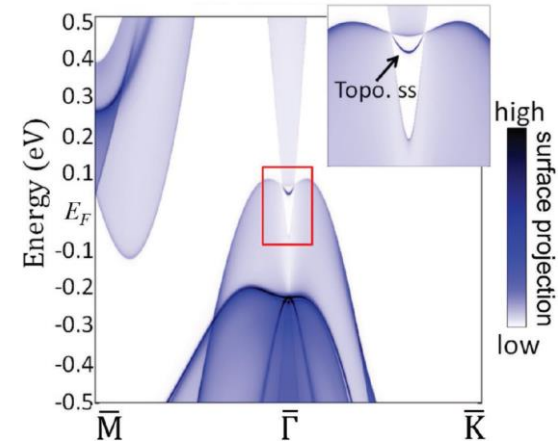
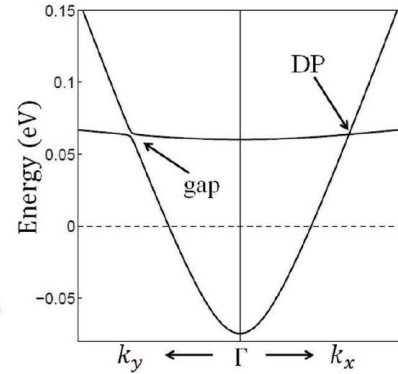
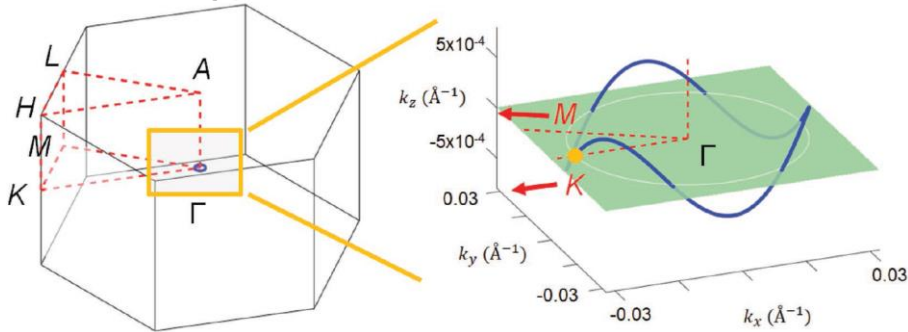
Type-II Weyl: A. A. Soluyanov et al., *Nature* volume 527, 495 (2016)

Type-II Dirac: T.-R. Chang et al., *Phys. Rev. Lett.* 119, 026404 (2017)

Type-II Nodal-line semimetal

28

Mg_3Bi_2



Acknowledgements (TCI)

29

Dr. Xiaoting Zhou
(NCKU)



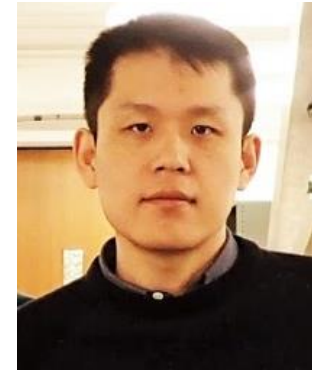
Chuang-Han Hsu
(NUS)



Prof. Hsin Lin
(Academia Sinica)



Dr. Su-Yang Xu
(MIT)



Prof. Liang Fu
(MIT)



X. Zhou et al., Phys. Rev. B 98, 241104(R) (2018)



MOST(Taiwan) Young Scholar Fellowship:
MOST Grant for the Columbus Program



NCTS
National Center for Theoretical Sciences
Physics Division 國家理論科學研究中心 物理組

Acknowledgements (Nodal-line)

30

Prof. R. J. Cava
(Princeton U.)



Prof. Weiwei Xie
(Louisiana State U.)



Prof. Guang Bian
(University of Missouri)



T.-R. Chang et al., Advanced Science (2018), DOI: 10.1002/advs.201800897



MOST(Taiwan) Young Scholar Fellowship:
MOST Grant for the Columbus Program

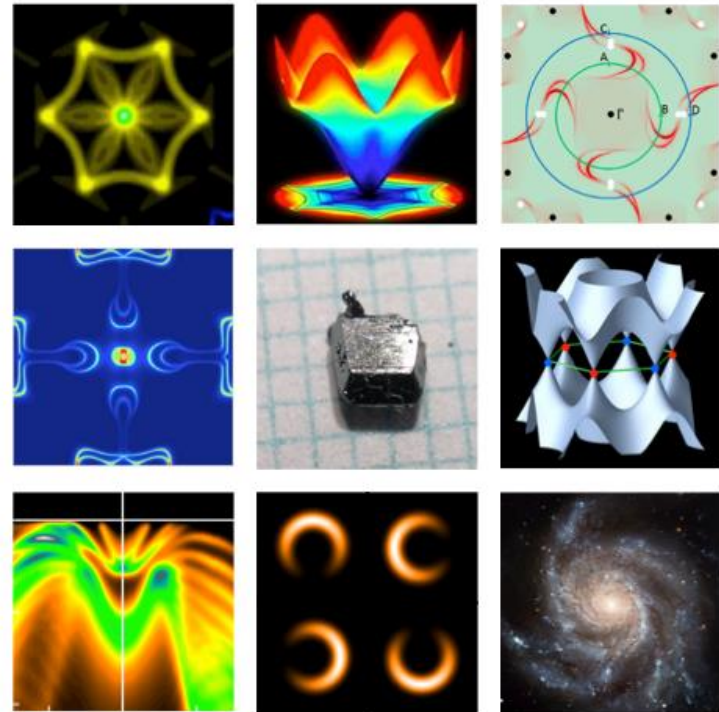


國立成功大學
National Cheng Kung University



National Center for Theoretical Sciences
Physics Division 國家理論科學研究中心 物理組

To see a world in a grain of sand ... —William Blake



Thank you !