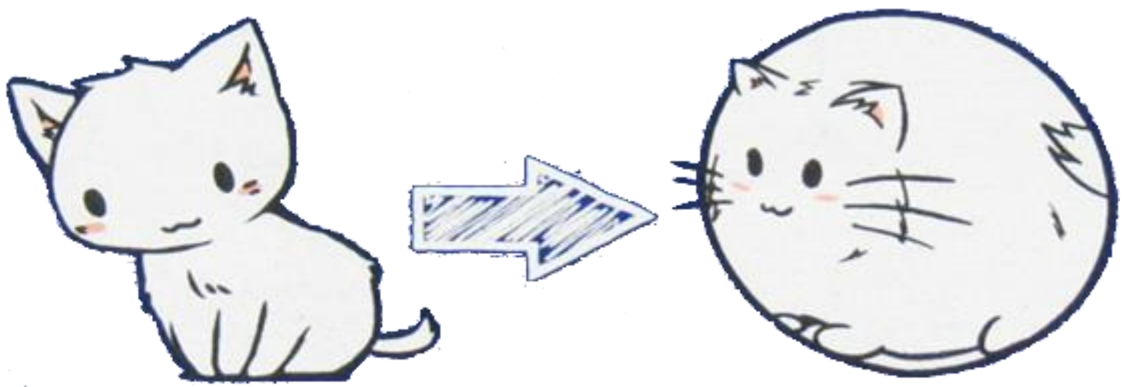
Topological Materials II



Department of physics, National Tsing Hua University

Tay-Rong Chang (張泰榕)

2016/May./26

Outline

1. Introduction

Band theory

Topology in condensed matter physics

Basics properties: Robust, invariant number, gapless surface states

Comparing with Landau's approach

Density functional theory (DFT)

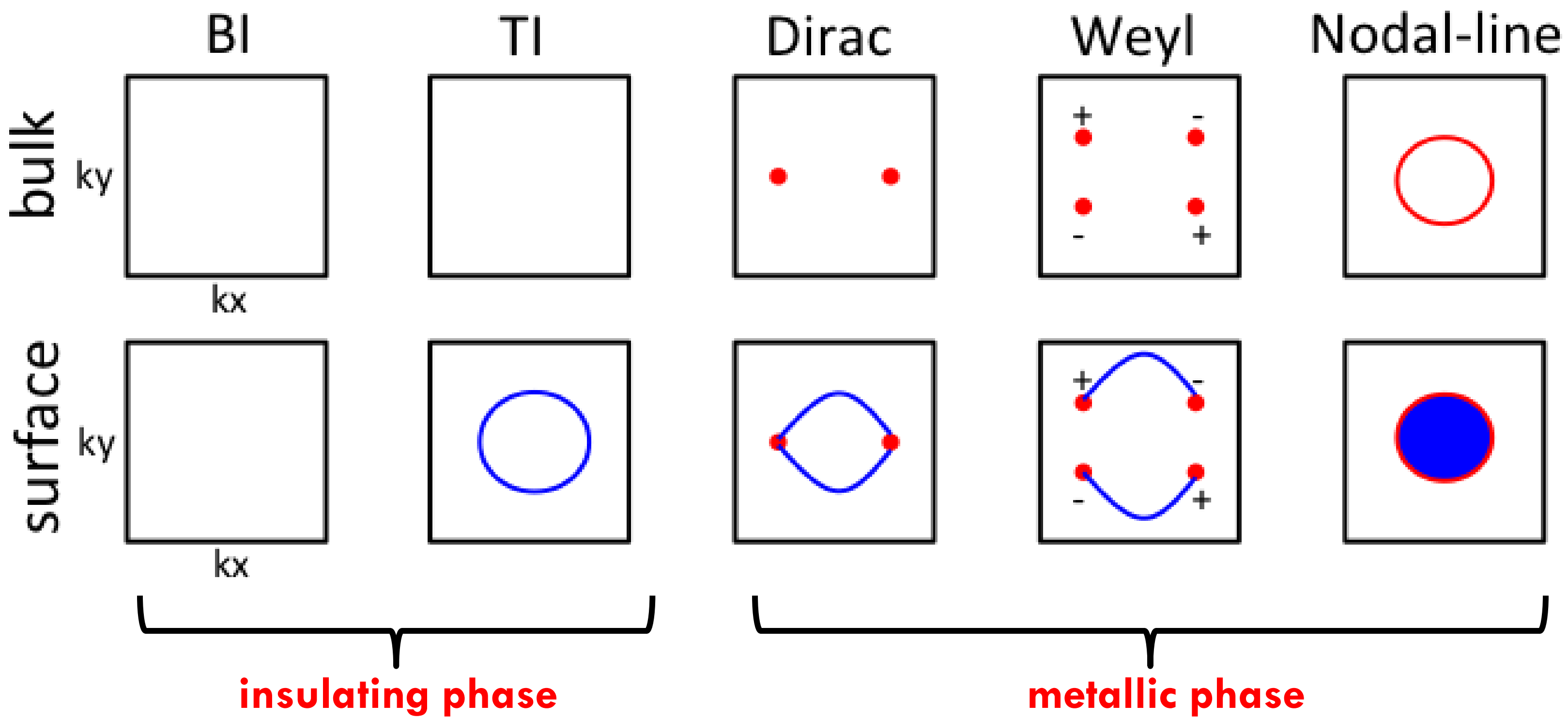
2. Topological insulator (quantum spin Hall insulator)

Strong topological insulator, weak topological insulator, topological crystalline insulator, topological Kondo insulator, quantum anomalous Hall effect…etc

3. Topological semimetal

3D Dirac semimetal, Weyl semimetal, Nodal-line semimetal, topological superconductor, New Fermion

Topological phases



Red: bulk bands

Blue: surface bands

Weyl semimetal

1. Introduction

Band theory

Topology in condensed matter physics

Basics properties: Robust, invariant number, gapless surface states

Comparing with Landau's approach

Density functional theory (DFT)

2. Topological insulator (quantum spin Hall insulator)

Strong topological insulator, weak topological insulator, topological crystalline insulator, topological Kondo insulator, quantum anomalous Hall effect…etc

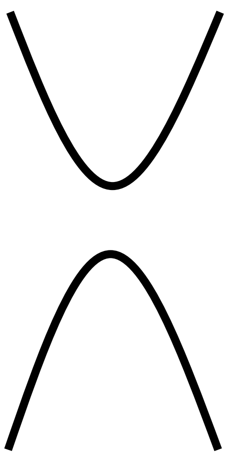
3. Topological semimetal

3D Dirac semimetal, Weyl semimetal, Nodal-line semimetal, topological superconductor, New Fermion

Weyl Fermion

4 x 4 matrix

$$H = \begin{pmatrix} v\vec{\sigma}\cdot\vec{k} & m \\ m & -v\vec{\sigma}\cdot\vec{k} \end{pmatrix}$$

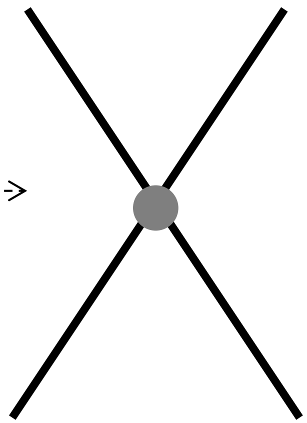


Dirac

if m = 0

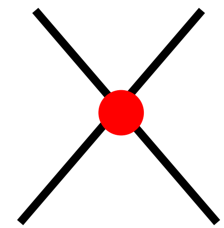
4 x 4 matrix

$$H = \begin{pmatrix} v\vec{\sigma}\cdot\vec{k} & 0 \\ 0 & -v\vec{\sigma}\cdot\vec{k} \end{pmatrix}$$

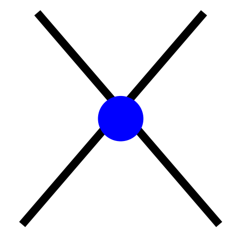


2 x 2 matrix

$$v\vec{\sigma}\cdot\vec{k}$$



Weyl



$$-v\vec{\sigma}\cdot\vec{k}$$

where $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

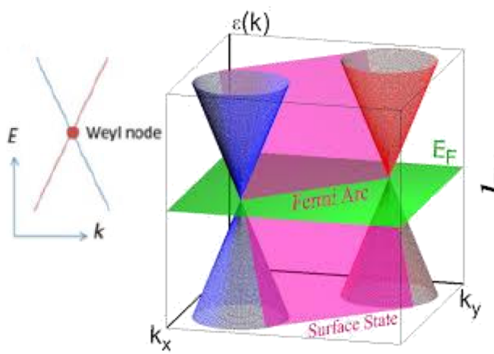
Nielsen-Ninomiya theorem: (Nuclear Physics B185 (1981) 20-40)

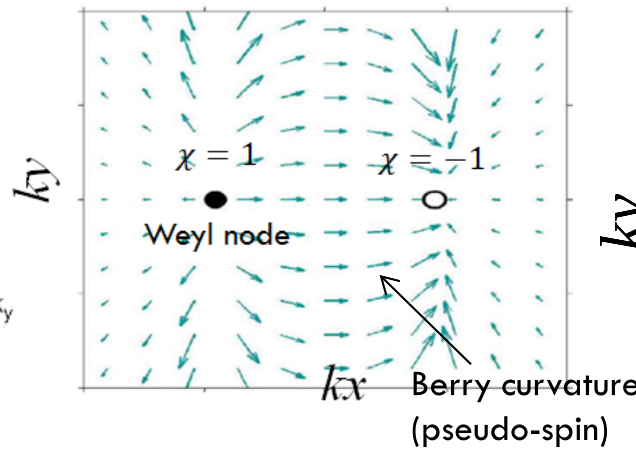
Equal numbers of χ =+1 and -1 WFs.

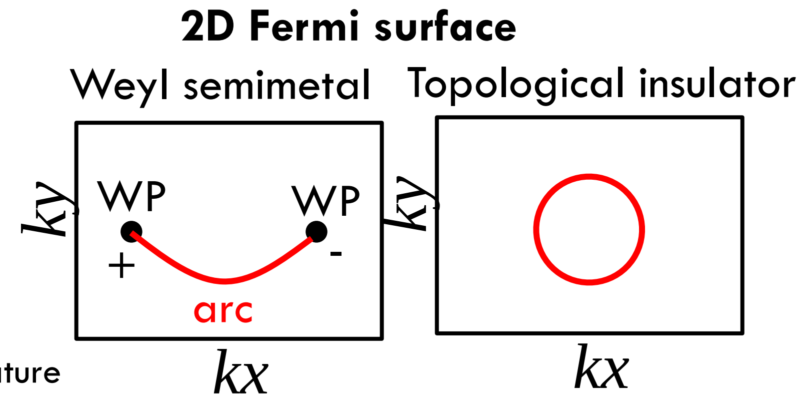
Weyl semimetal

Weyl semimetals:

1. Provide the realization of Weyl fermions
2. Extend the classification of topological phases of matter beyond insulators
3. Magnetic monopole in k-space (topological number called “chiral charge”)
4. Host exotic Fermi arc surface states







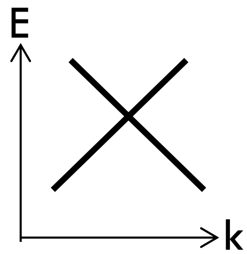
Weyl semimetal (topological phase)

(1) robust (2) topological invariant number (3) gapless surface states

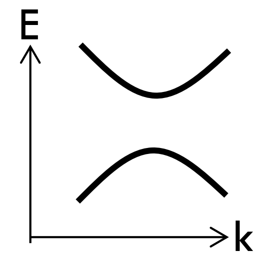
Weyl semimetal (robust)

2D $H = k_1\sigma_x + k_2\sigma_y$ $H = k_1\sigma_x + k_2\sigma_y + \underline{m\sigma_z}$

Graphene



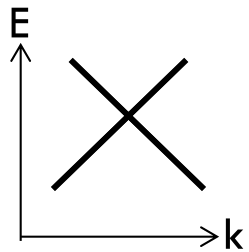
perturbation



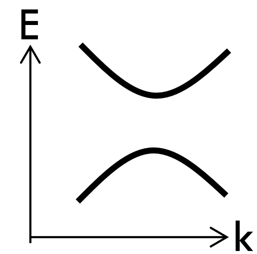
Weyl semimetal (robust)

2D $H = k_1\sigma_x + k_2\sigma_y$ $H = k_1\sigma_x + k_2\sigma_y + m\sigma_z$

Graphene



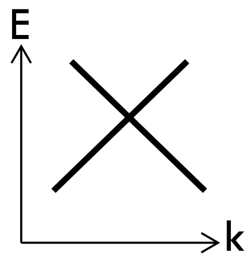
perturbation



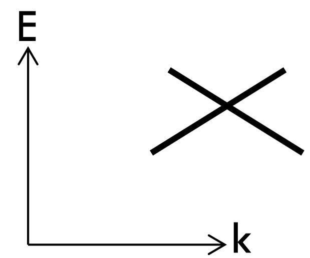
3D $H = k_1\sigma_1 + k_2\sigma_2 + k_3\sigma_z$

$$H = k_1\sigma_x + k_2\sigma_y + k_3\sigma_z + m\sigma_z$$
$$= k_1\sigma_x + k_2\sigma_y + (k_3 + m)\sigma_z$$
$$= k_1\sigma_x + k_2\sigma_y + k'_3\sigma_z$$

Weyl



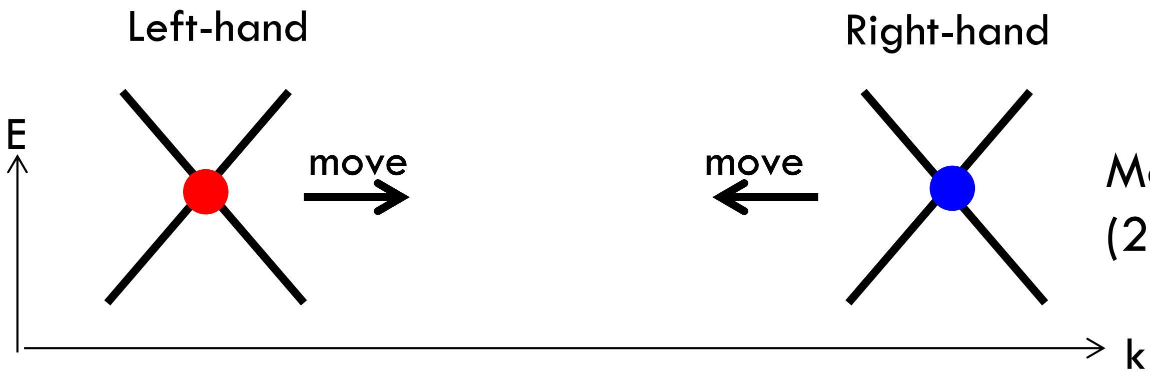
perturbation



In the presence of translation invariant, small perturbation cannot destroy the node. But only move the node.

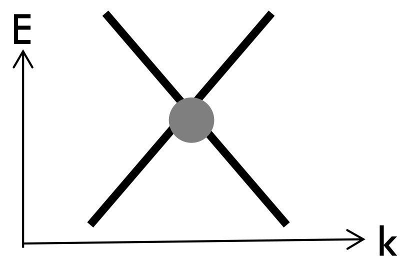
Weyl semimetal (annihilate)

Step 1



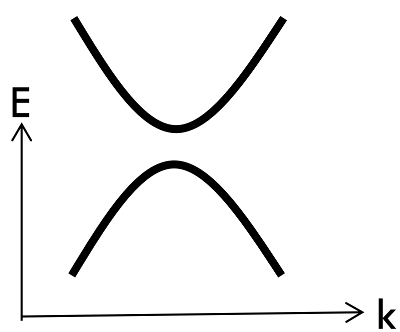
Move Weyl cones
(2x2 matrix)

Step 2



Two Weyl cones kiss
(4x4 matrix, m=0)

Step 3



open a gap
(4x4 matrix, m≠0)

Weyl semimetal (topological invariant number)

Chiral quantum number: χ

Berry connection

$$\boldsymbol{A}(\boldsymbol{k}) = \mathrm{i}\langle u(\boldsymbol{k})|\nabla_{\boldsymbol{k}} u(\boldsymbol{k})\rangle$$

Berry curvature

$$\boldsymbol{F}(\boldsymbol{k}) = \nabla_{\boldsymbol{k}} \times \boldsymbol{A}(\boldsymbol{k})$$

Chiral Charge

$$\frac{1}{2\pi} \oint_{FS} \boldsymbol{F}(\boldsymbol{k}) \cdot \mathrm{d}\boldsymbol{S}(\boldsymbol{k}) = \chi$$

$$\chi = integer$$

topological non-trivial

P. Hosur et al., C. R. Physique **14** (2013) 857

Weyl semimetal (topological invariant number)

Chiral quantum number: χ

Classical

Berry connection

$$\boldsymbol{A}(\boldsymbol{k}) = \mathrm{i}\langle u(\boldsymbol{k})|\nabla_{\boldsymbol{k}} u(\boldsymbol{k})\rangle \longleftrightarrow$$

Vector potential

A

Berry curvature

$$\boldsymbol{F}(\boldsymbol{k}) = \nabla_{\boldsymbol{k}} \times \boldsymbol{A}(\boldsymbol{k}) \longleftrightarrow$$

Magnetic field

$$\mathbf{B} = \nabla \times \mathbf{A}$$

Chiral Charge

$$\frac{1}{2\pi} \oint_{FS} \boldsymbol{F}(\boldsymbol{k}) \cdot \mathrm{d}\boldsymbol{S}(\boldsymbol{k}) = \chi \longleftrightarrow$$

Gauss's law for magnetism

$$\oiint_{\partial\Omega} \mathbf{B} \cdot \mathrm{d}\mathbf{S} = 0$$

$$\chi = integer$$

topological non-trivial

P. Hosur et al., C. R. Physique **14** (2013) 857

Weyl semimetal (pseduo-magnetic monopole)

Chiral quantum number: χ

Berry connection

$$\boldsymbol{A}(\boldsymbol{k}) = \mathrm{i}\langle u(\boldsymbol{k})|\nabla_{\boldsymbol{k}} u(\boldsymbol{k})\rangle$$

Berry curvature

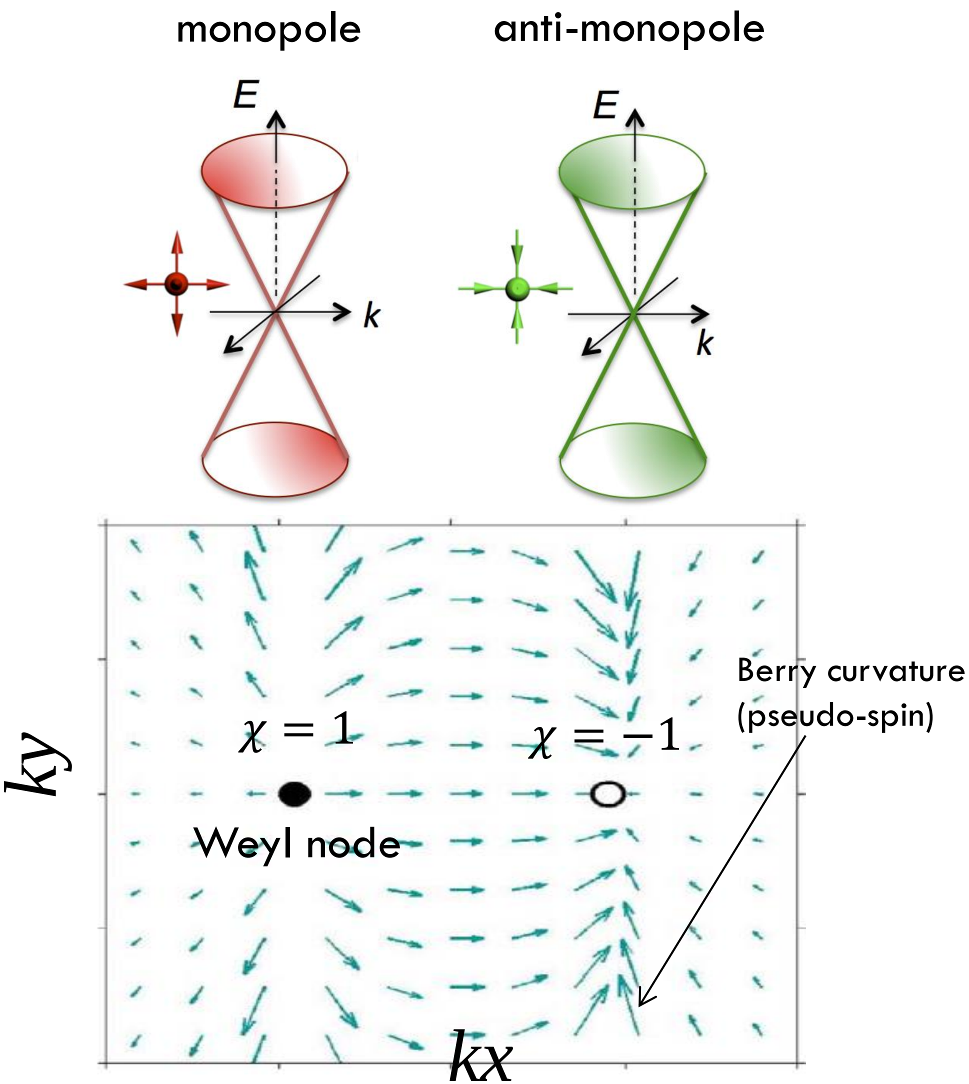
$$\boldsymbol{F}(\boldsymbol{k}) = \nabla_{\boldsymbol{k}} \times \boldsymbol{A}(\boldsymbol{k})$$

Chiral Charge

$$\frac{1}{2\pi}\oint_{FS} \boldsymbol{F}(\boldsymbol{k}) \cdot \mathrm{d}\boldsymbol{S}(\boldsymbol{k}) = \chi$$

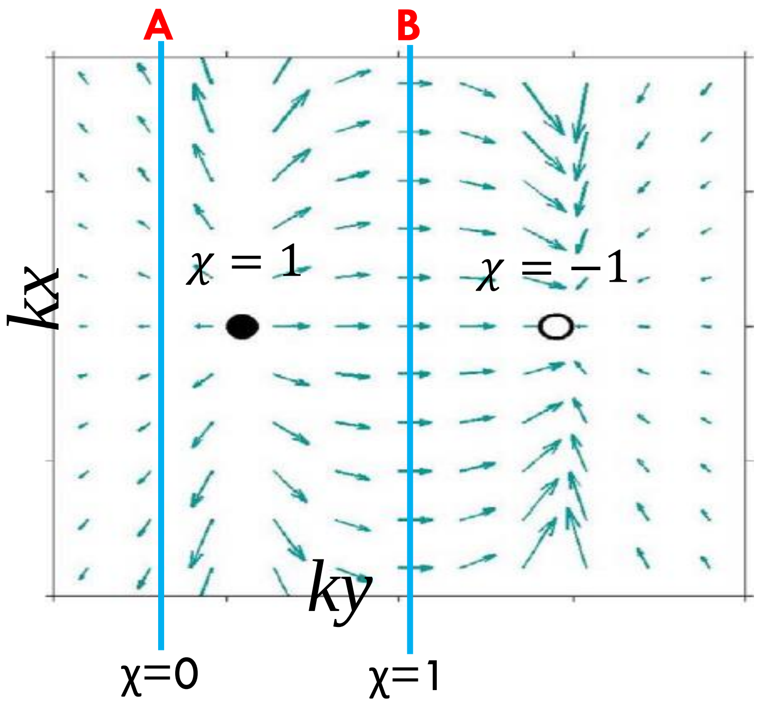
$$\chi = integer$$

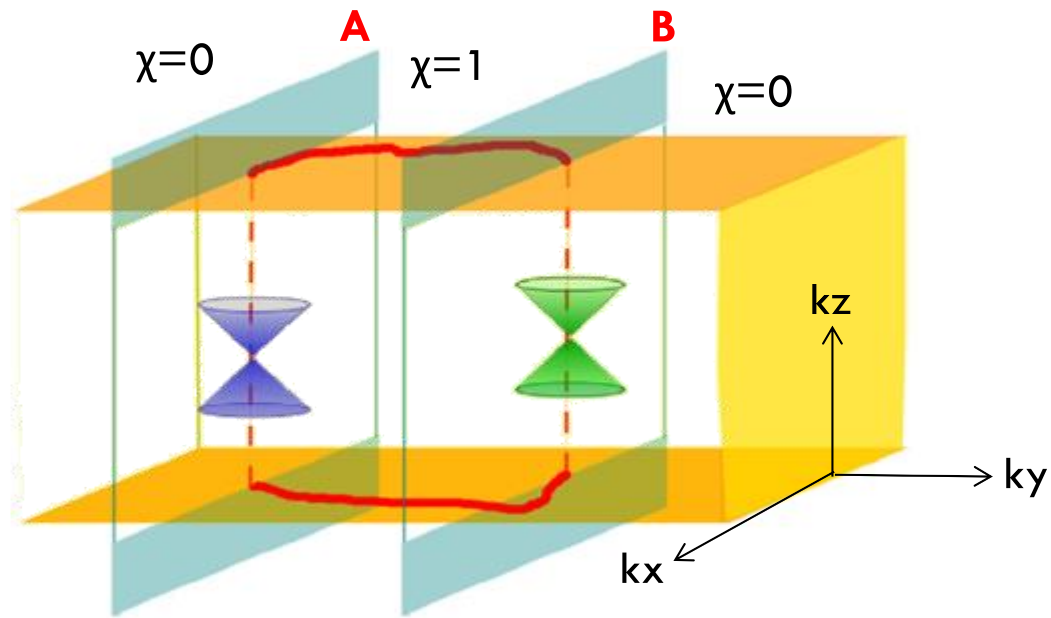
topological non-trivial



P. Hosur et al., C. R. Physique **14** (2013) 857

Weyl semimetal (Fermi arc)



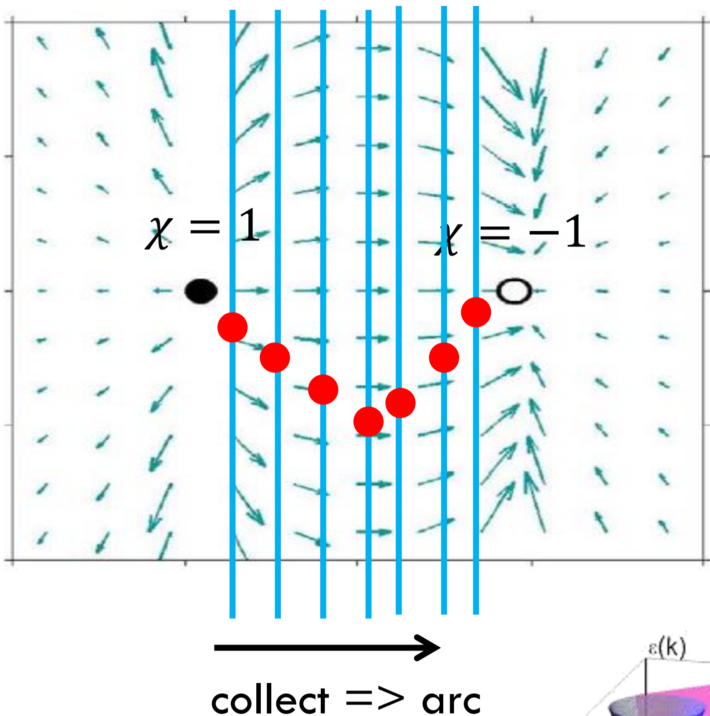


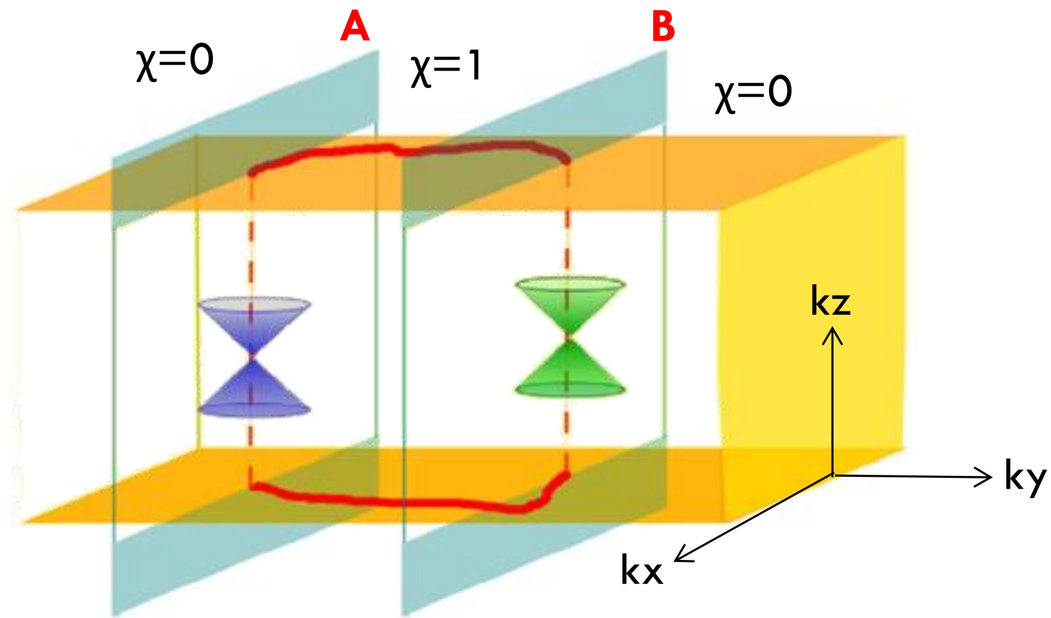
$$\frac{1}{2\pi}\oint_{FS} \boldsymbol{F}(\boldsymbol{k}) \cdot \mathrm{d}\boldsymbol{S}(\boldsymbol{k}) = \chi$$

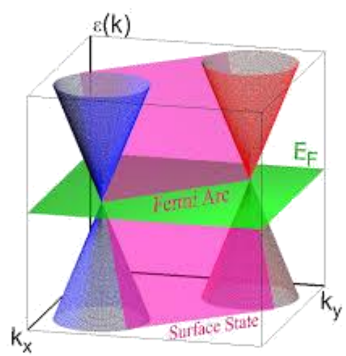
Berry curvature

A: χ=0 => topological trivial => no edge state
B: χ≠0 => topological non-trivial => edge state

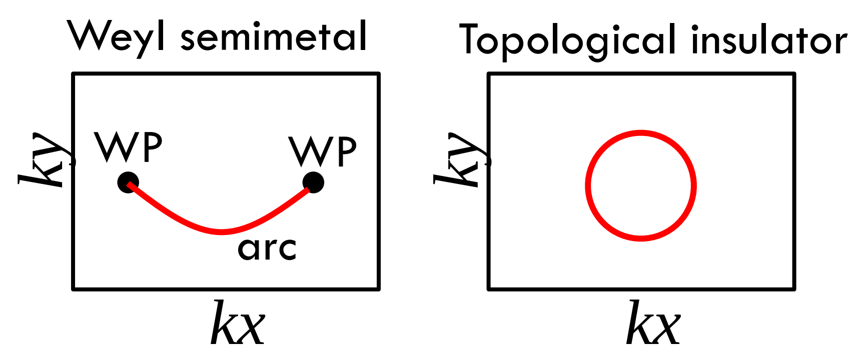
Weyl semimetal (Fermi arc)



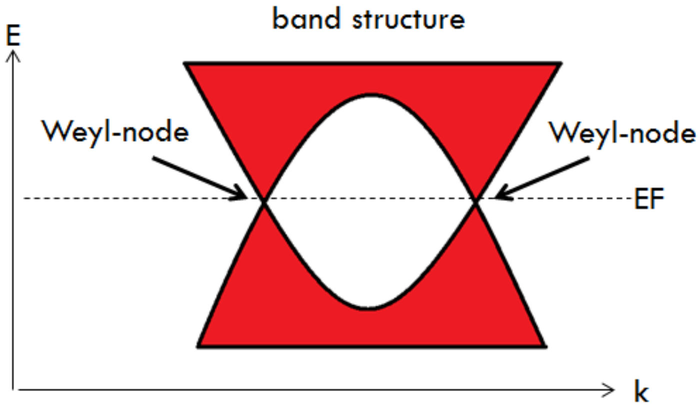


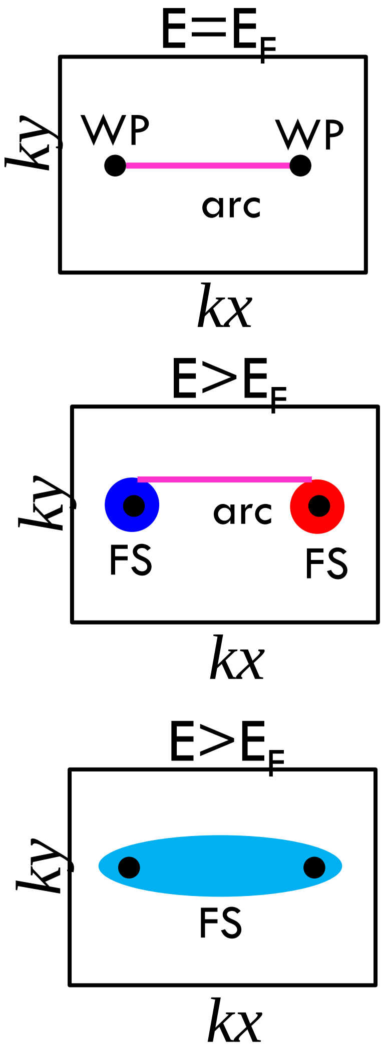


2D Fermi surface



Weyl semimetal (Fermi arc)



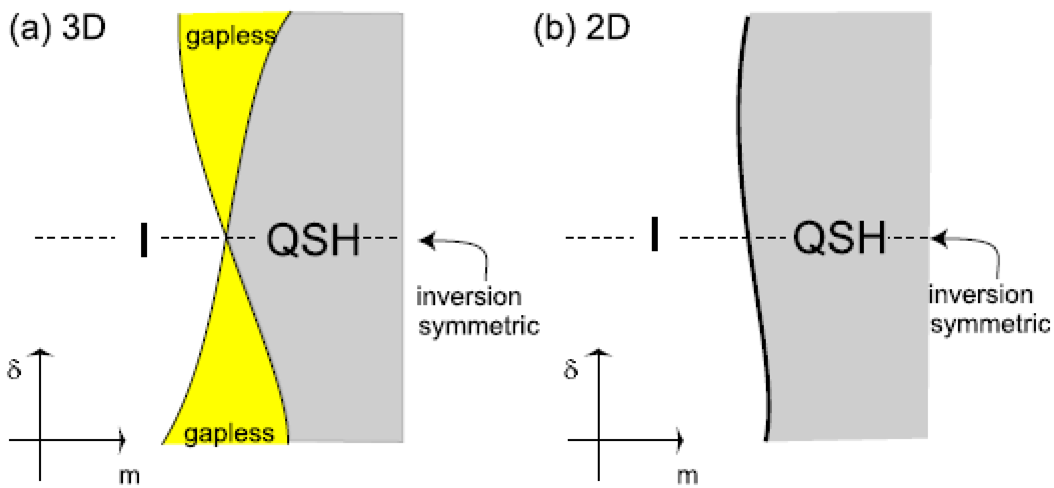


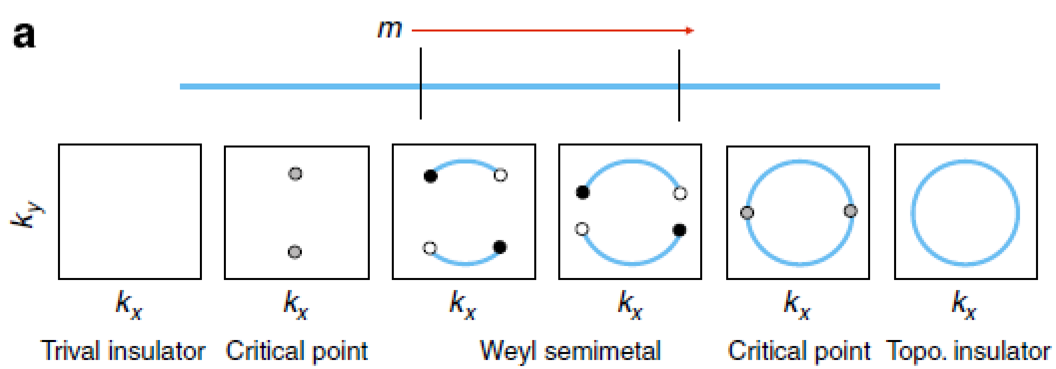
Some features of Weyl semimetal

1. Gapless linear band
2. Spin singly degenerate
3. FS = discrete points
4. Non-zero chiral charge
5. Fermi arc surface state

Previous works

S. Murakami et al., PRB **78**, 165313 (2008)



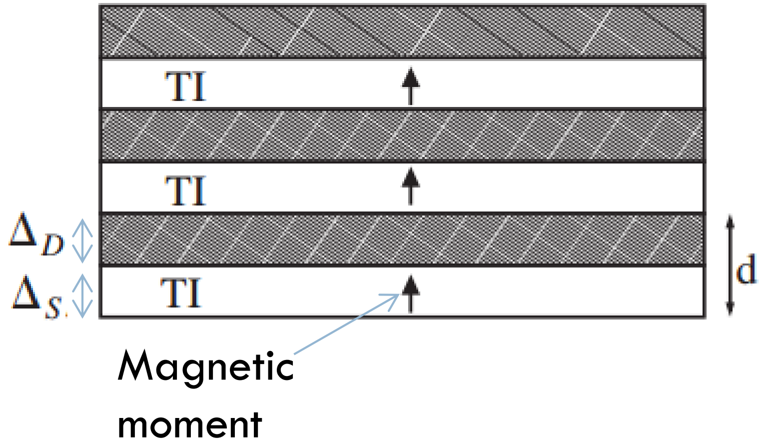


S.-N. Huang et al., Nat. commun. **6**, 7373 (2015)

Previous works

A. A. Burkov et al., PRL **107**, 127205 (2011)

TI-BI superlattice



$m_{c1}^2 = (\Delta_S - \Delta_D)^2 < m^2 < m_{c2}^2 = (\Delta_S + \Delta_D)^2$. Weyl semimetal

$m^2 < m_{c1}^2$ Band insulator

$m^2 > m_{c2}^2$ Topological insulator

Previous works

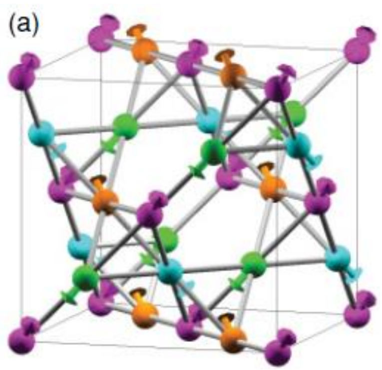
Selected for a Viewpoint in *Physics*

PHYSICAL REVIEW B **83**, 205101 (2011)

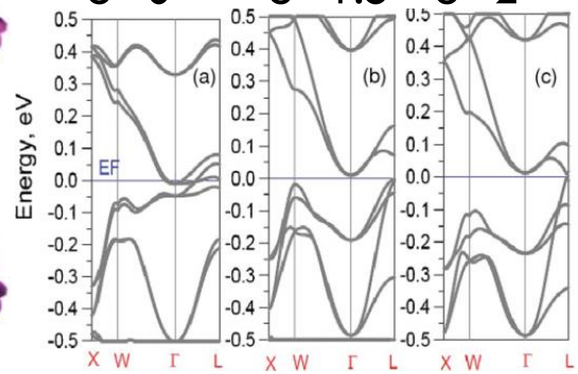
Topological semimetal and Fermi-arc surface states in the electronic structure of pyrochlore iridates

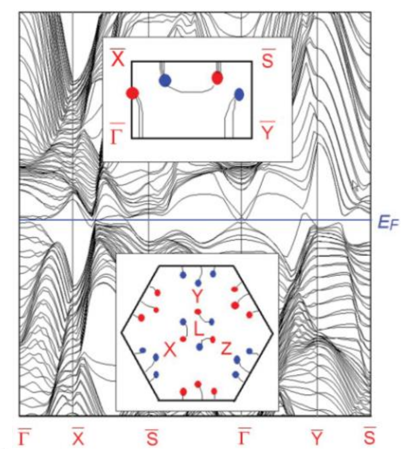
Xiangang Wan,[1] Ari M. Turner,[2] Ashvin Vishwanath,[2,3] and Sergey Y. Savrasov[1,4]

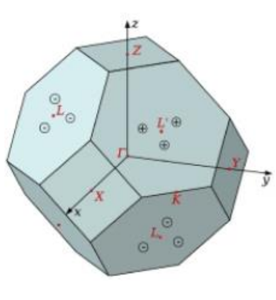
$Y_2Ir_2O_7$

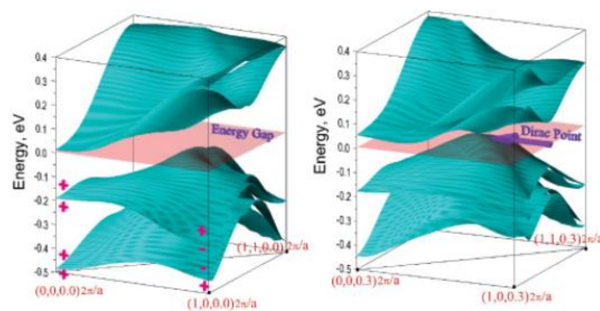


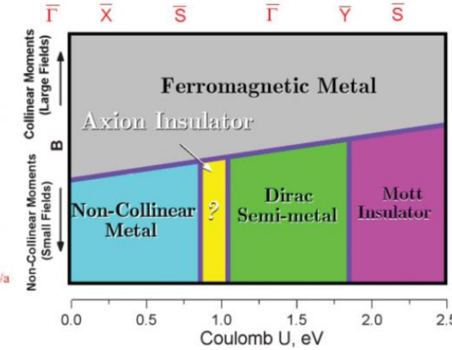
U=0 U=1.5 U=2







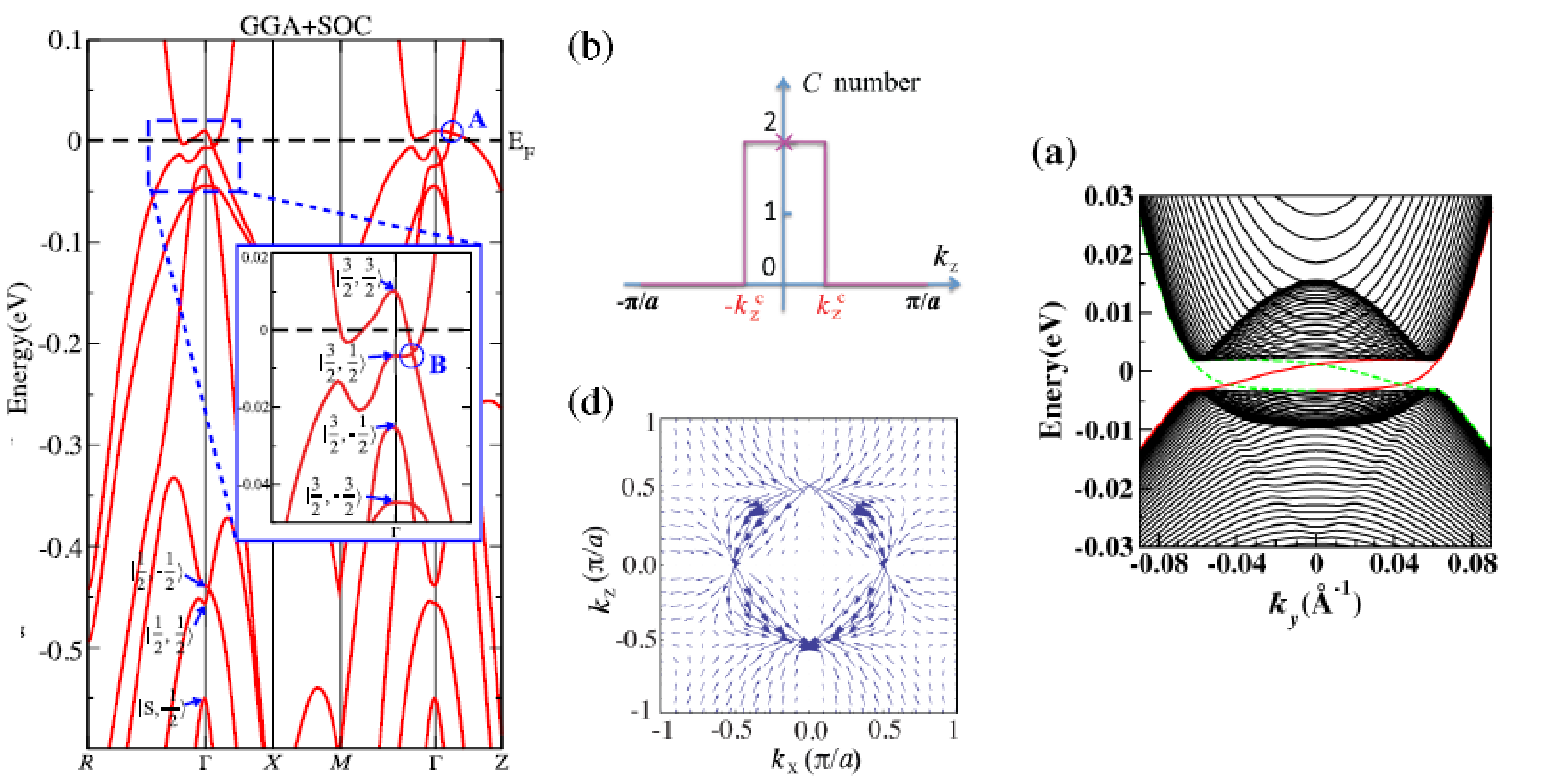




Previous works

PRL 107, 186806 (2011) PHYSICAL REVIEW LETTERS week ending 28 OCTOBER 2011

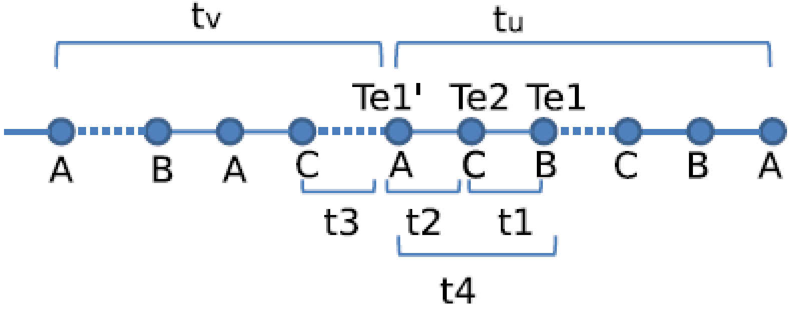
Chern Semimetal and the Quantized Anomalous Hall Effect in $HgCr_2Se_4$

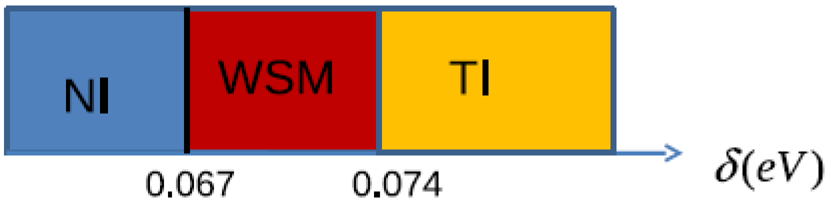


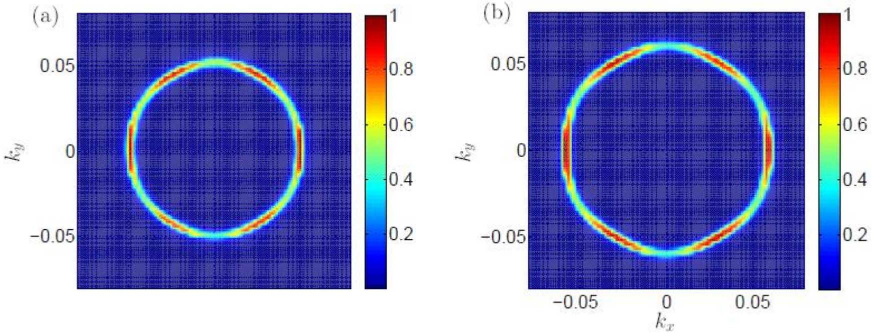
Previous works

J. Liu et al., PRB **90**, 155316 (2014)

$\mathrm{LaBi}_{1-x}\mathrm{Sb}_x\mathrm{Te}_3$ and $\mathrm{LuBi}_{1-x}\mathrm{Sb}_x\mathrm{Te}_3$ for $x \approx 38.5 - 41.9\%$ and $x \approx 40.5 - 45.1\%$ respectively.







The light of hope

ARTICLE

Received 24 Nov 2014 | Accepted 30 Apr 2015 | Published 12 Jun 2015
DOI: 10.1038/ncomms8373
OPEN

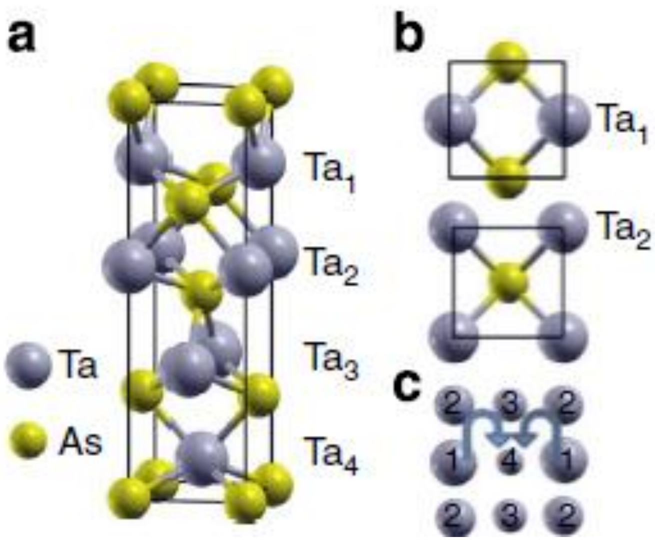
A Weyl Fermion semimetal with surface Fermi arcs in the transition metal monopnictide TaAs class

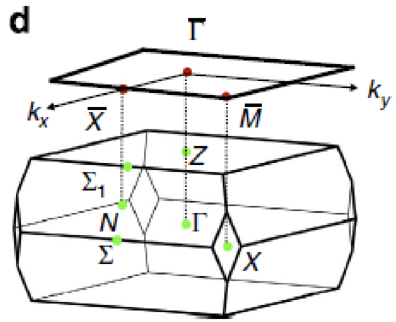
PHYSICAL REVIEW X 5, 011029 (2015)

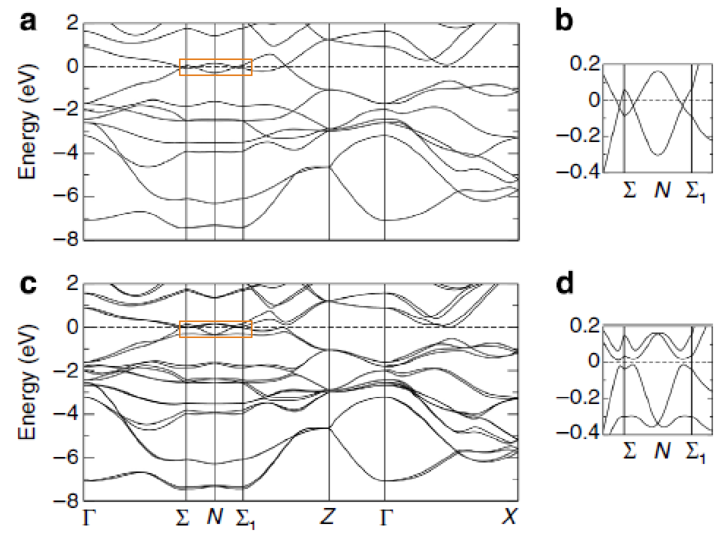
Weyl Semimetal Phase in Noncentrosymmetric Transition-Metal Monophosphides

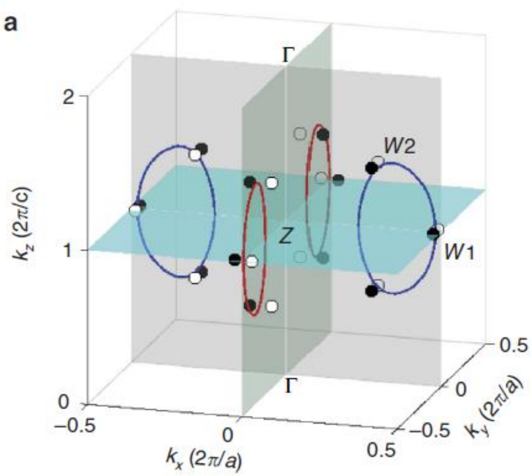
(Received 12 January 2015; published 17 March 2015)

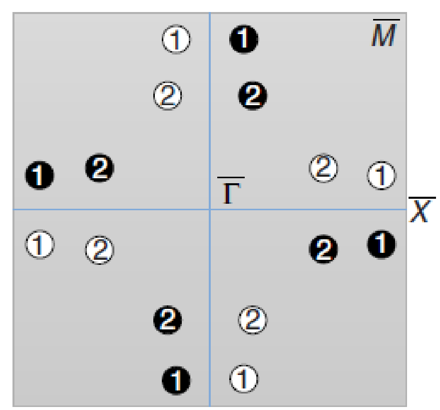
Weyl semimetal: TaAs

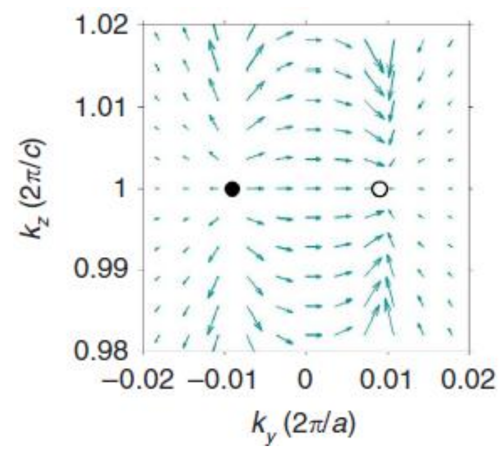




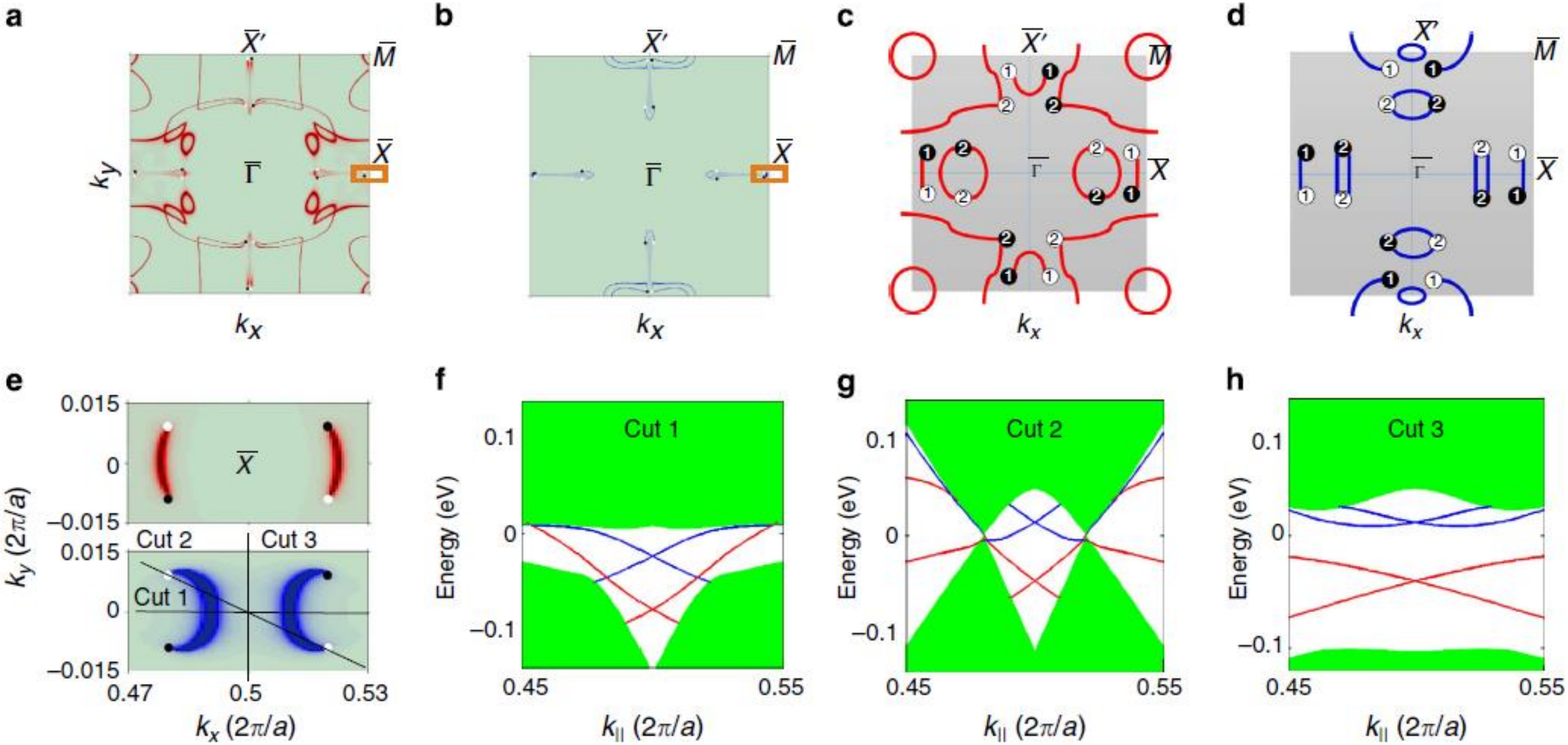








Weyl semimetal: TaAs

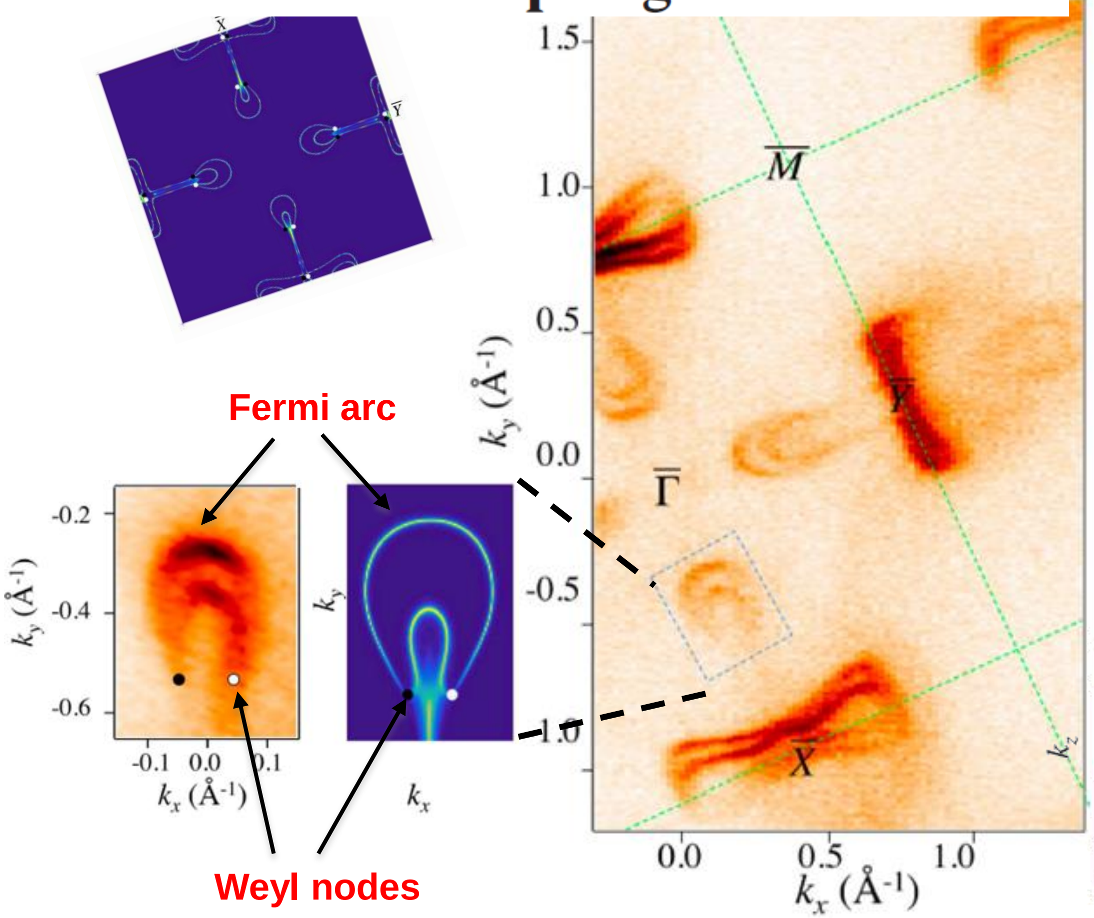


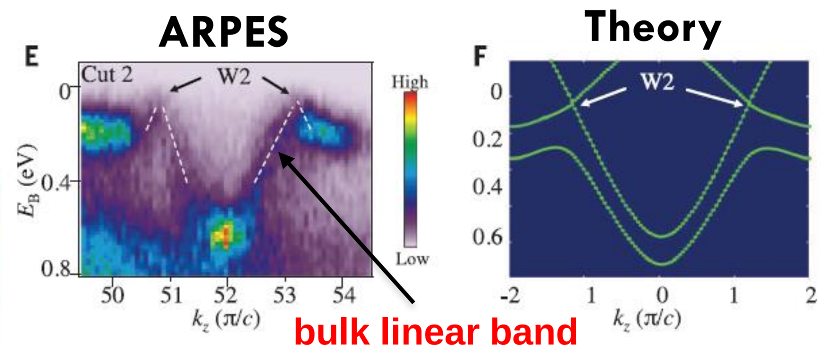
Weyl semimetal: TaAs (ARPES)

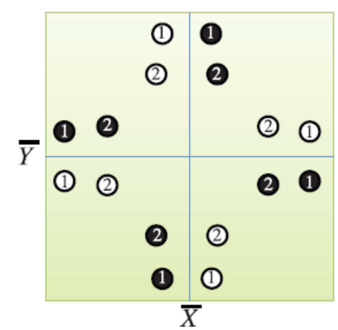
TOPOLOGICAL MATTER

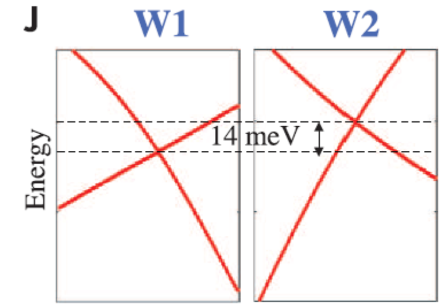
Science **349**, 613 (2015)

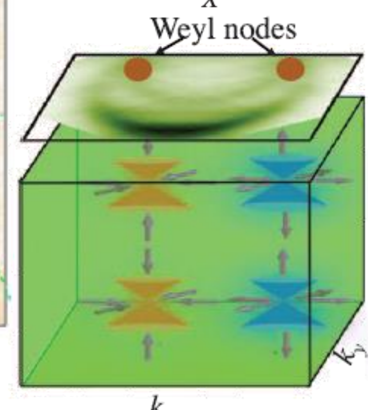
Discovery of a Weyl fermion semimetal and topological Fermi arcs











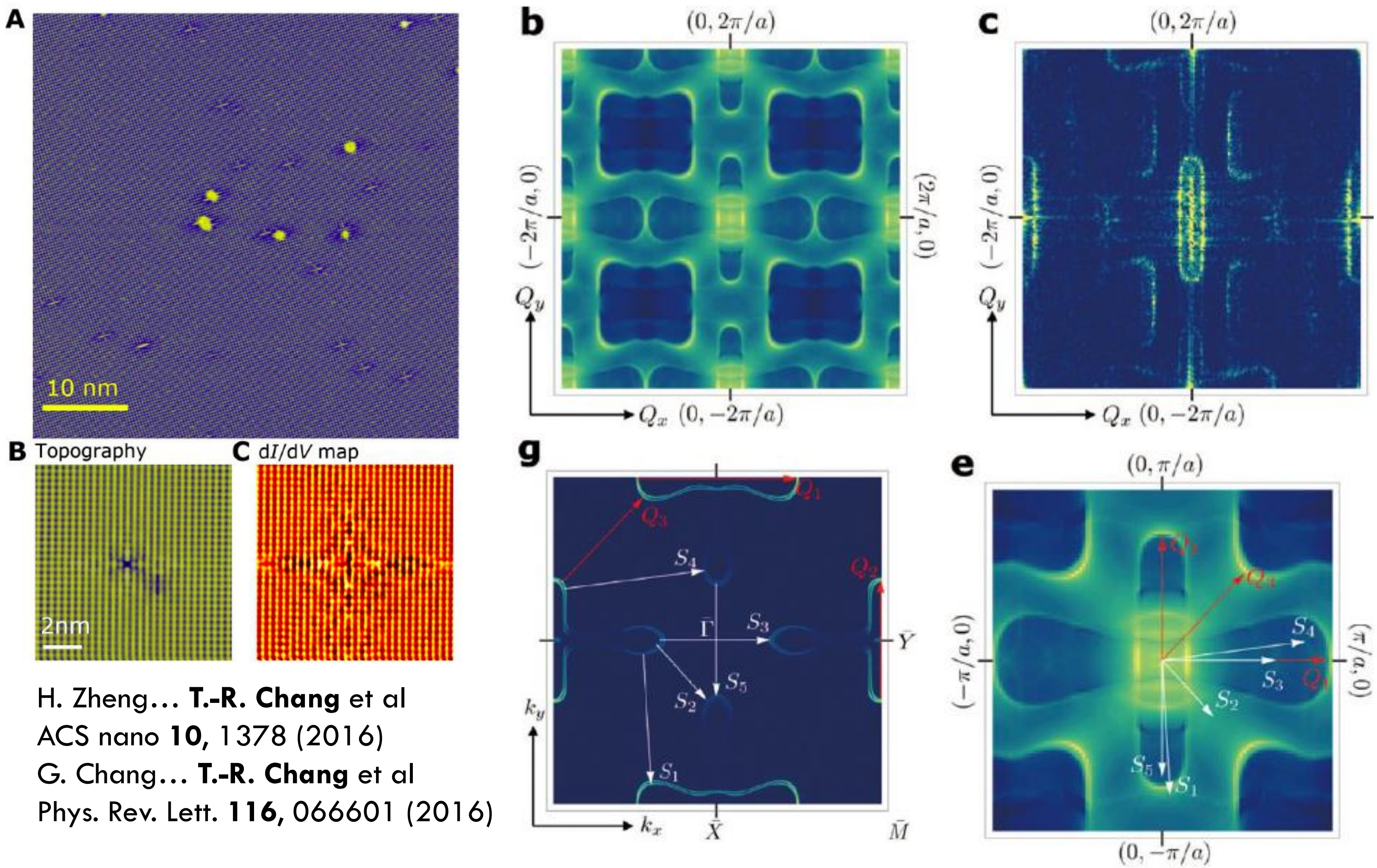
NbAs
S.-Y. Xu… **T.-R. Chang** et al
Nat. Phys. **11**, 748 (2015)

TaP
S.-Y. Xu… **T.-R. Chang** et al
Sci. Adv. **1**, e1051092 (2015)

NbP
I. Belopolski … **T.-R. Chang** et al
PRL **116**, 066802 (2016)

Weyl semimetal: NbP

EXP (STM) | **Theory** | **EXP (QPI)**



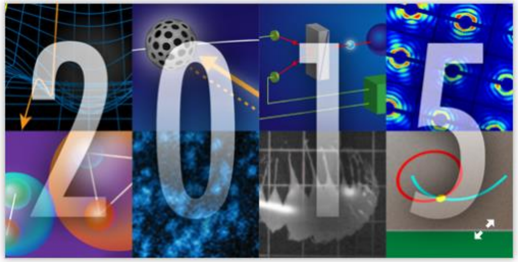
H. Zheng… **T.-R. Chang** et al
ACS nano **10**, 1378 (2016)
G. Chang… **T.-R. Chang** et al
Phys. Rev. Lett. **116**, 066601 (2016)

Highlights of the Year

Highlights of the Year

December 18, 2015 • *Physics* 8, 126

Physics picks its favorite stories from 2015.



Discovery of Weyl Semimetals

APS Physics
2015年7月24日

Two research teams have confirmed the existence of Weyl fermions—massless particles originally theorized as a solution to the Dirac equation. The findings are published in Science (http://go.aps.org/1gSk9EQ & http://go.aps.org/1gSI7RF) and in a forthcoming issue of APS's open access journal Physical Review X (http://go.aps.org/1JCGopq).

翻譯年糕

Weyl fermions are spotted at long last

Solution to the Dirac equation detected 85 years after it was predicted

PHYSICSWORLD.COM

PRINCETON UNIVERSITY | Research A to Z | Contac

Research at Princeton

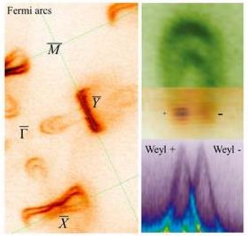
Research Areas
Affiliated National Labs
News & Events
Features
Podcasts
Faculty Focus
Spotlights
In the Media
Events
Featured Video
News Archive
Newsletter
DISCOVERY: Research at Princeton
Celebrate Princeton Invention
REPORTS

News

Discovery of Weyl fermion named a 'breakthrough of the year' by Physics World magazine

Posted Dec 11, 2015 by Catherine Zandonella, Office of the Dean for Research — Share — Print

The discovery of an elusive massless particle theorized 85 years ago has been named one of the Top Ten Breakthroughs of the Year by Physics World magazine. The Weyl fermion, a form of quasiparticle, could give rise to faster and more efficient electronics because of its unusual ability to behave as monopole and anti-monopole inside a crystal.



The magazine honored three groups, M. Zahid Hasan of Princeton University, Marin Soljačić of the Massachusetts Institute of Technology, and Zhong Fang and Hongming Weng of the Chinese Academy of Sciences, for their pioneering work on Weyl fermions.

Princeton University's M. Zahid Hasan, professor

ScienceNews
MAGAZINE OF THE SOCIETY FOR SCIENCE & THE PUBLIC

NEWS CONDENSED MATTER, PARTICLE PHYSICS

Elusive particle shows up in 'semimetal'

Weyl fermions detected in tantalum arsenide

BY ANDREW GRANT 2:00PM, JULY 16, 2015

Magazine issue: Vol. 188, No. 4, August 22, 2015, p. 11

chemistryworld

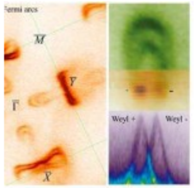
Elusive fermion found at long last

16 July 2015 Ida Emilie Steinmark

TODAY AT BERKELEY LAB

Physics World Names Weyl Fermion Research as a 'Top Ten Breakthrough of 2015'

DECEMBER 16, 2015



Advanced Light Source user M. Zahid Hasan is one of three physicists whose efforts to observe Weyl fermions, an elusive massless particle theorized 85 years ago, were recognized by Physics World. Weyl fermions have been regarded as possible building blocks of other subatomic particles. The top 10 were chosen by a panel of Physics World editors and reporters. More>

physicsworld
TOP 10
BREAKTHROUGH
2015

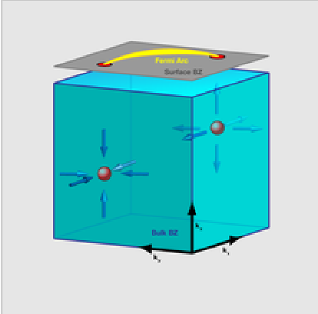
Advertisement

Weyl semimetal

From Wikipedia, the free encyclopedia

Weyl fermions are massless chiral fermions that play an important role in quantum field theory and the standard model. They may be thought of as a building block for fermions in quantum field theory, and were predicted from a solution to the Dirac equation derived by Hermann Weyl.[1] For example, one-half of a charged Dirac fermion of a definite chirality is a Weyl fermion.[2] They have not been observed as a fundamental particle in nature. Weyl fermions may be realized as emergent quasiparticles in a low-energy condensed matter system.[3][4]

Contents [hide]

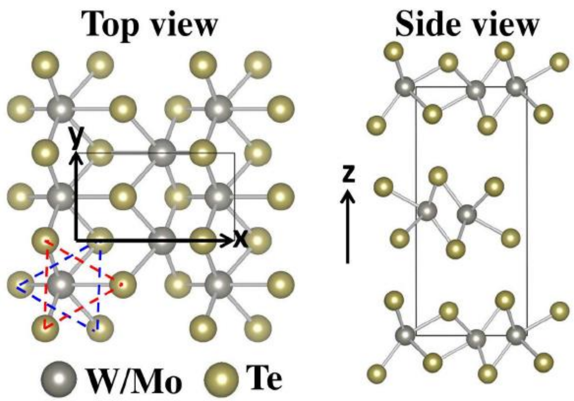


A schematic of the Weyl semimetal state, which include the Weyl nodes and the Fermi arcs. The Weyl nodes are momentum space monopoles and anti-monopoles. The sketch is adapted from Ref.[5]

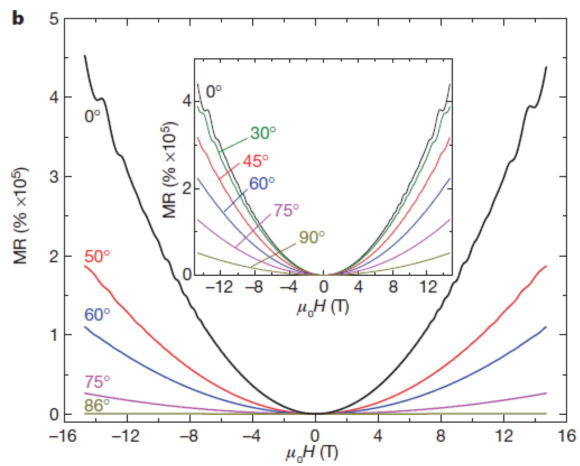
Experimental discovery [edit]

A **Weyl semimetal** is a solid state crystal whose low energy excitations are Weyl fermions.[6][7] A Weyl semimetal enables the first-ever realization of Weyl fermions.[8] It is a topologically nontrivial phase of matter that broadens the topological classification beyond topological insulators.[4] The Weyl fermions at zero energy correspond to points of bulk band degeneracy, the Weyl nodes that are separated in momentum space. Weyl fermions have distinct chiralities, either left handed or right handed. In a Weyl semimetal crystal, the chiralities associated with the Weyl nodes can be understood as topological charges, leading to monopoles and anti-monopoles of Berry curvature in momentum space, which (the splitting) serve as the topological invariant of this phase.[6] Comparing to the Dirac fermions in graphene or on the surface of topological insulators, Weyl fermions in a Weyl semimetal are the most robust electrons and do not depend on symmetries except the translation symmetry of the crystal lattice. Hence the Weyl fermion quasiparticles in a Weyl semimetal possess a

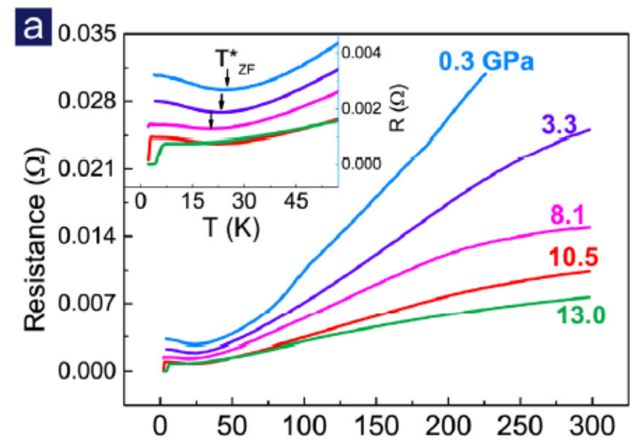
WTe_2: Weyl candidate



M. N. Ali et al, Nature **514**, 205 (2014)



D. Kang et al., Nat. com. **6**, 7804 (2015)



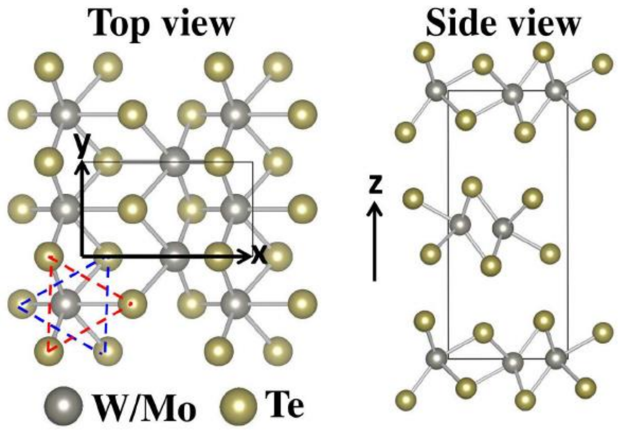
PRB **58**, 2788 (1998)

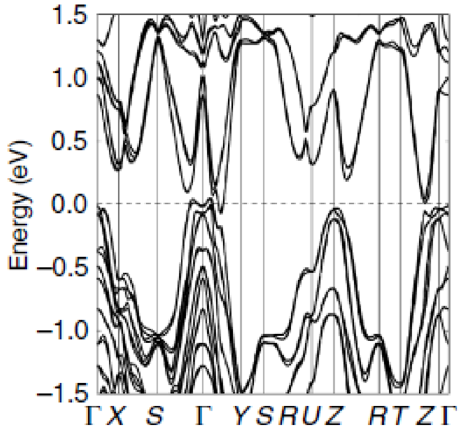
Quantum magnetoresistance

A. A. Abrikosov
Materials Science Division, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, Illinois 60439
(Received 26 September 1997; revised manuscript received 9 March 1998)

An explanation is proposed of the unusual magnetoresistance, linear in magnetic field and positive, observed recently in nonstoichiometric silver chalcogenides. The idea is based on the assumption that these substances are basically gapless semiconductors with a linear energy spectrum. Most of the excess silver atoms form metallic clusters which are doping the remaining material to a very small carrier concentration, so that even in a magnetic field as low as 10 Oe, only one Landau band participates in the conductivity.

WTe_2: Weyl candidate

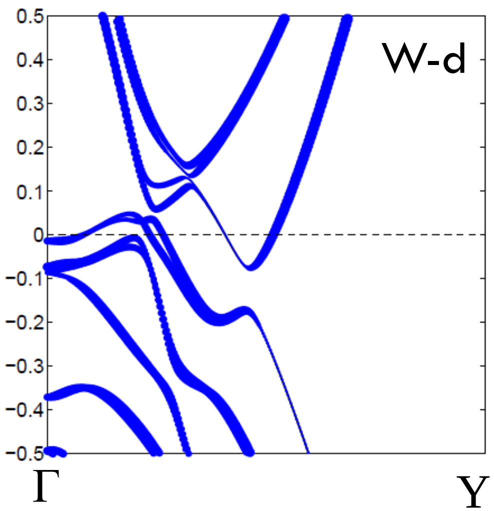


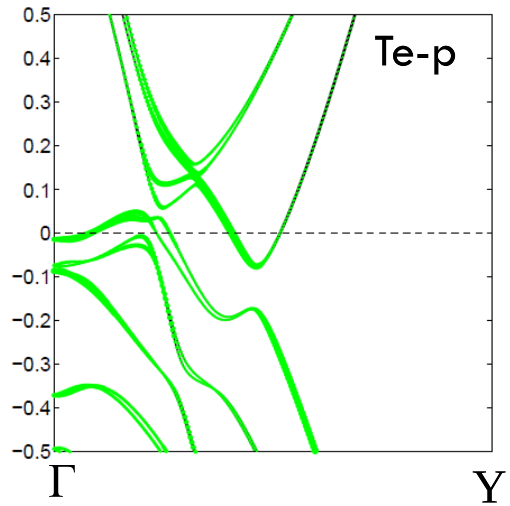


Symmetry operation of WTe_2

1. C_2 (glide)
2. ky=0 mirror
3. kx=0 mirror (glide)
4. time-reversal

no inversion symmetry



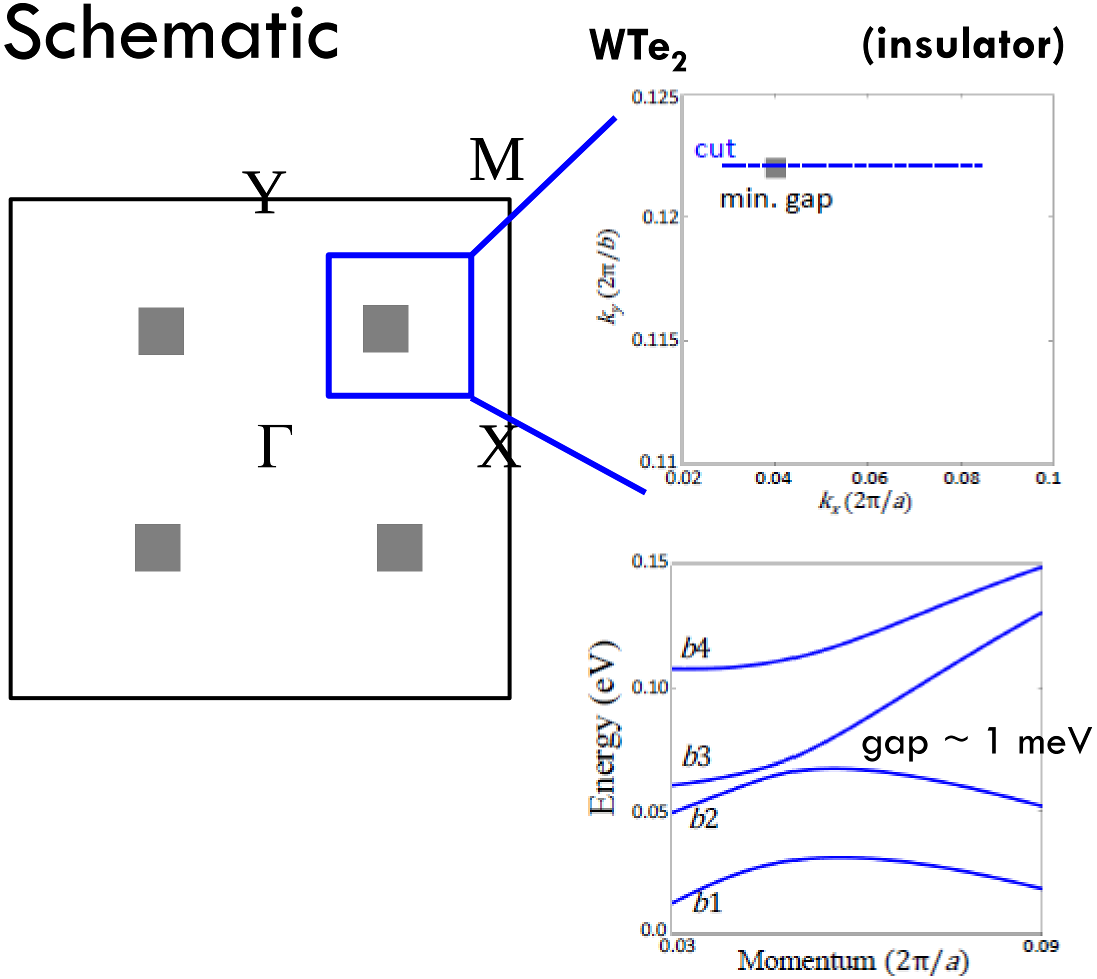


Weyl candidate

- No crystal inversion symmetry
- SOC band inversion gap on mirror plane

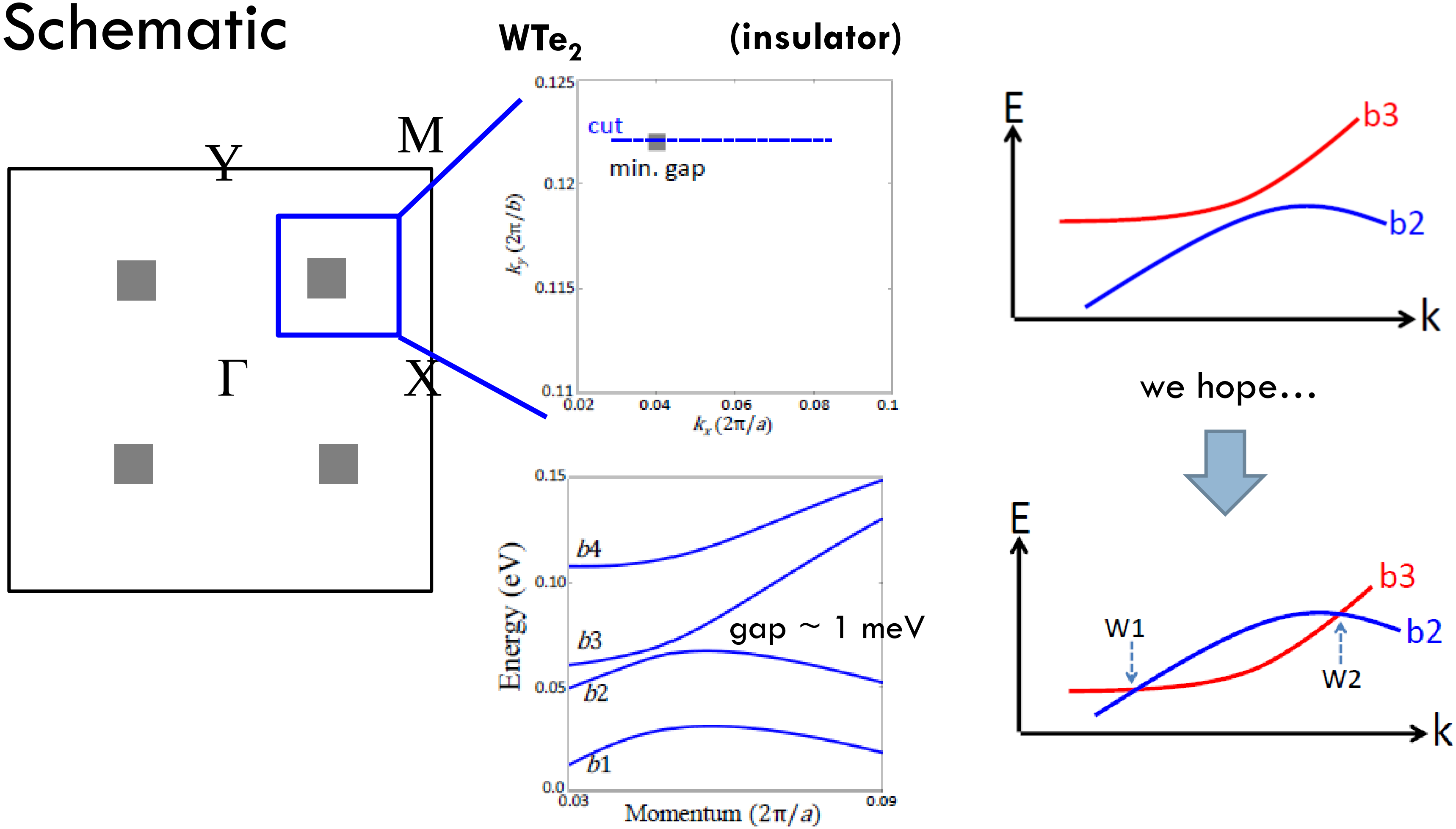
WTe_2: Weyl candidate

Schematic



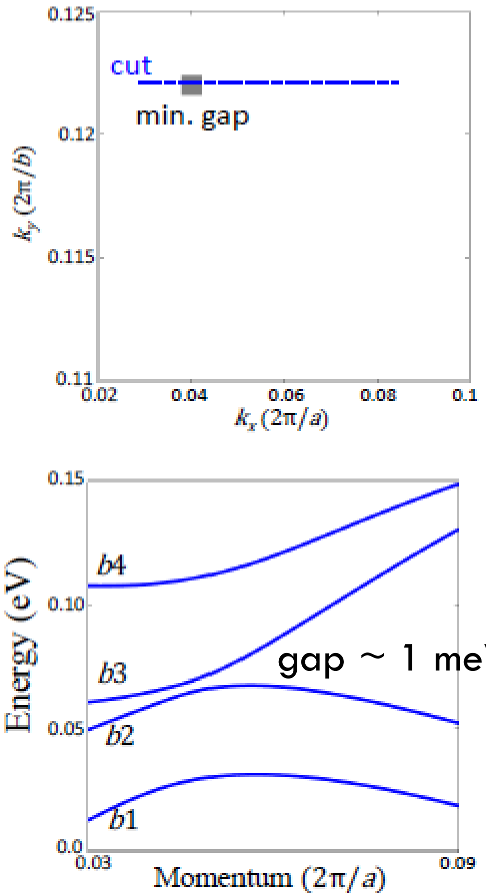
WTe_2: Weyl candidate

Schematic



Weyl state in $Mo_xW_{1-x}Te_2$

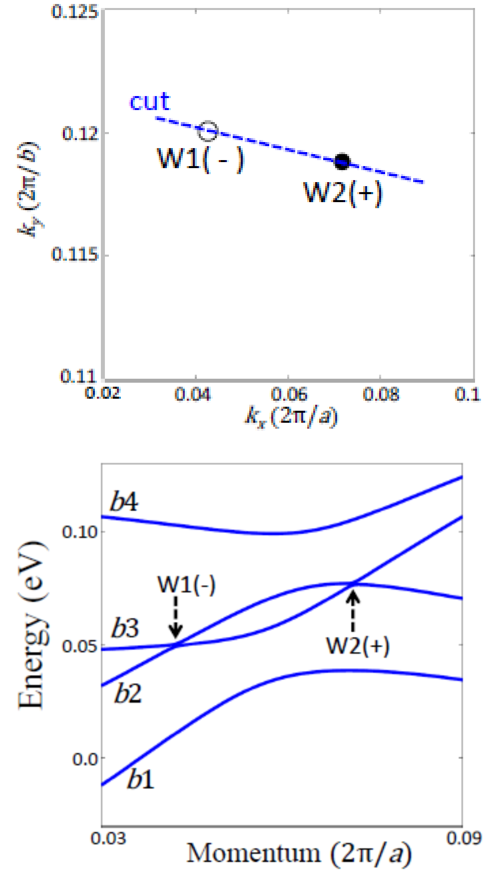
WTe_2 (insulator)



reduce strength of SOC
and/or
lattice constants
=> Weyl phase in WTe_2

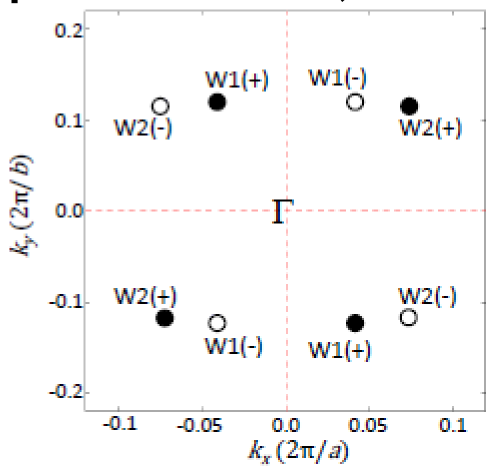
Mo doping

$Mo_{0.2}W_{0.8}Te_2$ (Weyl)

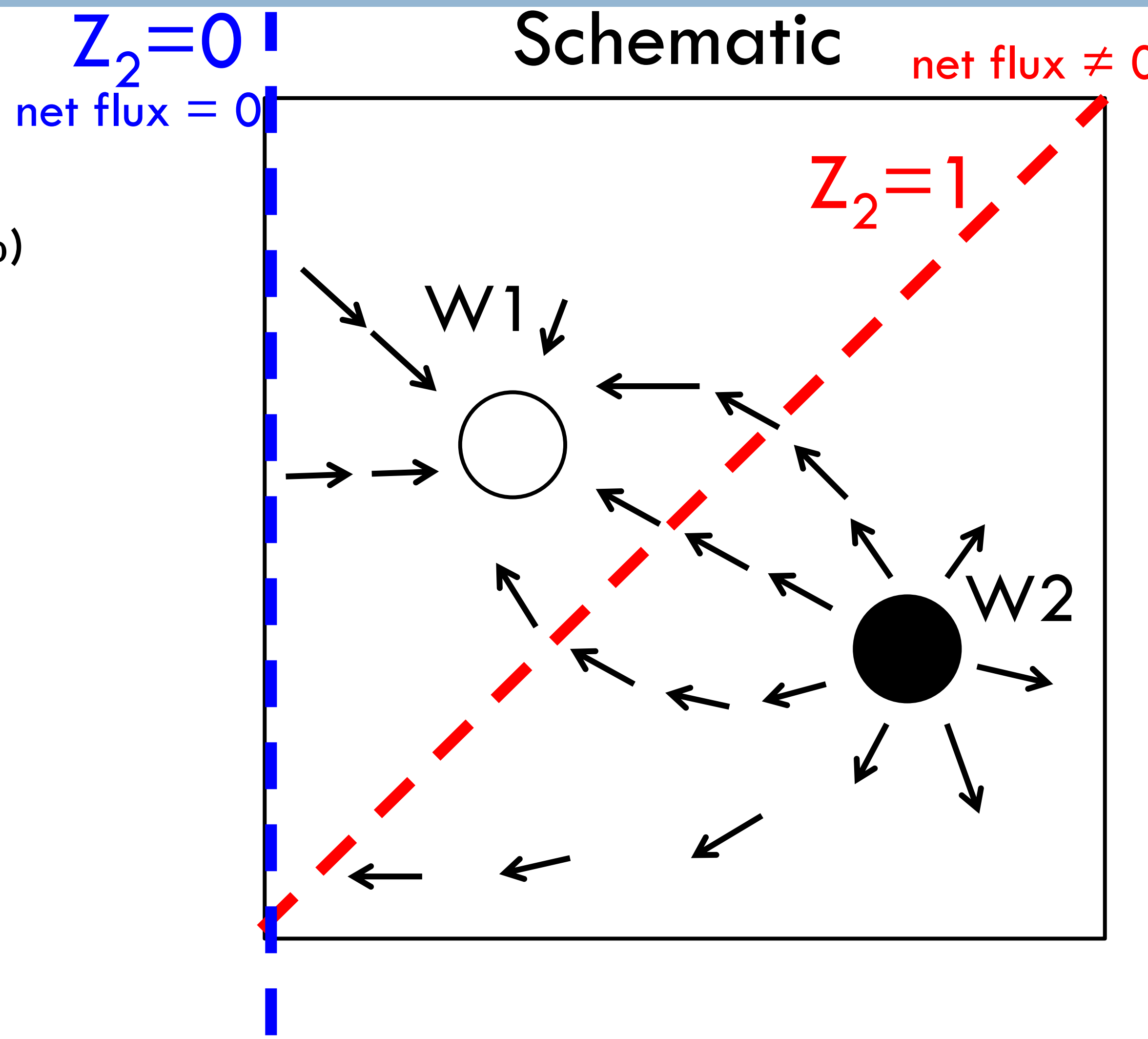


Weyl state in $Mo_xW_{1-x}Te_2$

position of WPs (Mo 20%)

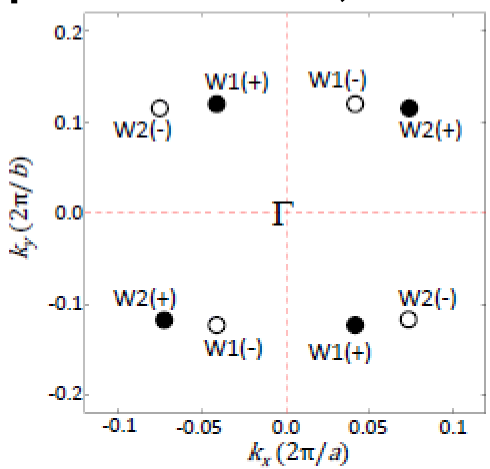


$C_{2T}=C_2{*}T$



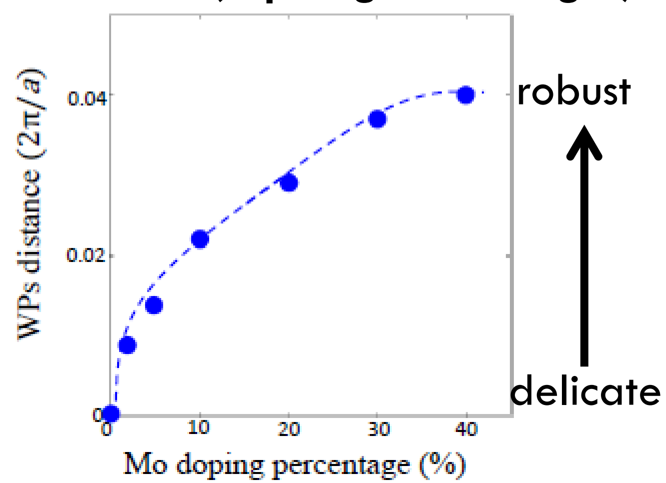
Weyl state in $Mo_xW_{1-x}Te_2$

position of WPs (Mo 20%)

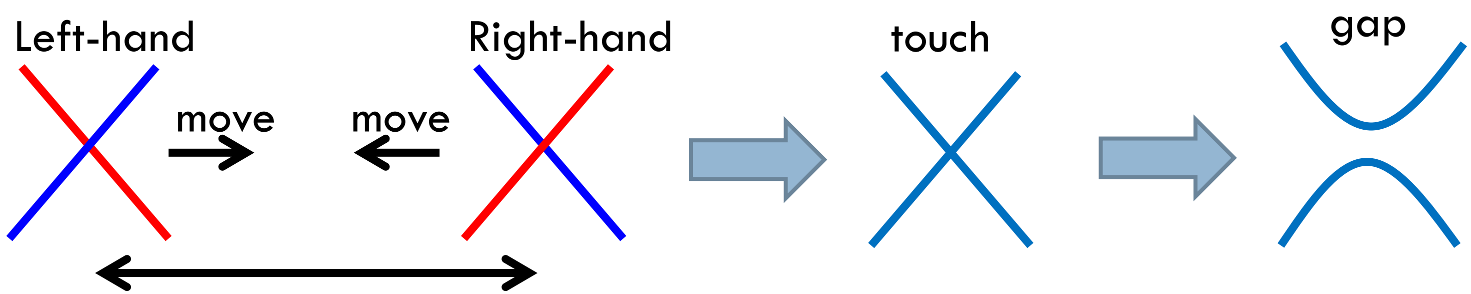


$C_{2T}=C_2{*}T$

WPs distance (topological strength)



topological strength can be tuned by varying Mo doping concentration

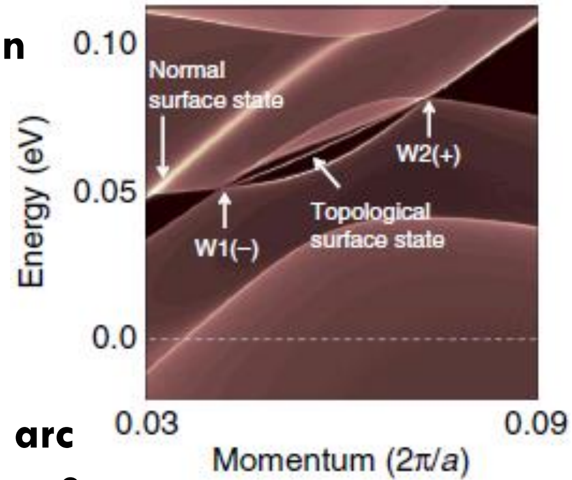


WPs distance = topological strength

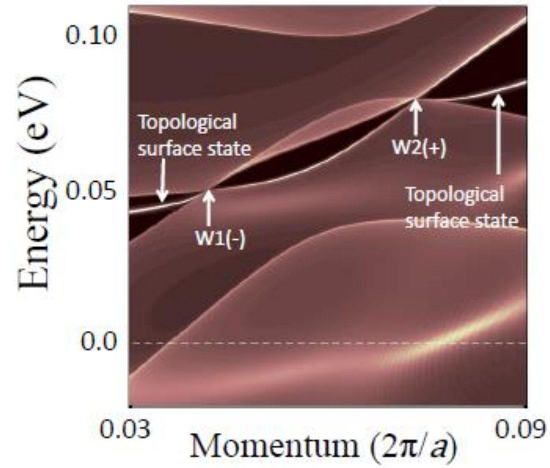
Weyl state in $Mo_xW_{1-x}Te_2$

Surface spectral weight simulation

surface onsite = 0

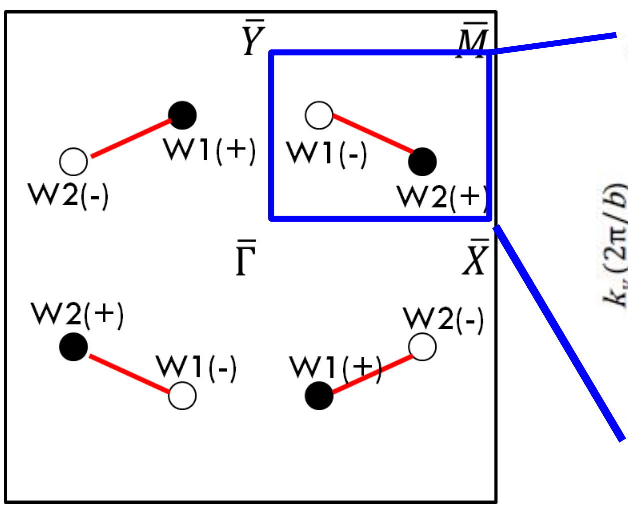


surface onsite = -0.11 eV

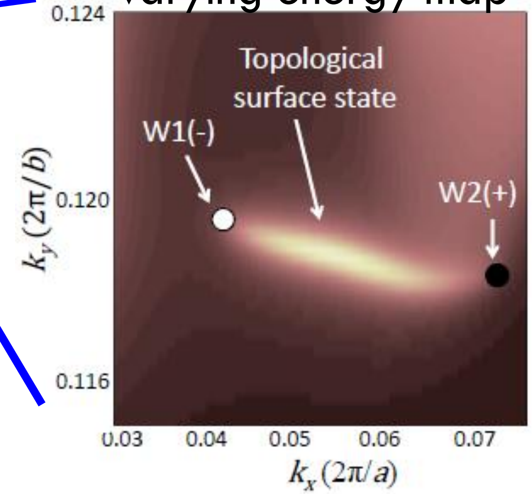


Schematic of Fermi arc

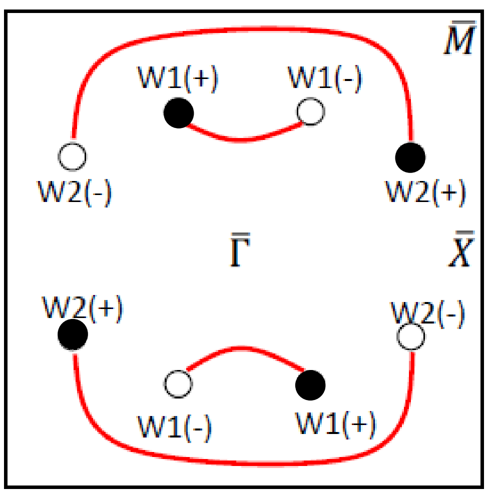
surface onsite = 0



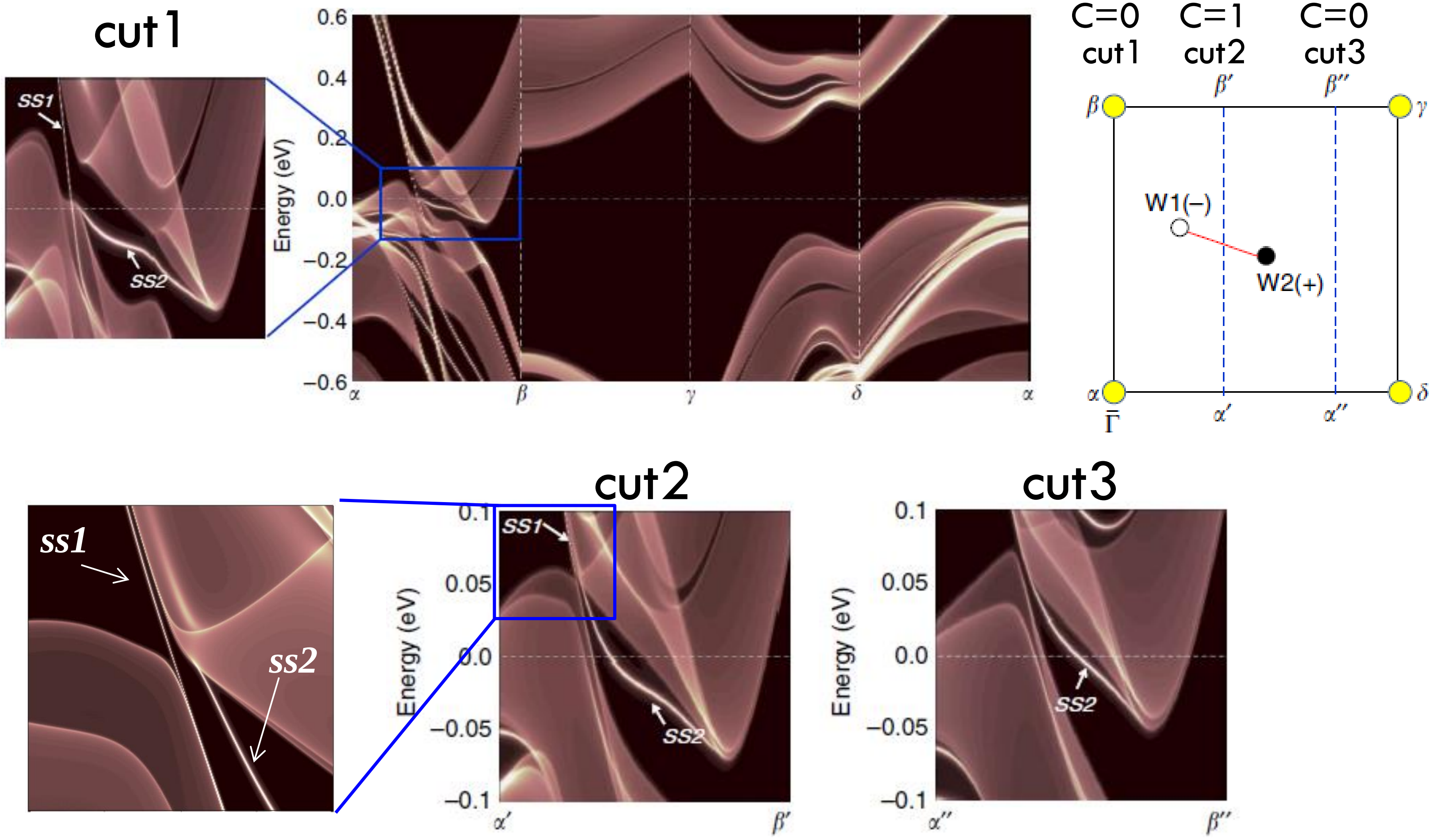
varying energy map



surface onsite = -0.11 eV



Weyl state in $Mo_xW_{1-x}Te_2$



nature COMMUNICATIONS

ARTICLE

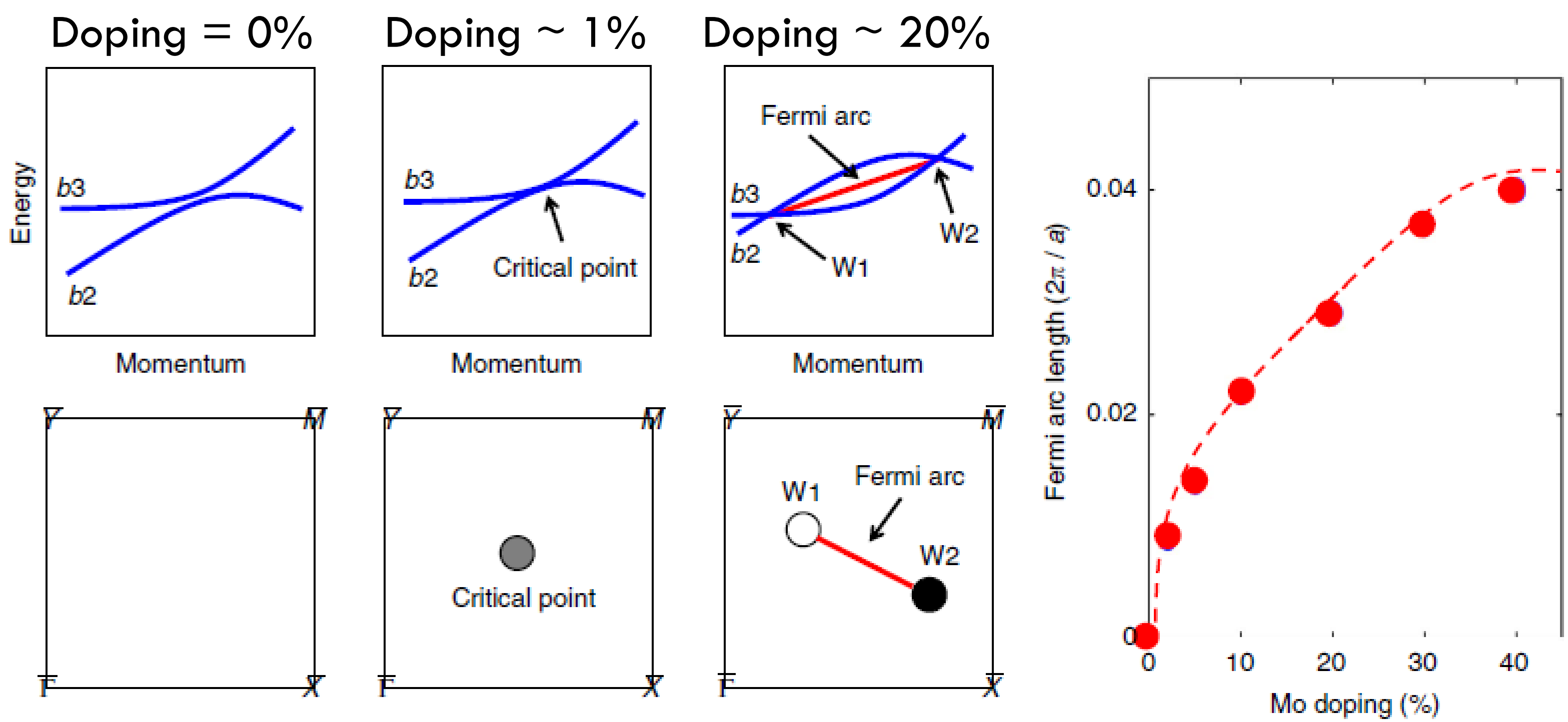
Received 23 Sep 2015 | Accepted 7 Jan 2016 | Published 15 Feb 2016

DOI: 10.1038/ncomms10639

OPEN

Prediction of an arc-tunable Weyl Fermion metallic state in $Mo_xW_{1-x}Te_2$

Tay-Rong Chang *et al. Nat. Commun.* ***7****, 10639 (2016)*



topological strength can be tuned by varying Mo doping concentration

Weyl state in $Mo_xW_{1-x}Te_2$

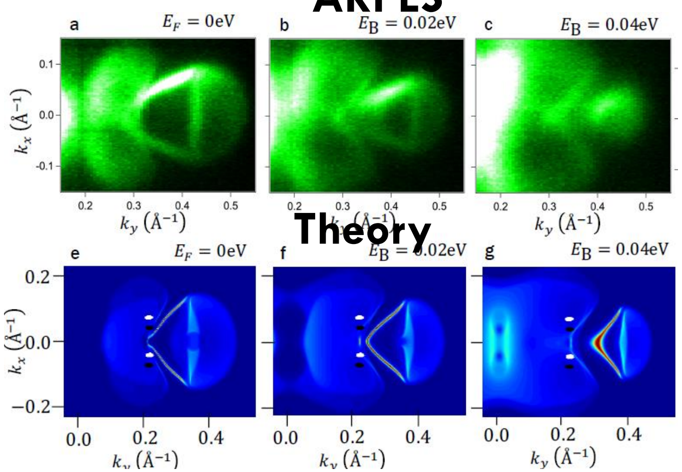
arXiv.org > cond-mat > arXiv:1604.07079

Condensed Matter > Mesoscale and Nanoscale Physics

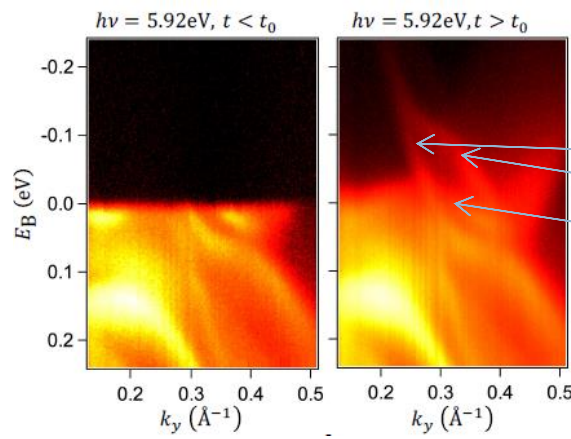
Measuring Chern numbers above the Fermi level in the Type II Weyl semimetal $Mo_xW_{1-x}Te_2$

*I. Belopolski … **T.-R. Chang** et al*

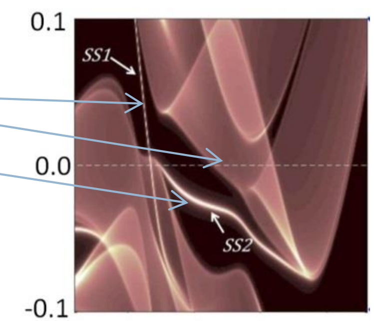
ARPES



time-resolve ARPES



Theory



$MoWTe_2$ is a Weyl semimetal
arXiv:1604.01706, arXiv:1603.08508, arXiv:1604.00139, arXiv:1604.04218, arXiv:1604.02116, and arXiv:1604.07079

Type-II Weyl semimetal

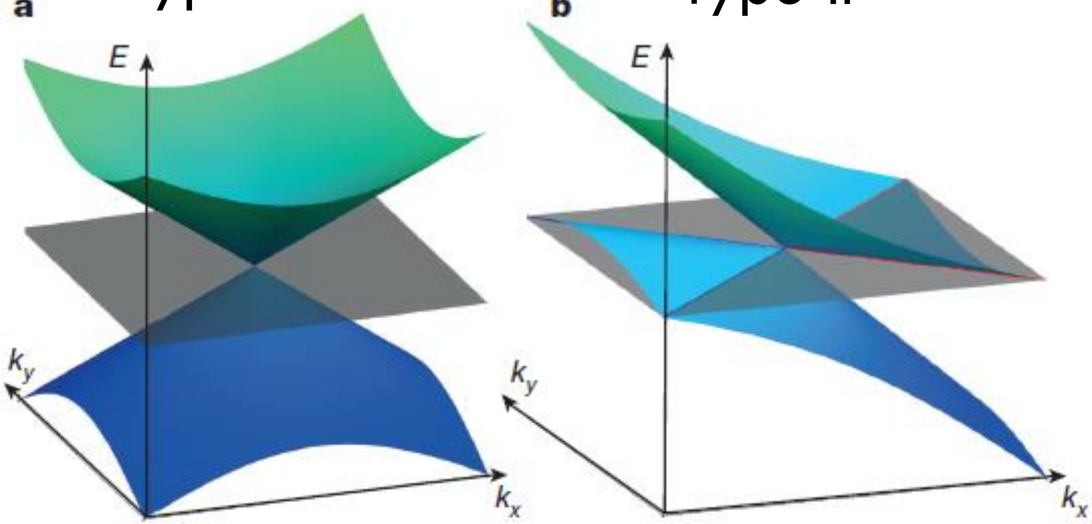
LETTER

doi:10.1038/nature15768

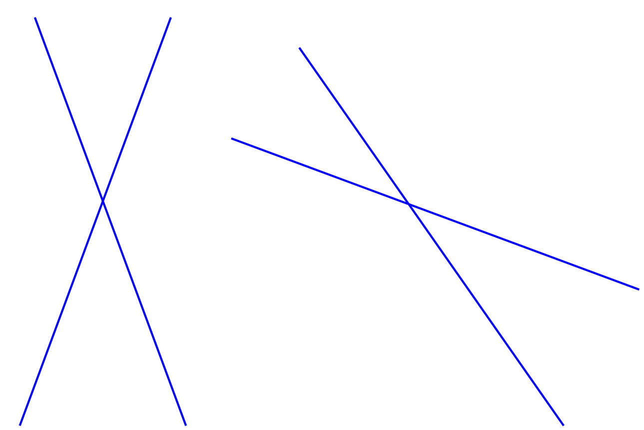
Type-II Weyl semimetals

Alexey A. Soluyanov[1], Dominik Gresch[1], Zhijun Wang[2], QuanSheng Wu[1], Matthias Troyer[1], Xi Dai[3] & B. Andrei Bernevig[2]

Type-I Type-II



Type-I Type-II



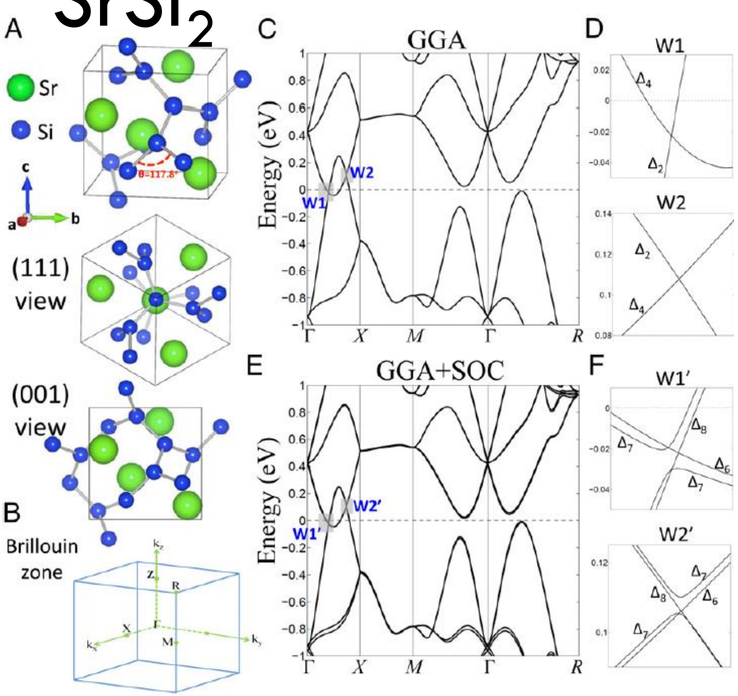
Weyl+symmetry: High chiral charge

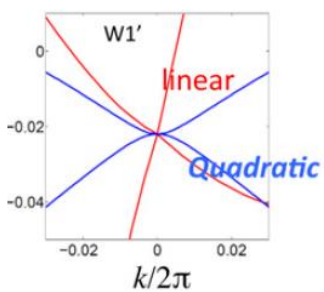
1180–1185 | PNAS | February 2, 2016 | vol. 113 | no. 5

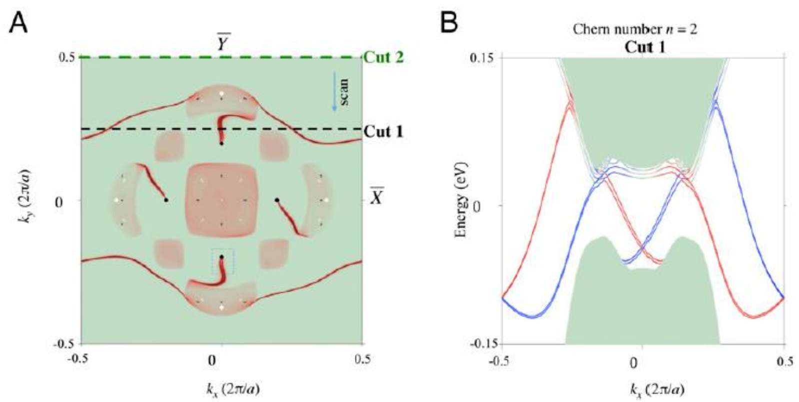
New type of Weyl semimetal with quadratic double Weyl fermions

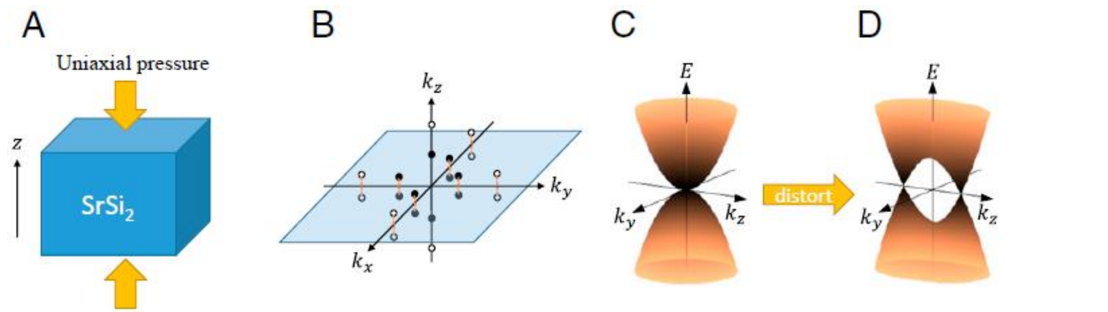
*S.-M. Huang … **T.-R. Chang** et al*

$SrSi_2$

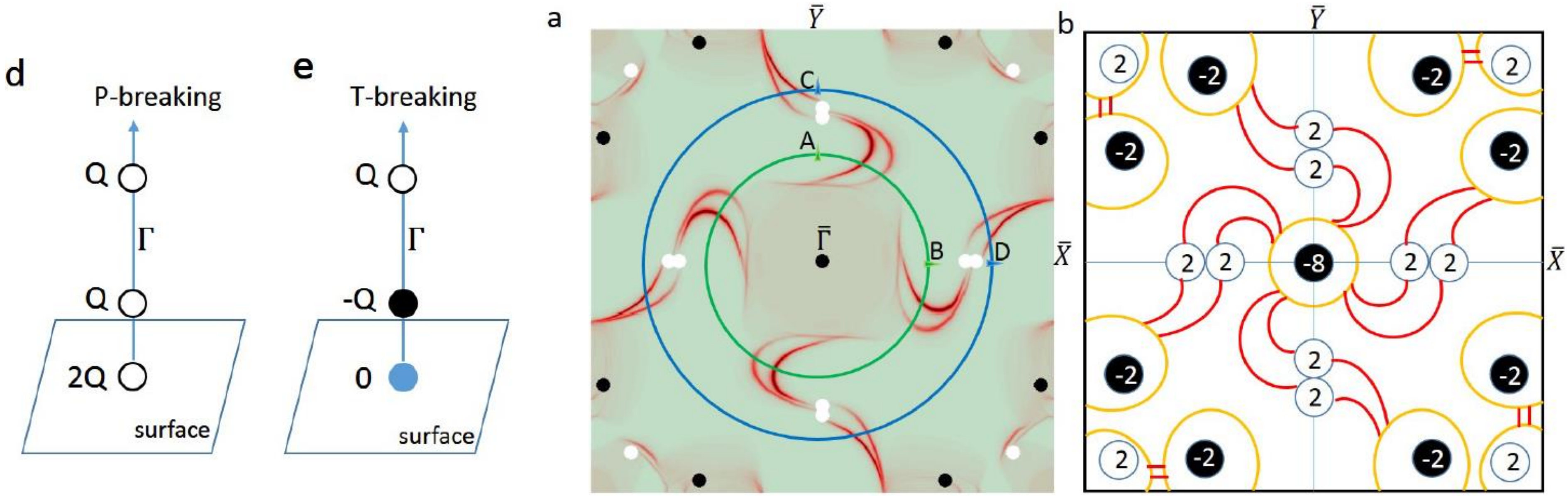








Weyl+symmetry: High chiral charge



Nodal-line semimetal

1. Introduction

Band theory

Topology in condensed matter physics

Basics properties: Robust, invariant number, gapless surface states

Comparing with Landau's approach

Density functional theory (DFT)

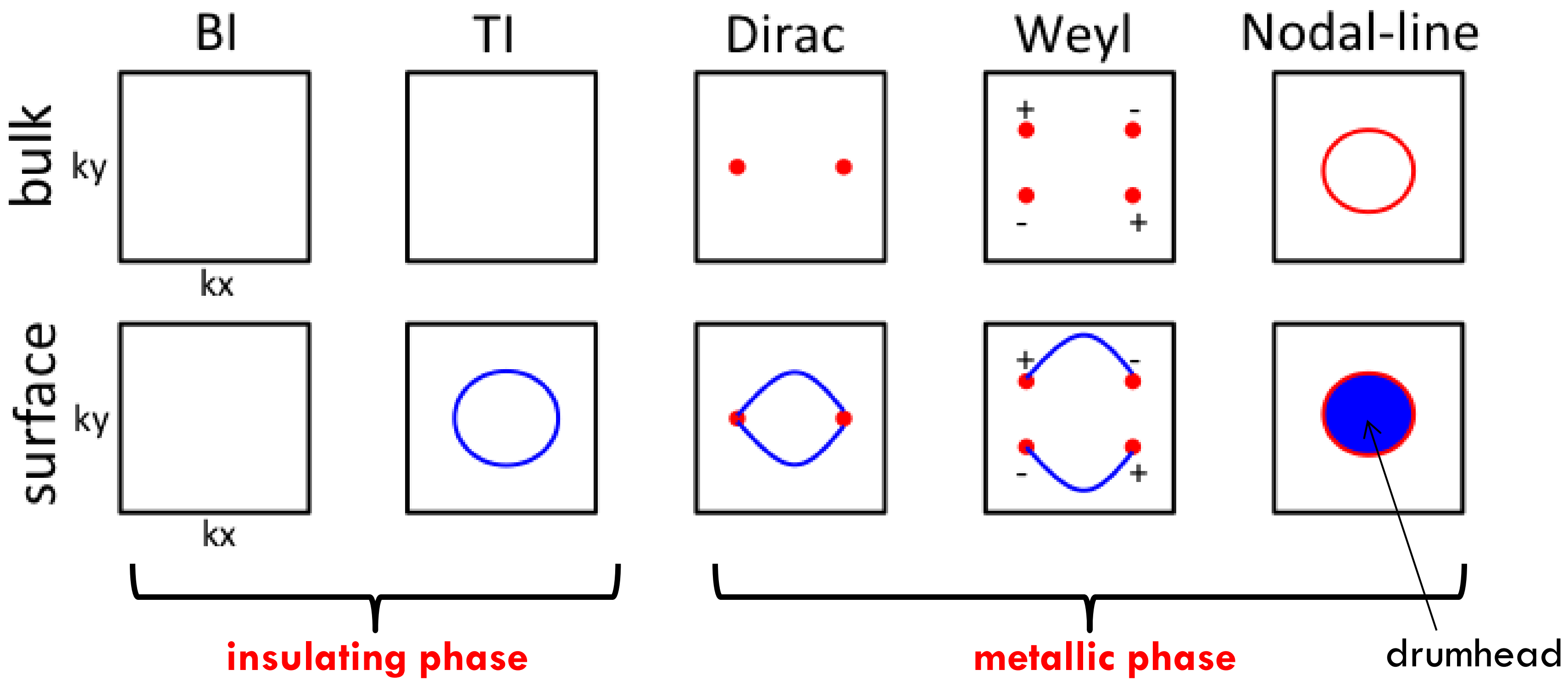
2. Topological insulator (quantum spin Hall insulator)

Strong topological insulator, weak topological insulator, topological crystalline insulator, topological Kondo insulator, quantum anomalous Hall effect…etc

3. Topological semimetal

3D Dirac semimetal, Weyl semimetal, Nodal-line semimetal, topological superconductor, New Fermion

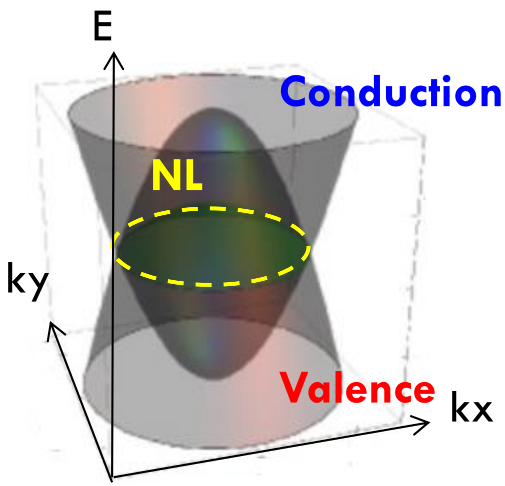
Topological phases

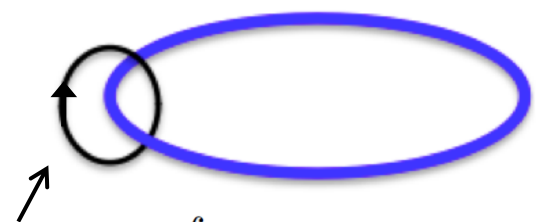


Red: bulk bands

Blue: surface bands

Nodal-line semimetal: topology





$$\gamma = i\oint_C \langle \psi(\mathbf{k})|\nabla\psi(\mathbf{k})\rangle \cdot \mathrm{d}\mathbf{k}$$

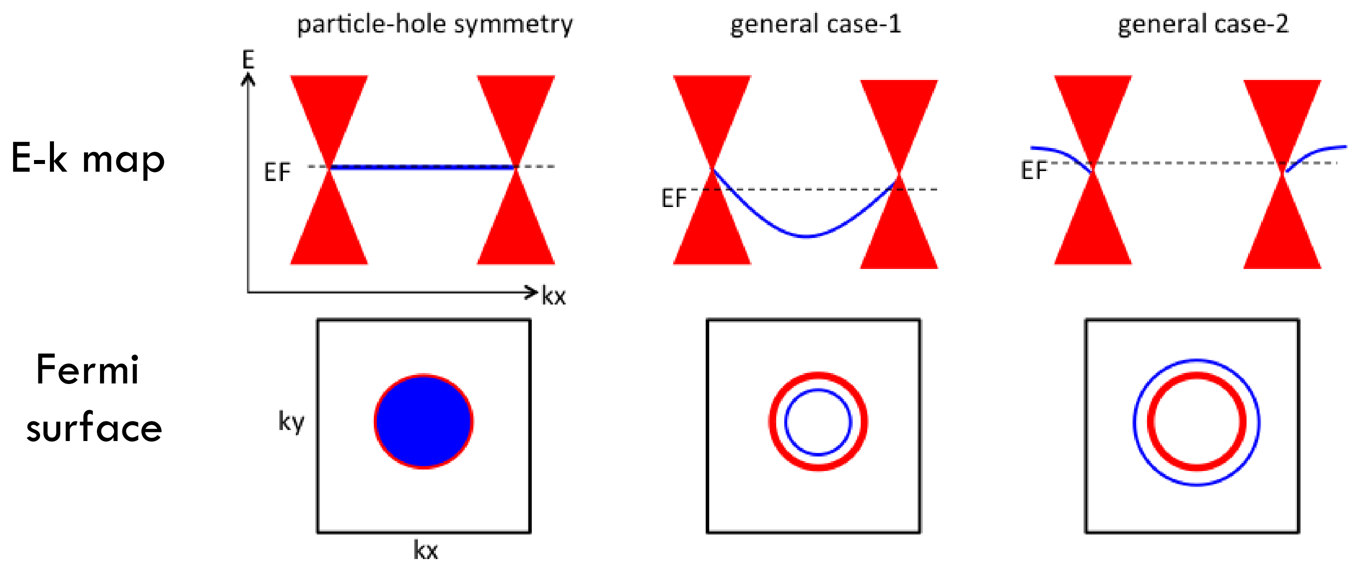
Chan *et al.*, arXiv:1510.02759 (2015)

winding number

$g/p = \pm 1$

bulk-boundary correspondece

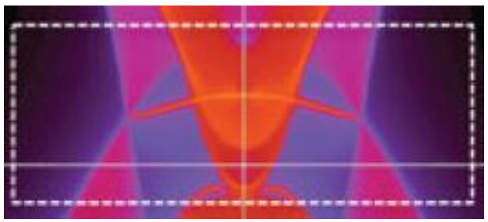
topo. surface states



Previous works

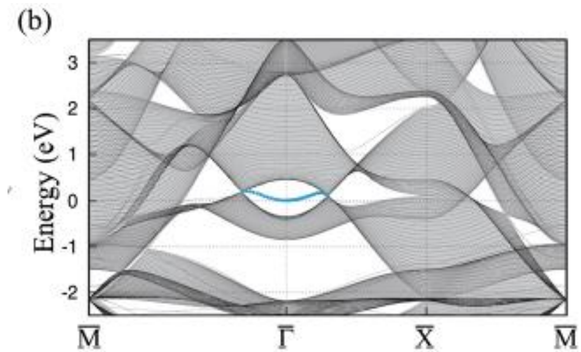
Cu_3PdN
PRL **115**, 036807 (2015)

without SOC

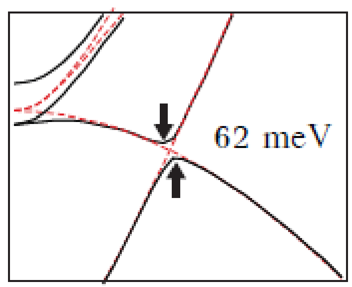


with SOC

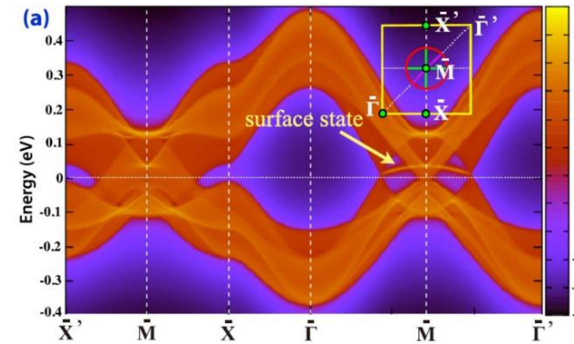
Cu_3ZnN
PRL **115**, 036806 (2015)



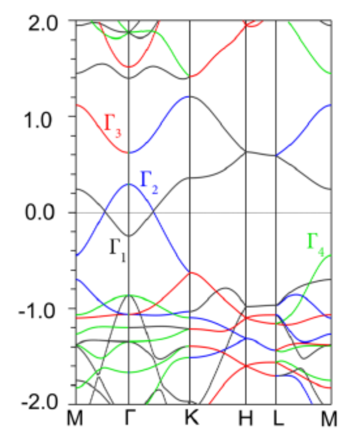
SOC gap



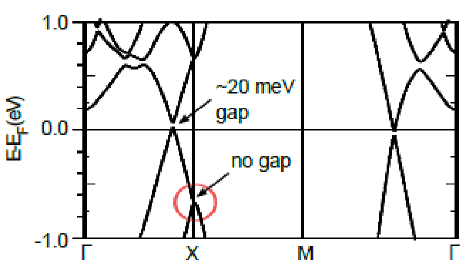
Graphene Networks
PRB **92**, 045108 (2015)



Ca_3P_2
APL Mat. **3**, 083602 (2015)



ZrSiS
arXiv:1509.00861 (2015)



Without SOC => Nodal-Line

With SOC => gap (or partially gapless)

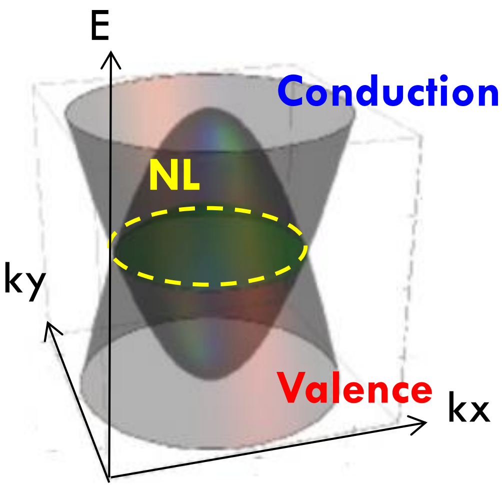
Strategy

(1) Layer structure
avoid complex 3D band structure

(2) Breaking either time-reversal symmetry or inversion symmetry
coexistence of both TR and I symmetries is too restrictive for a line touching to occur

(3) planer-like crystalline symmetry
rotational symmetry protect a part of band touching points

Simplest case:
the crossing points of two paraboloids bands.



Nodal-line candidate

RAPID COMMUNICATIONS

PHYSICAL REVIEW B **89**, 020505(R) (2014)

Noncentrosymmetric superconductor with a bulk three-dimensional Dirac cone gapped by strong spin-orbit coupling

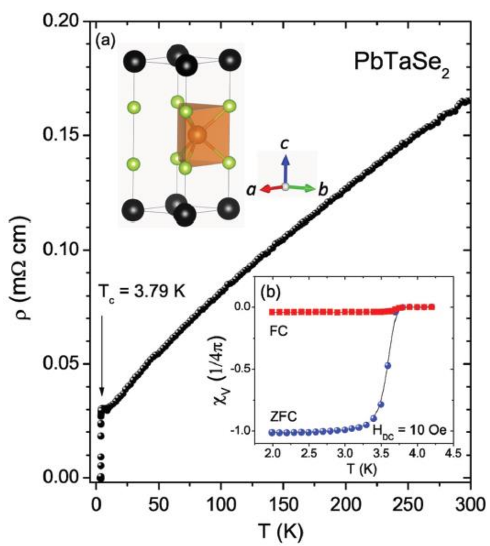
Mazhar N. Ali,[1,*] Quinn D. Gibson,[1] T. Klimczuk,[2,3] and R. J. Cava[1,†]

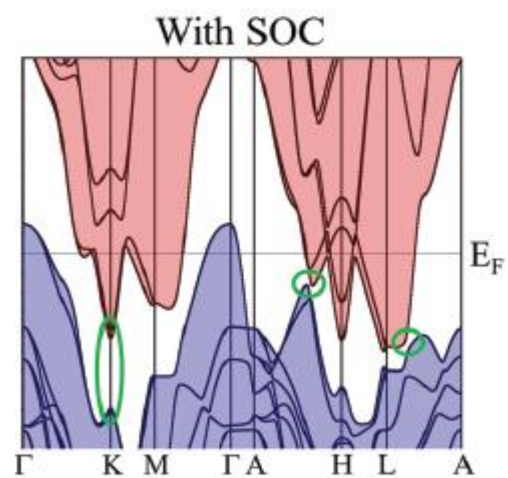
[1]*Department of Chemistry, Princeton University, Princeton New Jersey, 08544, USA*

[2]*Faculty of Applied Physics and Mathematics, Gdansk University of Technology, Narutowicza 11/12, 80-233 Gdansk, Poland*

[3]*Institute of Physics, Pomeranian University, Arciszewskiego, 76-200 Slupsk, Poland*

(Received 30 October 2013; revised manuscript received 27 December 2013; published 14 January 2014)





Nodal-line candidate: $PbTaSe_2$

nature COMMUNICATIONS

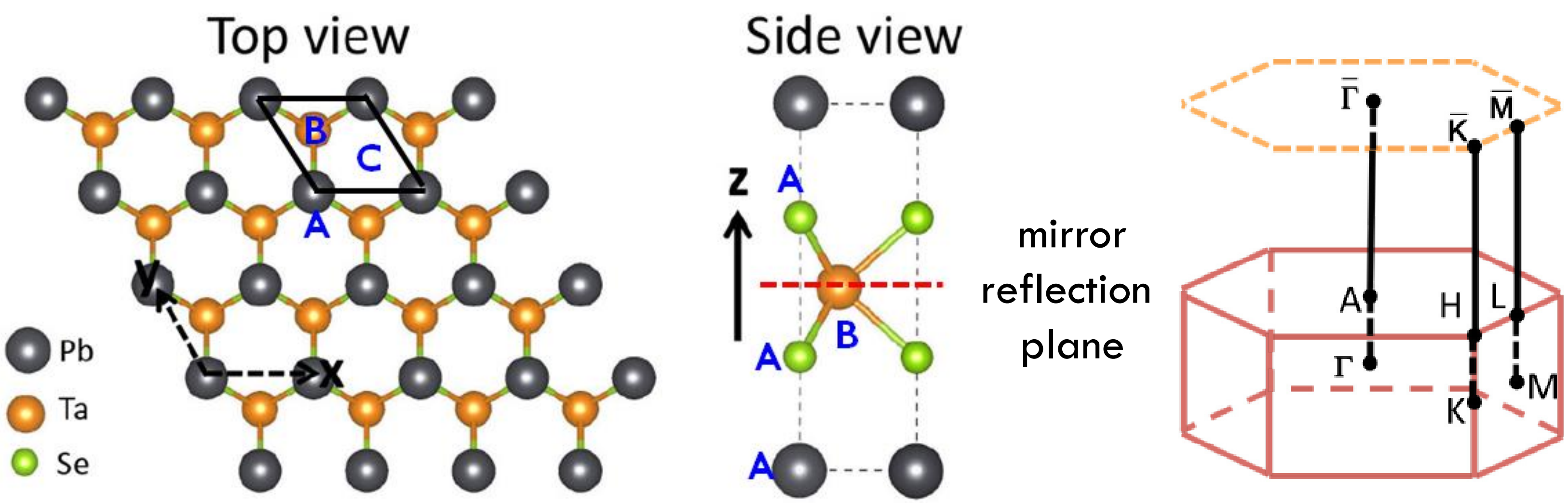
ARTICLE

Received 16 Nov 2015 | Accepted 28 Dec 2015 | Published 2 Feb 2016

DOI: 10.1038/ncomms10556 OPEN

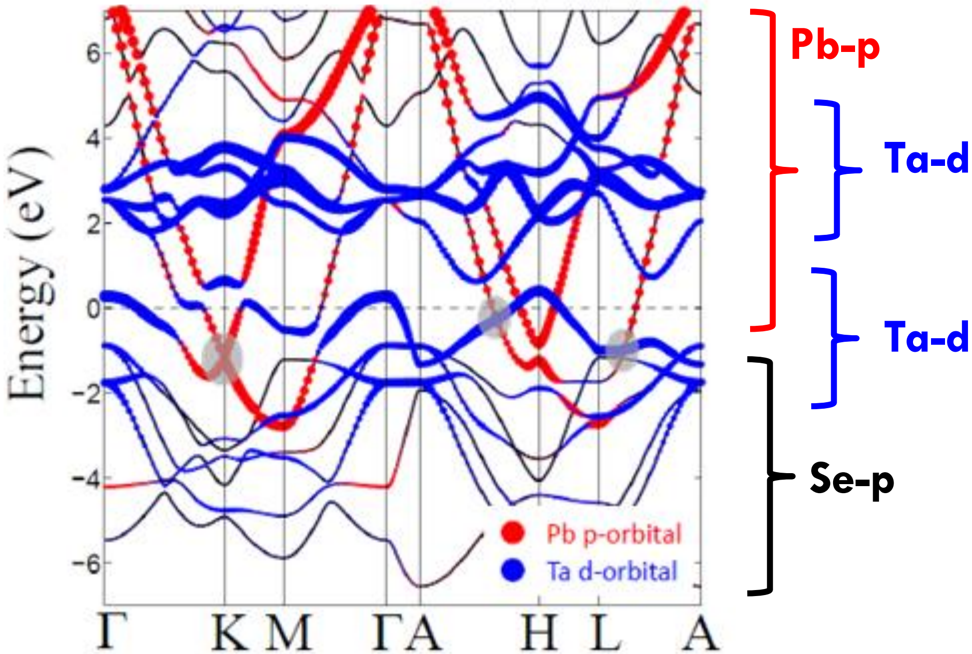
Topological nodal-line fermions in spin-orbit metal $PbTaSe_2$

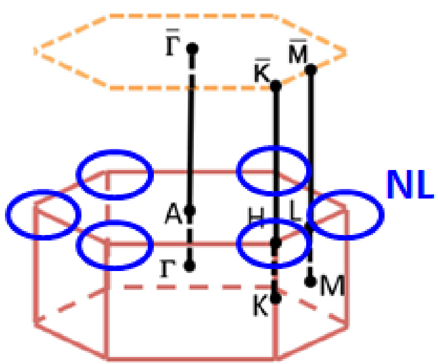
G. Bian, ***Tay-Rong Chang**** *et al. Nat. Commun.* ***7****, 10556 (2016)*

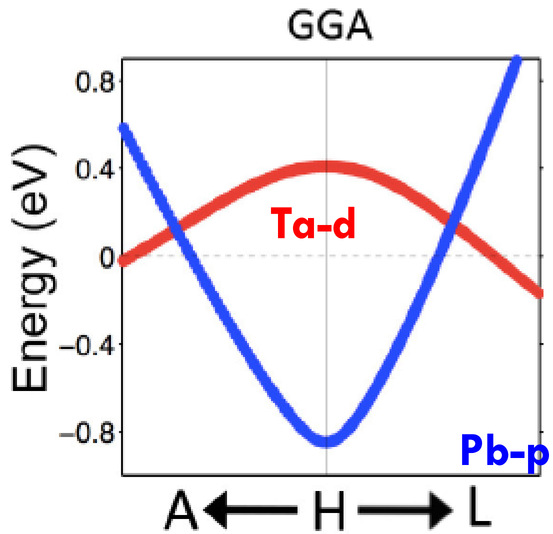


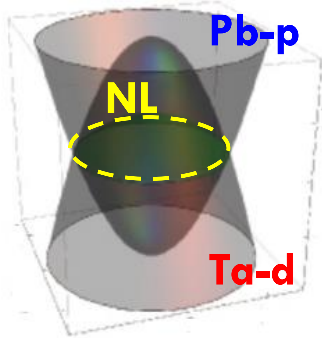
Nodal-line (spinless): $PbTaSe_2$

GGA w/o SOC









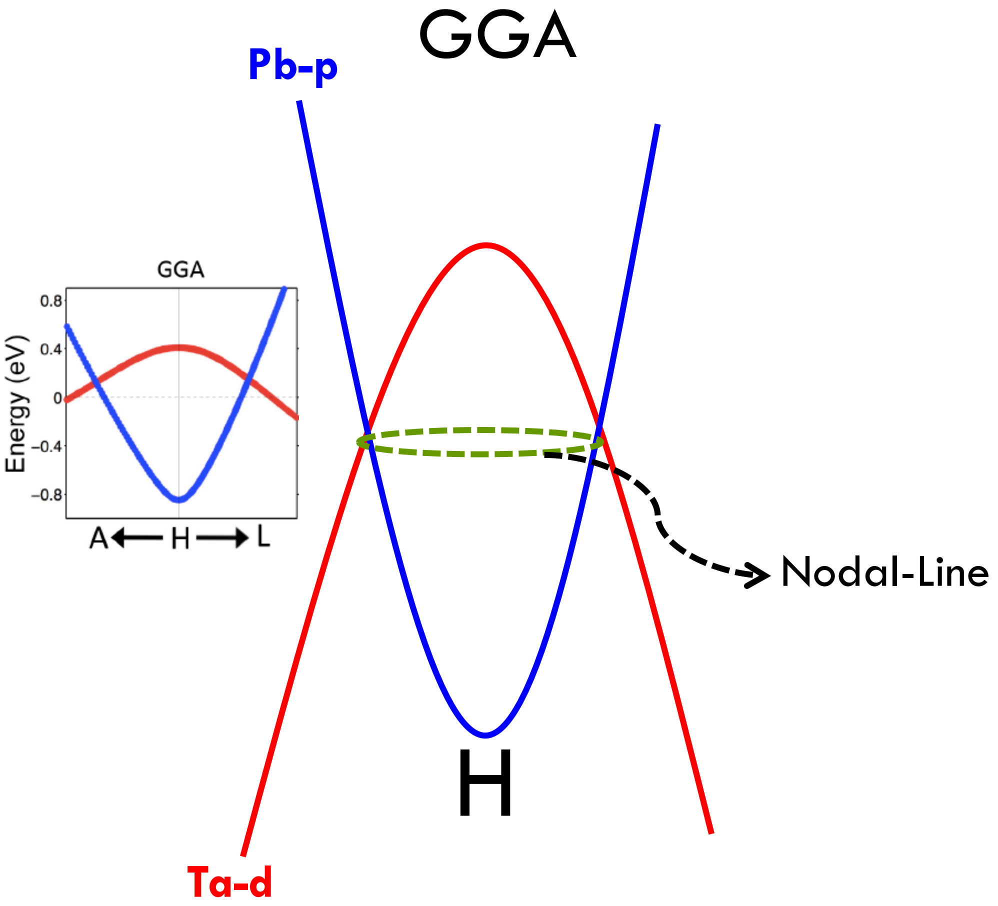
SOC

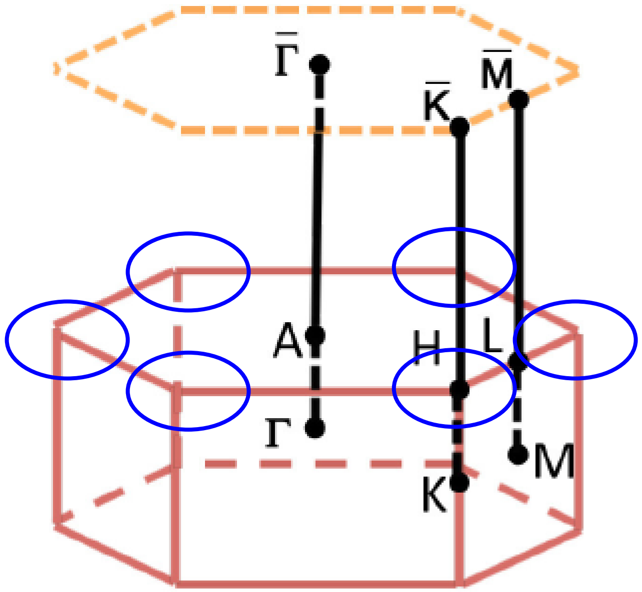
gaped out ?

or

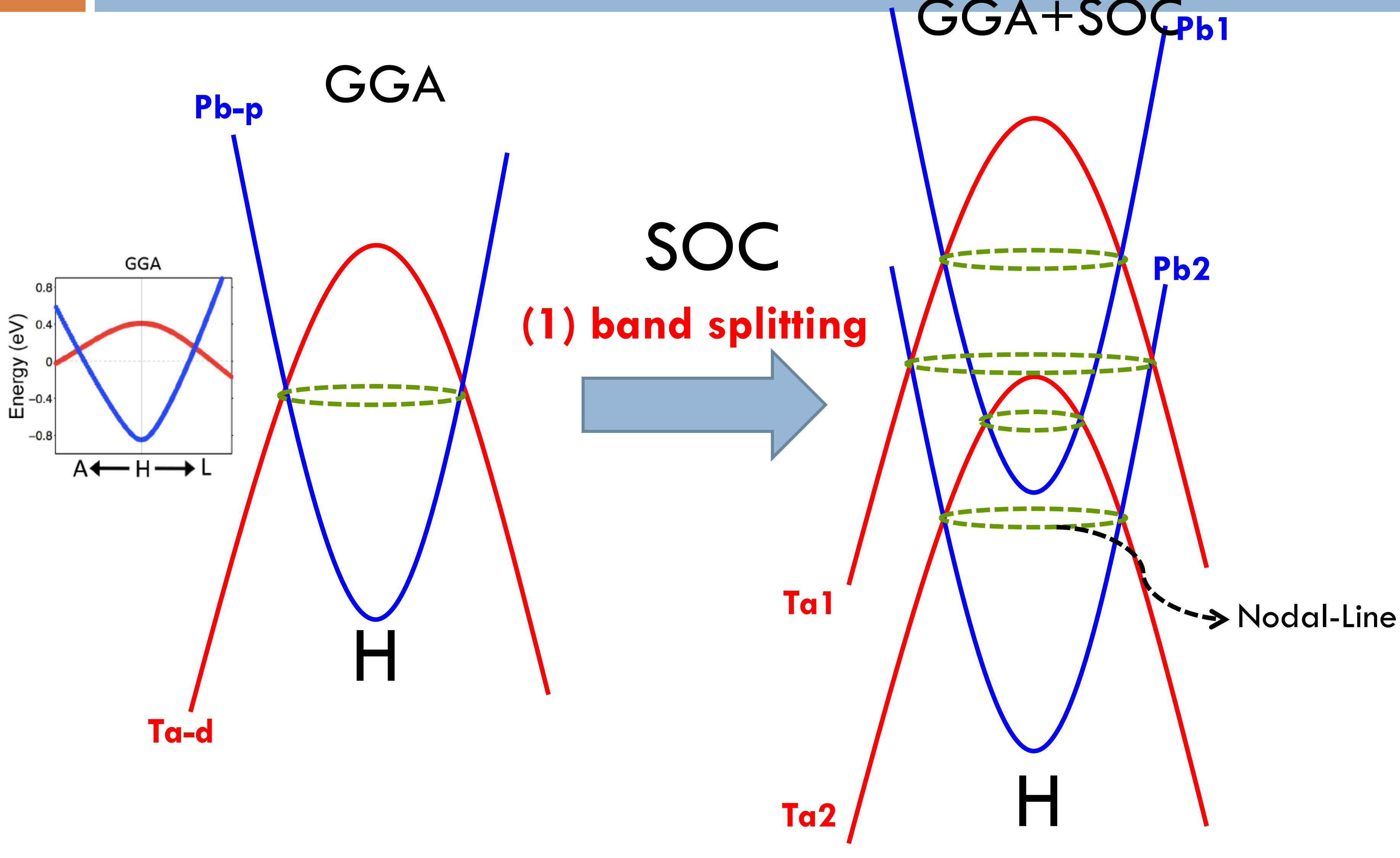
NL survived?

NL evolve under SOC

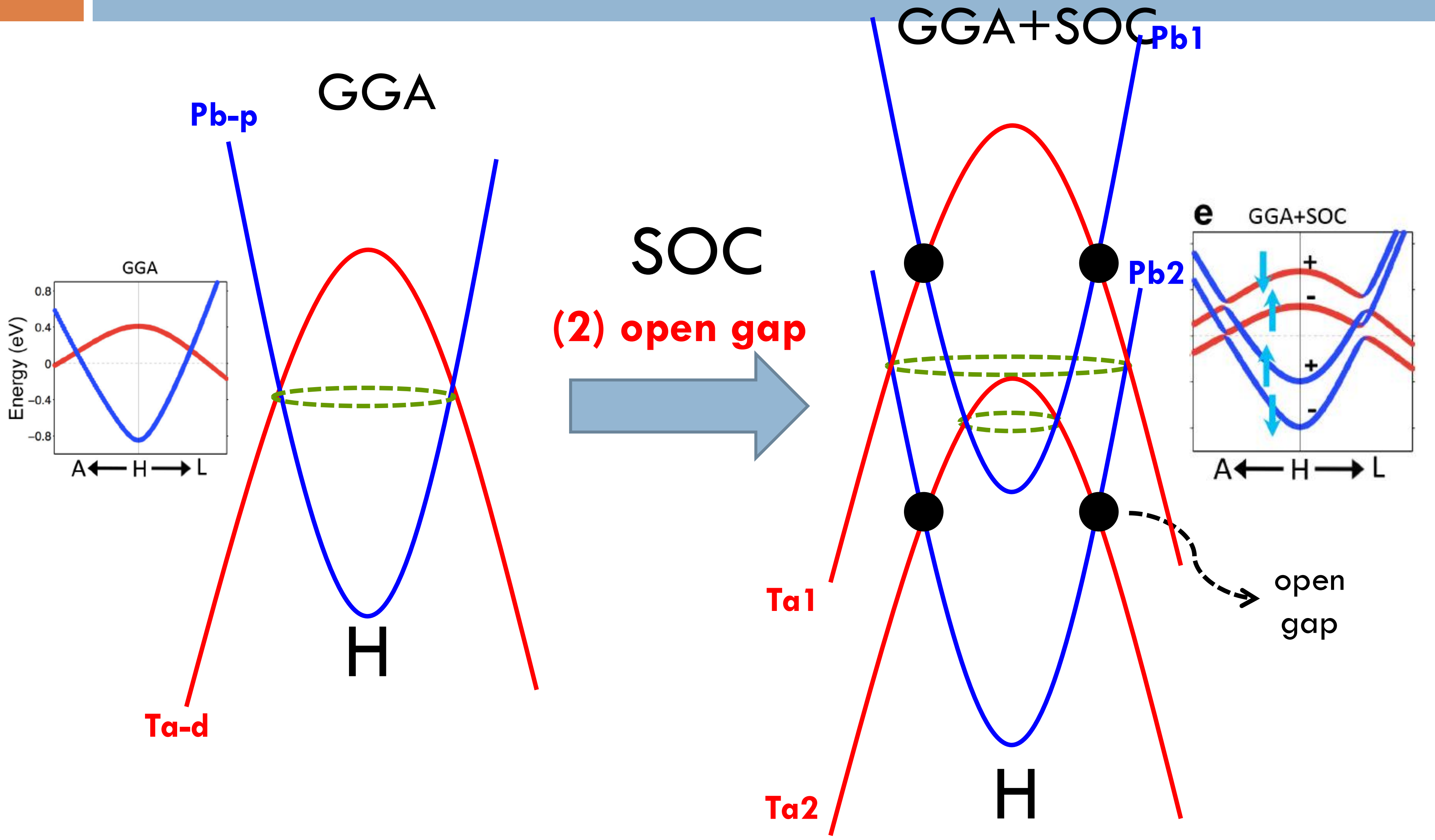




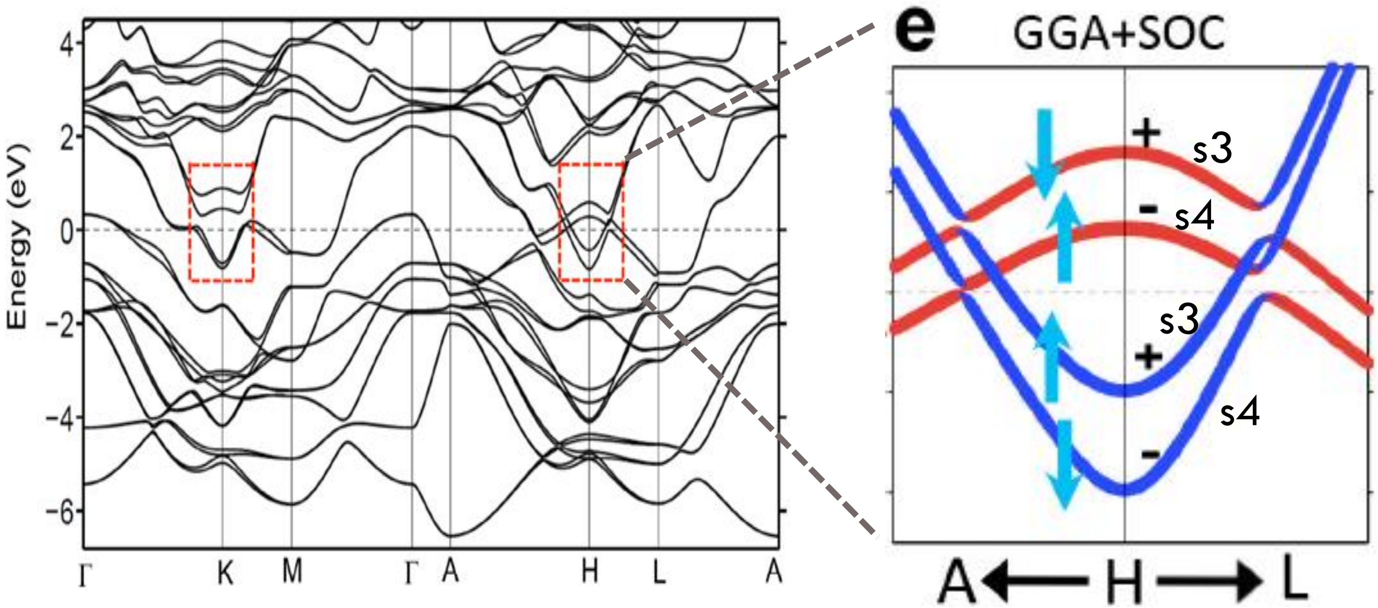
NL evolve under SOC



NL evolve under SOC



Nodal-line (spinful): $PbTaSe_2$



↑: spin up along z axis

↓: spin down along z axis

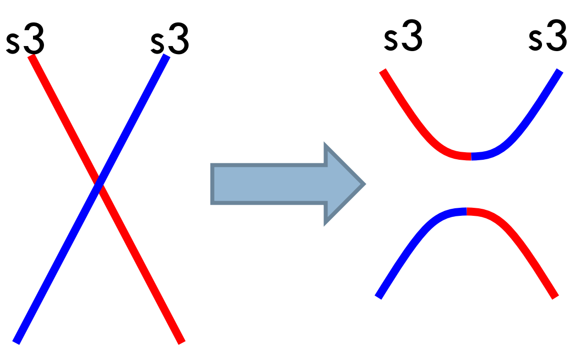
● Pb-p_x/p_y

● Ta-d_{xy}/d_{x2-y2}

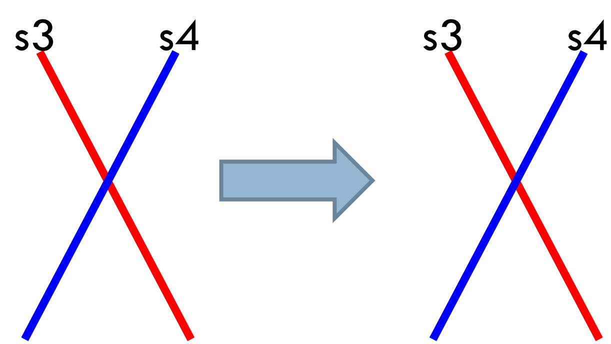
+,-: mirror eigenvalues

Nodal lines are protected by mirror symmetry!

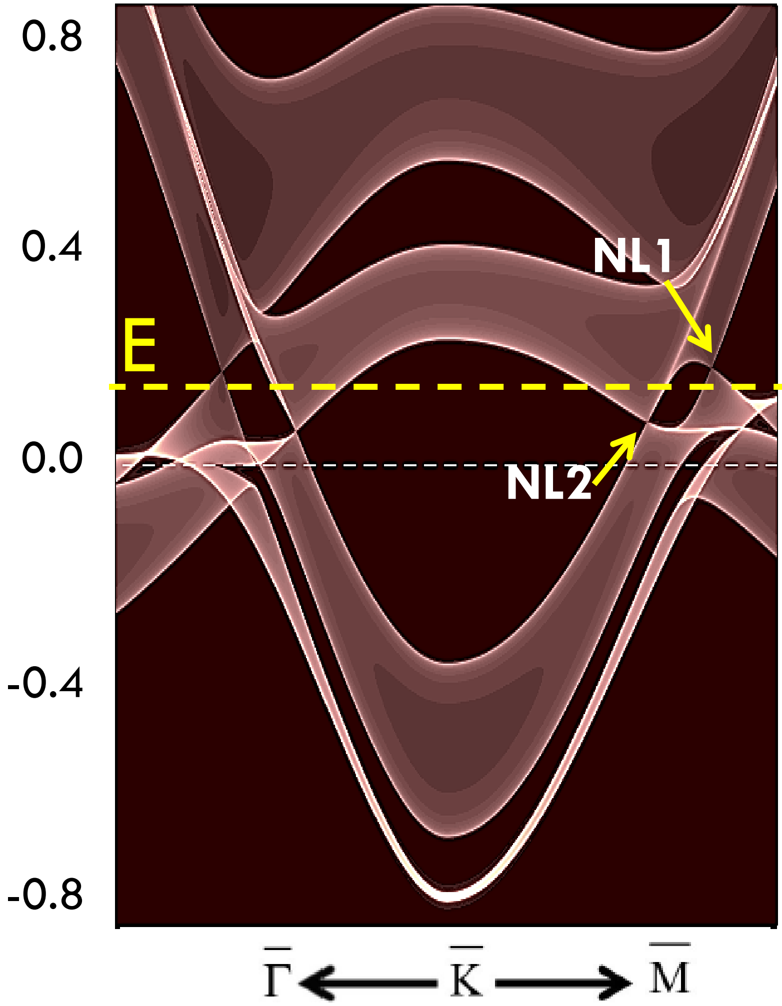
Same eig. values => gap

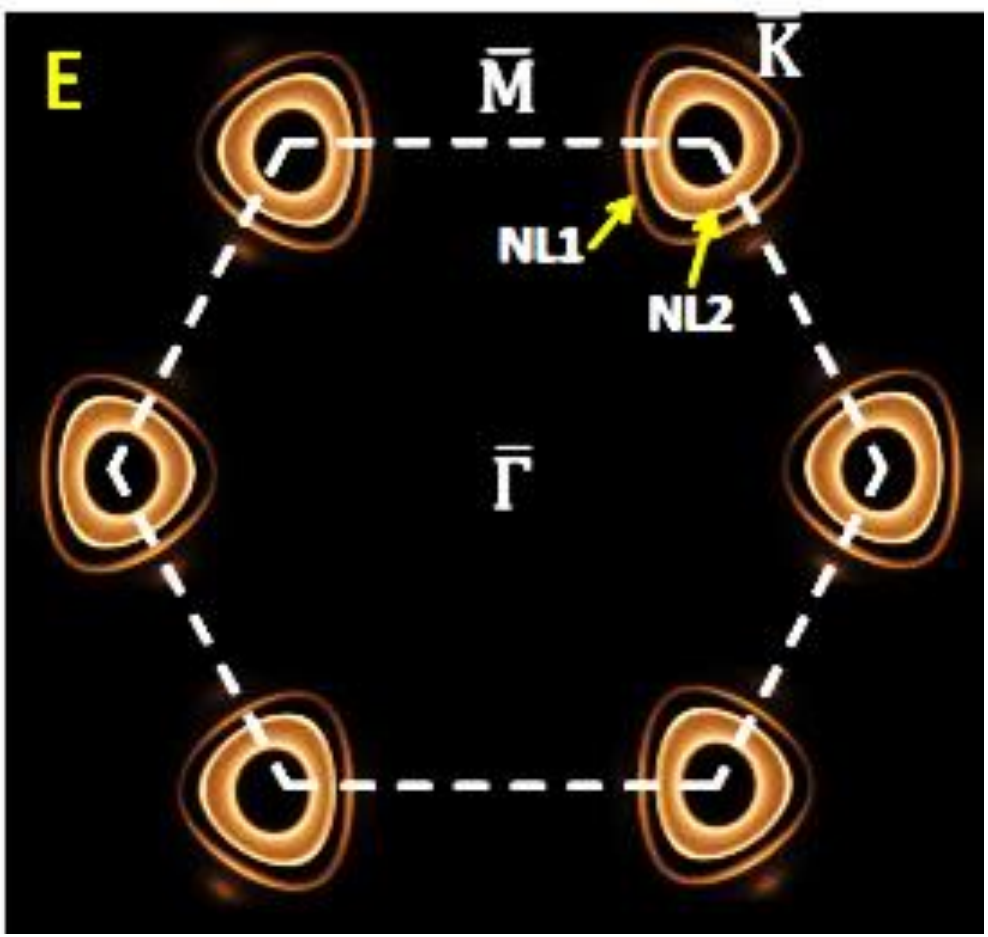


Different eig. values => crossing

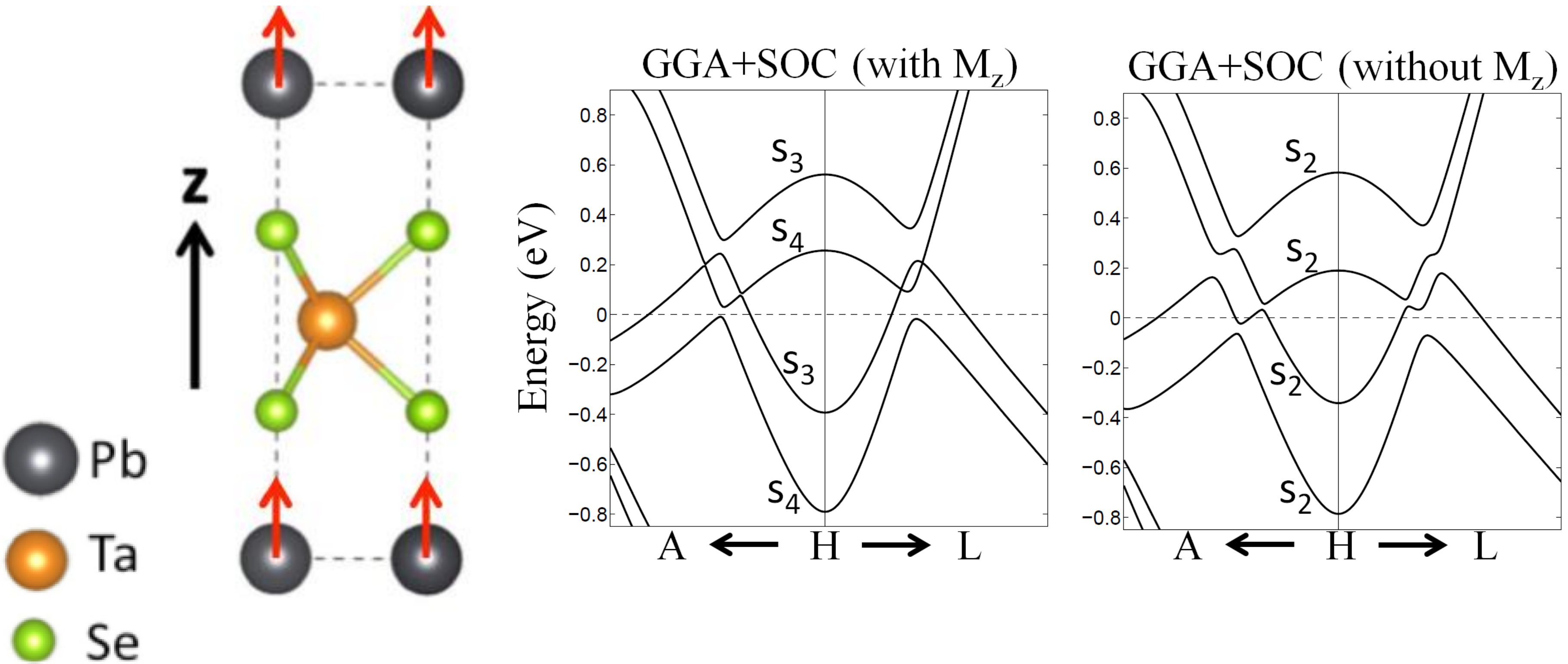


Nodal-line: $PbTaSe_2$



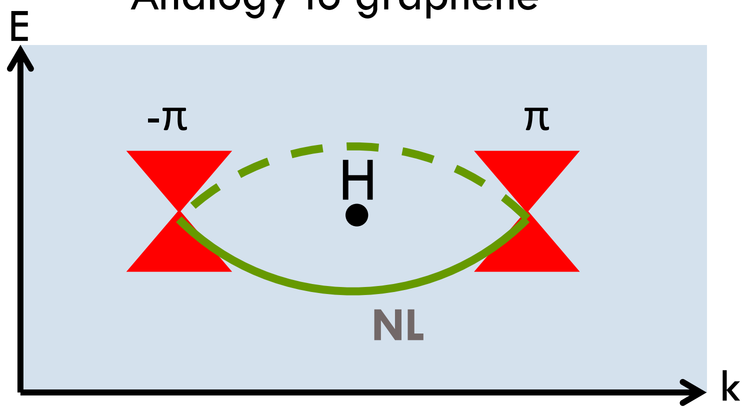


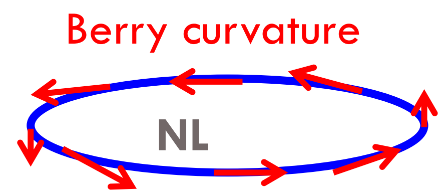
Nodal-line: $PbTaSe_2$



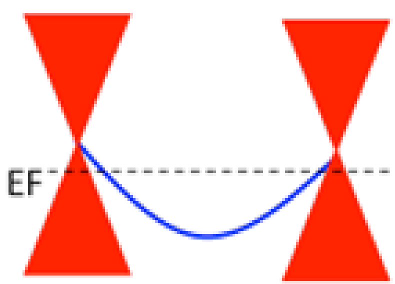
Nodal-line $PbTaSe_2$: topology

Analogy to graphene

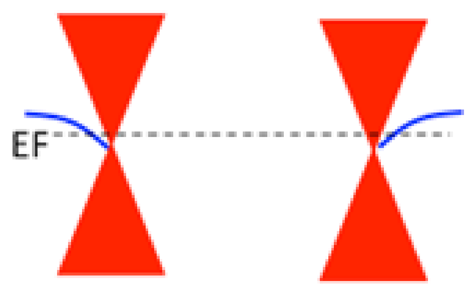




general case-1



general case-2



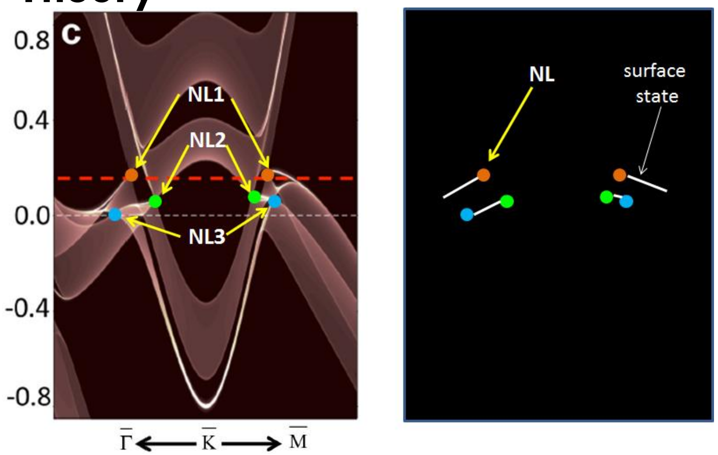
nodal line

$$\gamma = i \oint_C \langle \psi(\mathbf{k}) | \boldsymbol{\nabla} \psi(\mathbf{k}) \rangle \cdot d\mathbf{k}$$

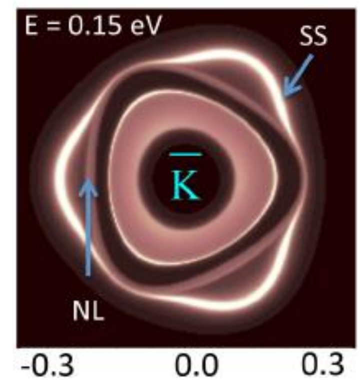
Chan *et al.*, arXiv:1510.02759 (2015)

Nodal-line $PbTaSe_2$: surface states

Theory Se-termination



Theory



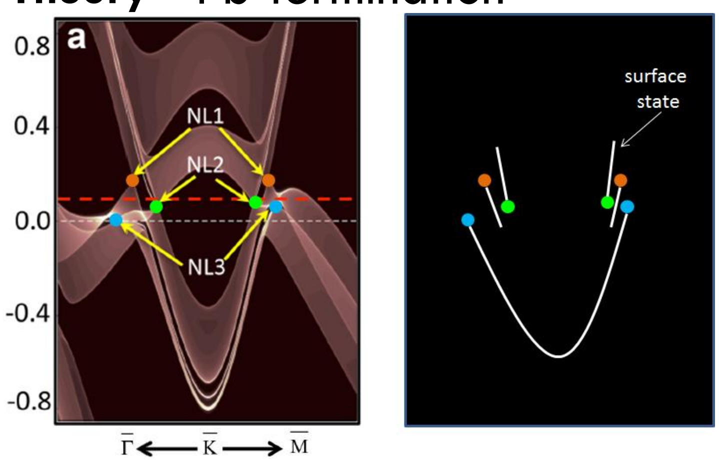
winding number

$$g/p = \pm 1$$

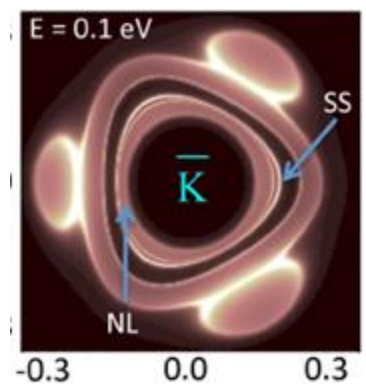
bulk-boundary correspondece

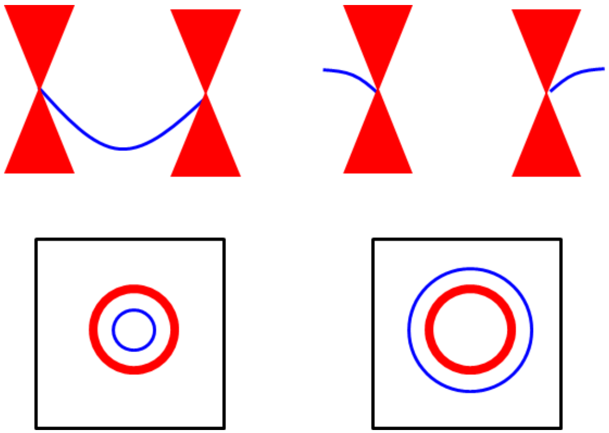
topo. surface states

Theory Pb-termination

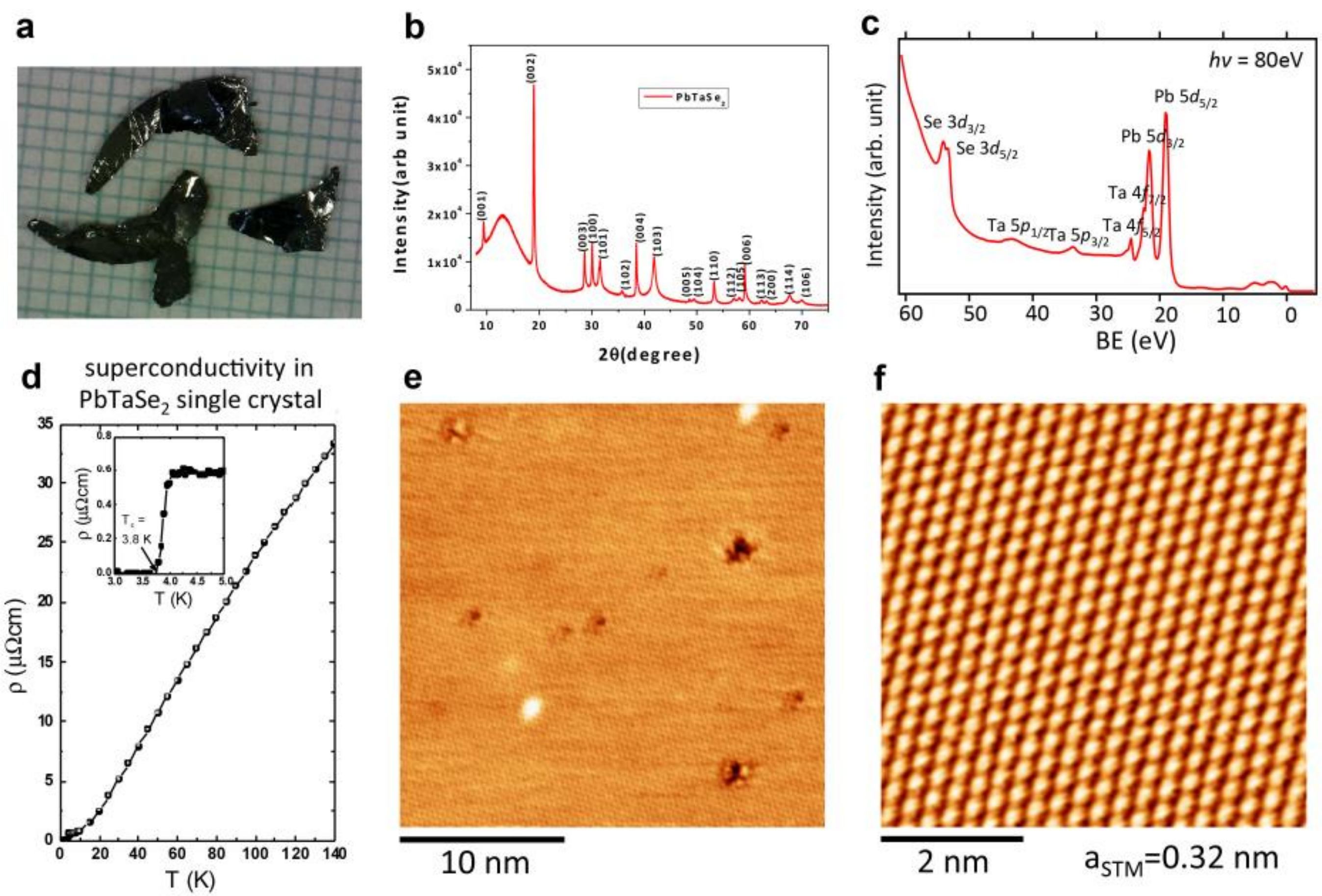


Theory



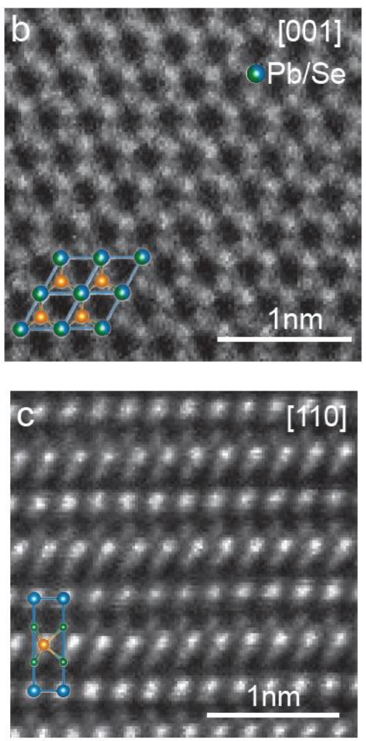


Nodal-line $PbTaSe_2$: Experiments

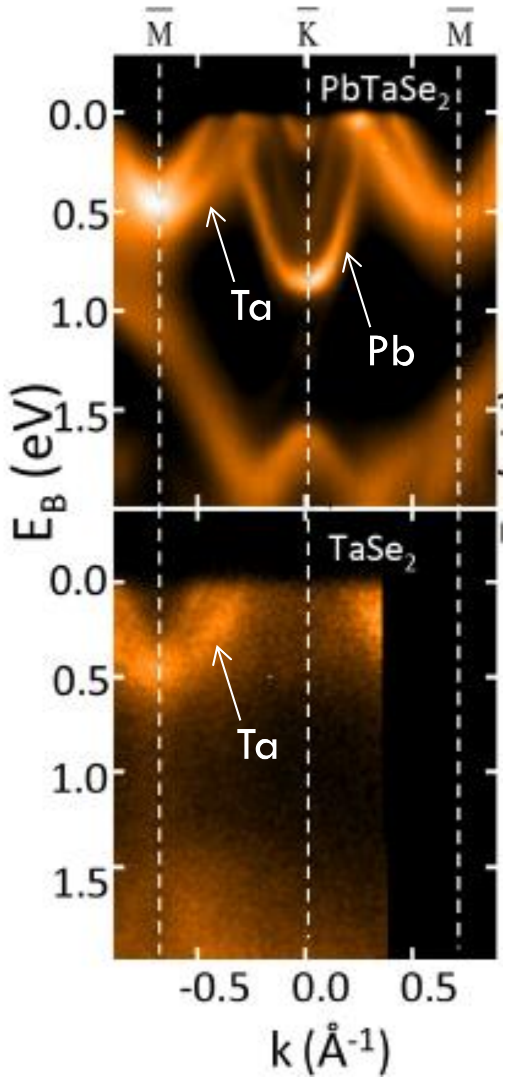


S.-Y. Guan, P.-J. Chen, M.-W. Chu et al, unpublished

STEM

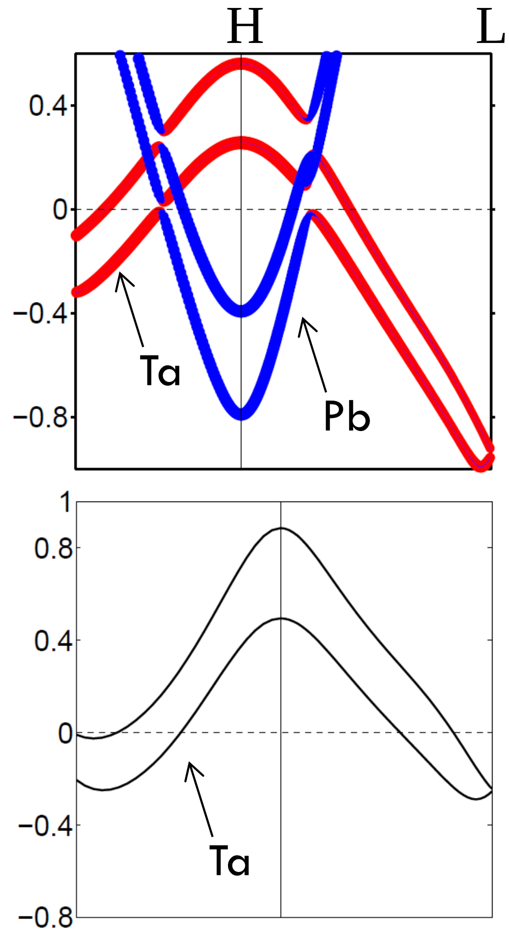


Nodal-line $PbTaSe_2$: Experiments



$PbTaSe_2$

$TaSe_2$

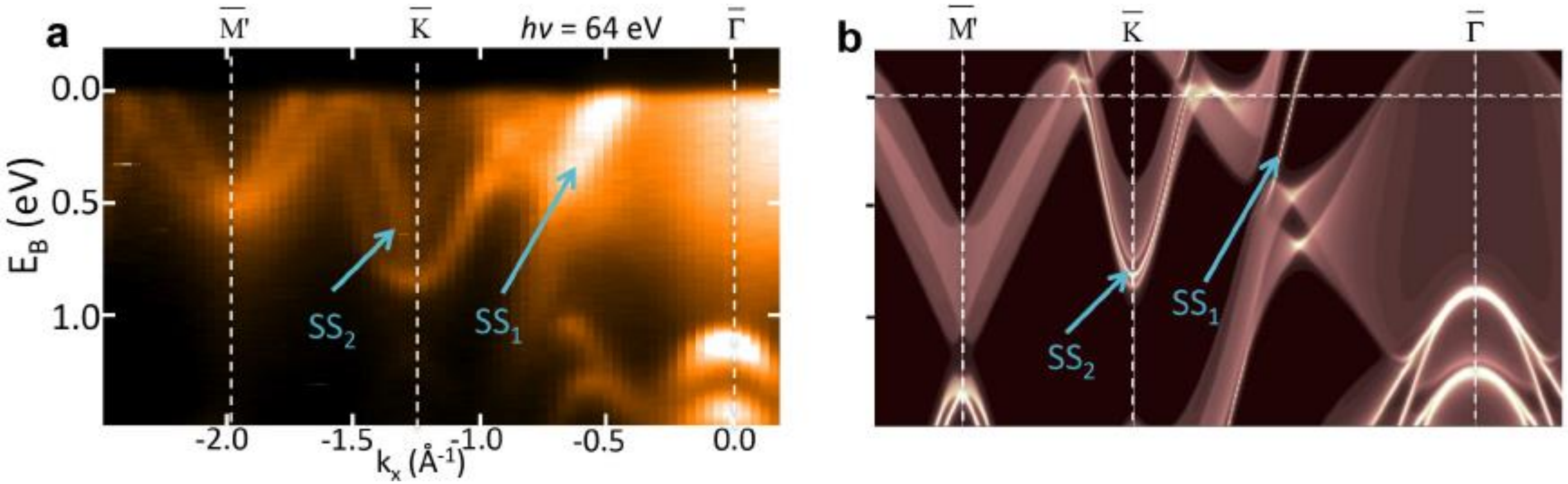


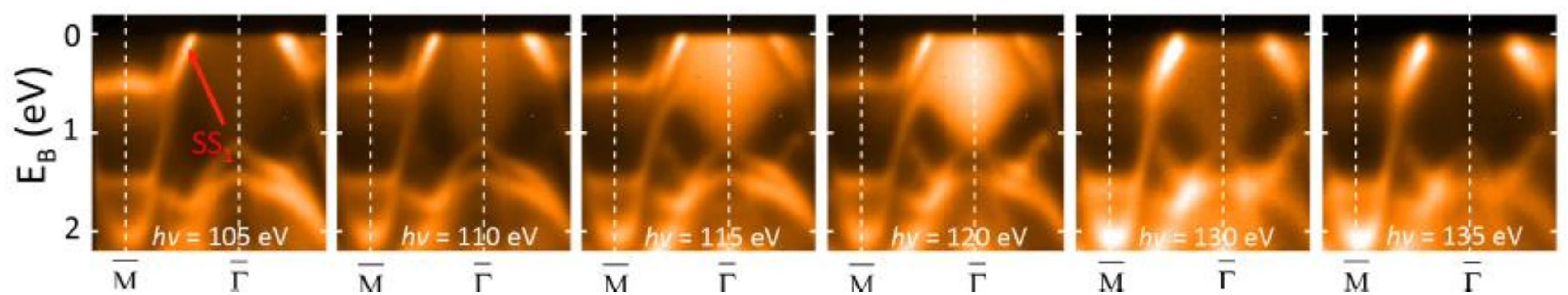
$PbTaSe_2$

$TaSe_2$

Nodal-line $PbTaSe_2$: Experiments

ARPES **1^{st}-principles**

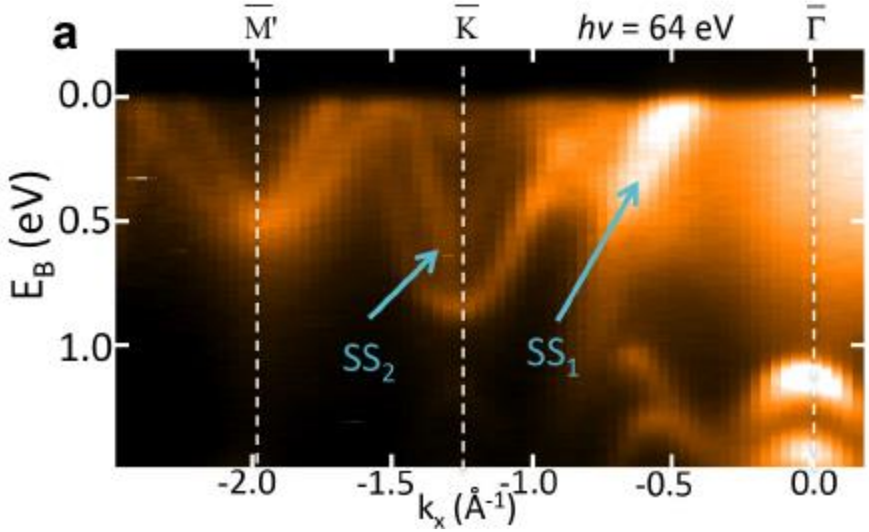


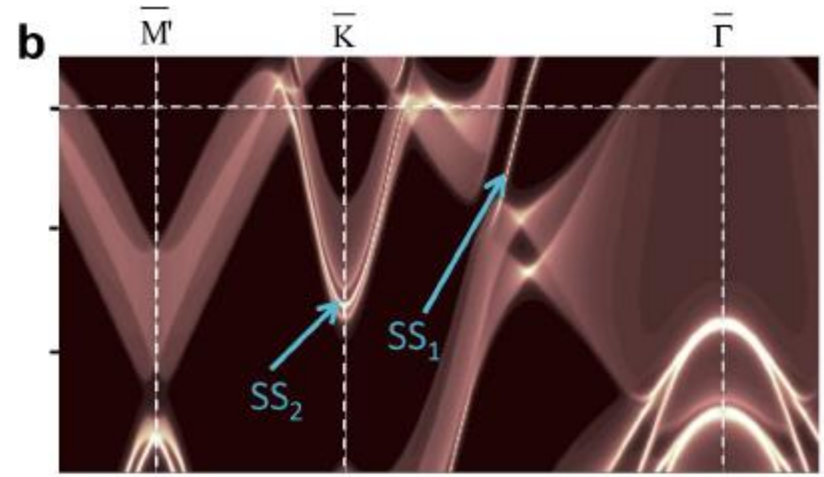


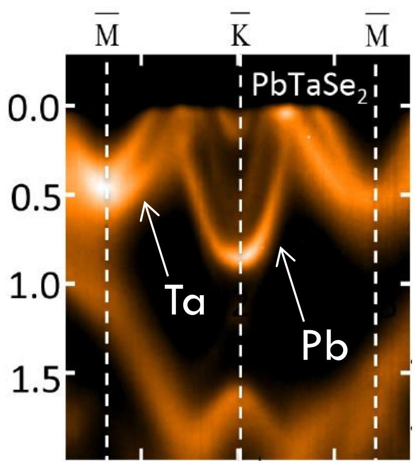
Nodal-line $PbTaSe_2$

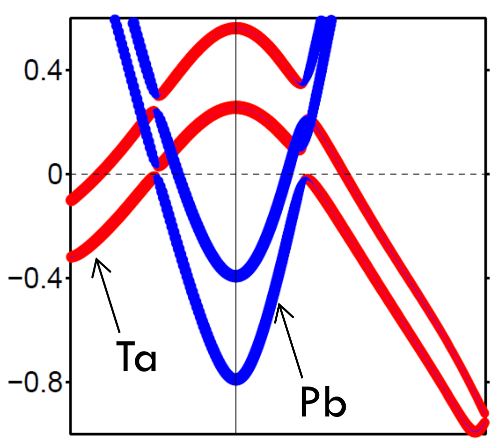
ARPES

1^{st}-principles









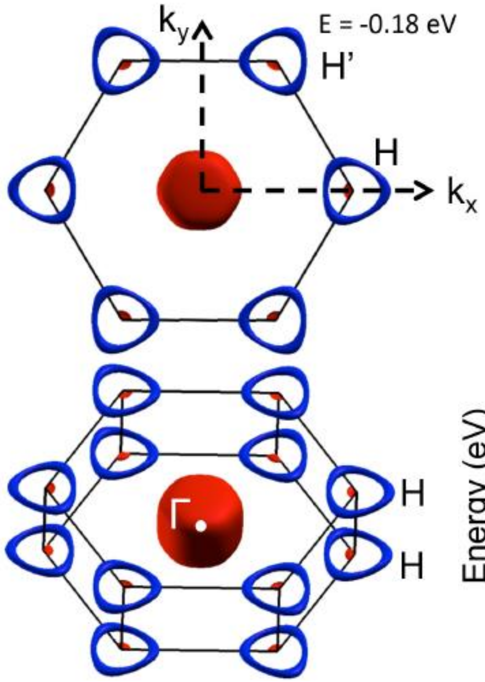
Editor: Nodal-line shape band appearing near Fermi level hosts unique properties in topological matter, which has yet to be confirmed in real materials. Here, the authors report the existence of topological nodal-line states in the non-centrosymmetric single-crystalline spin-orbit semimetal $PbTaSe_2$.

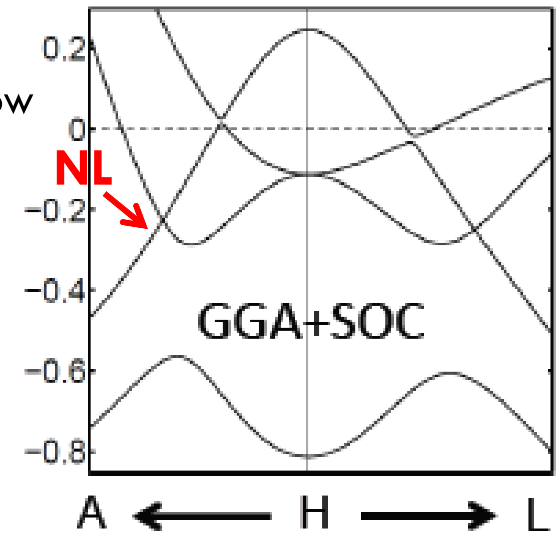
Nodal-line semimetal: $TlTaSe_2$

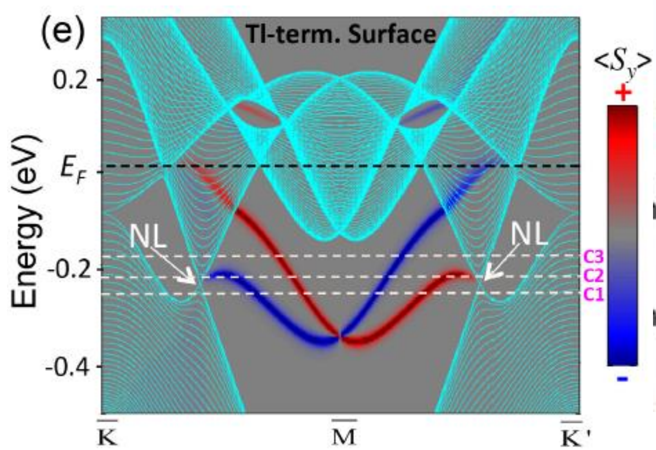
PRB ***93****, 12113 (R) (2016)*

(1) Single Nodal-ring below EF

(2) Exotic surface states







surface spectral weight