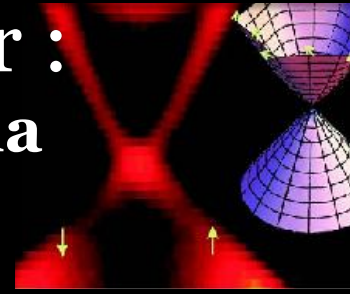
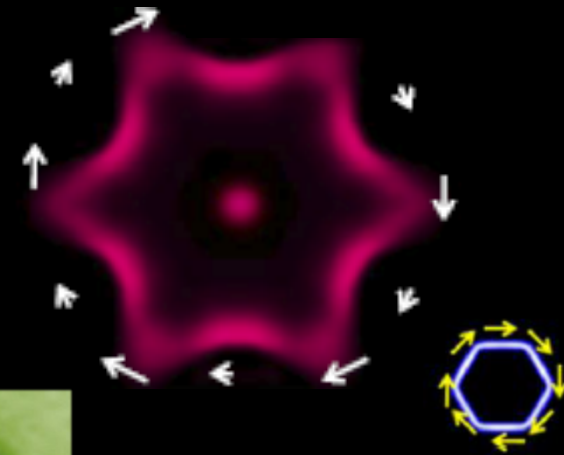


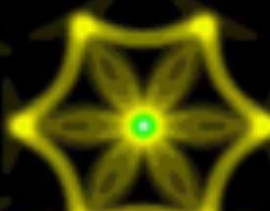
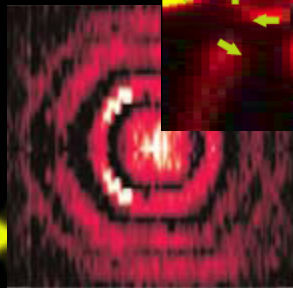
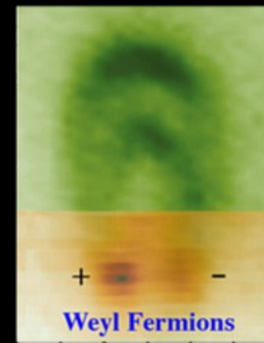
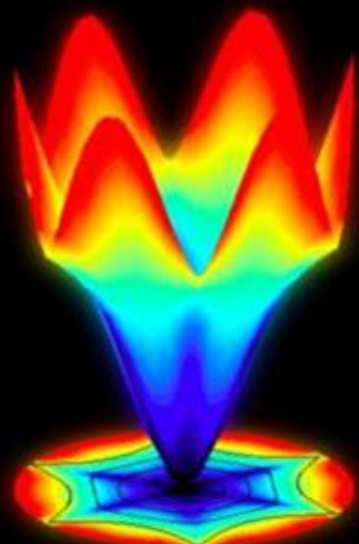
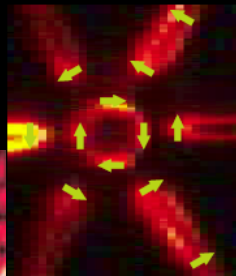
New Topological Phases of Matter : Platform for emergent Dirac, Majorana and Weyl fermions



Physics Colloquium
California Inst. of Technology
October, 2016



M.Z. Hasan
Princeton Univ.



Topological Phases Theory:

Thouless et.al., PRL 1982; Laughlin, PRL 1983

Haldane, PRL 1983 (SPT) & *Haldane*, PRL 1988 (QAHE)

Kane, Mele; PRL 2005, *Kane, Mele, Fu*; PRL 05 -> PRL 07
and many others....

Experiments :

2D : *von Klitzing et.al.*, PRL 1980

Int. **QHE**

Tsui et.al., PRL 1982

Frq. QHE

Konig et.al, (Molenkamp) Sci' 2007

Spin QHE

Chang et.al., (Q.Xue) Science 2013

Anom **QHE**

3D: *Hsieh et., (MZH)* KITP'2007, Nature 2008

TSS, TI (3D-TI)

Xu et.al., (MZH) Science'15, Science 2015

FermiArc, Weyl

and others...

+ **Superconductivity**

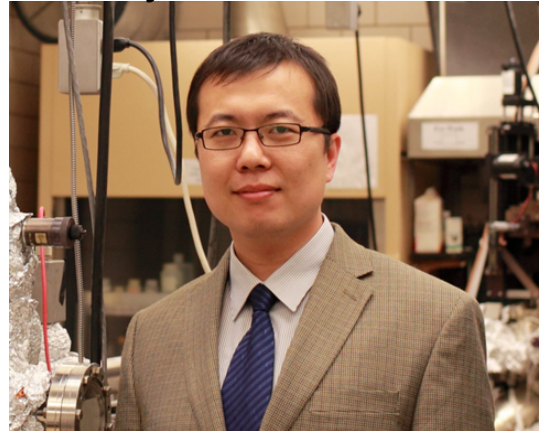
ARPES team on **Topo. Fermions (Weyl, Dirac, TNL)**

Weyl-Semimetals + Superconductivity **TNL**-Semimetals

Dirac-Semimetals



Su-Yang Xu



Guang Bian



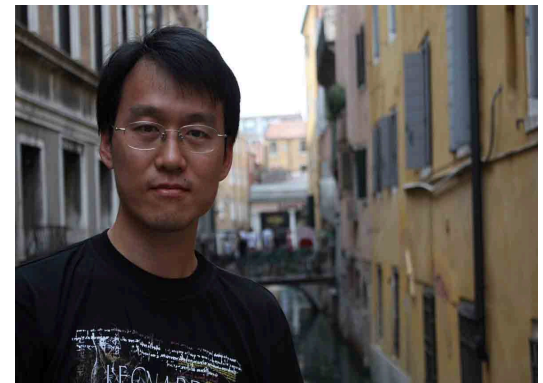
Madhab Neupane



Ilya Belopolski



Nasser Alidoust



Hao Zheng

S. Xu, G. Bian, M. Neupane, I. Belopolski, N. Alidoust, H. Zheng C. Liu, D. Sanchez

(previously) D.Hsieh (CalTech), L.A.Wray (SLAC/NYU), D.Qian (Shanghai)

Samples: R. Sanker (India), C. Zhang, Shuang Jia (Peking), F.C Chou (Taiwan)

FP/DFT: G. Bian, S. Xu, I. Belopolski, MZH + A. Bansil (NEU), S. Huang, H. Lin (NUS)

Insulators



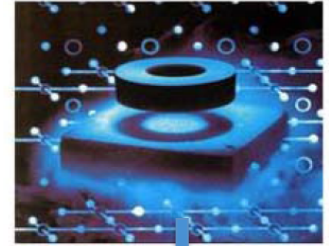
Magnets



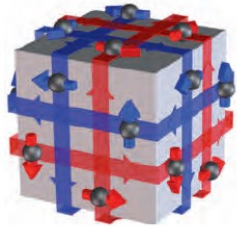
Metals/Semimetals



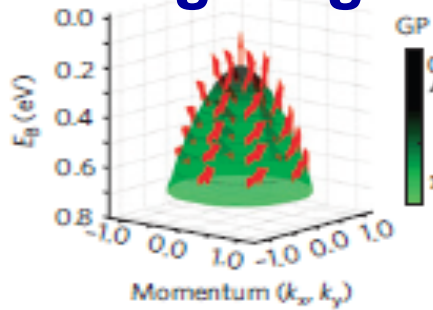
Superconductors



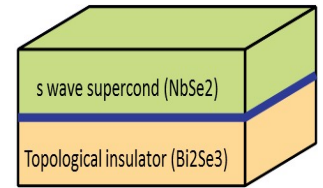
Topo Insulators



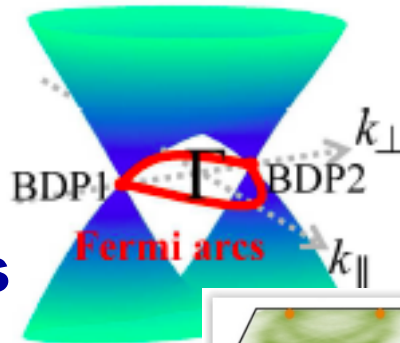
Hedgehog Magnet



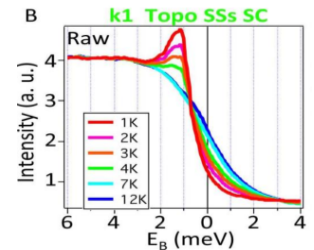
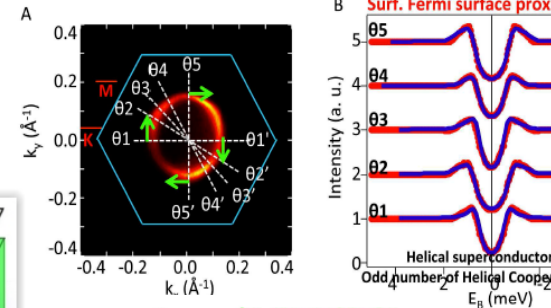
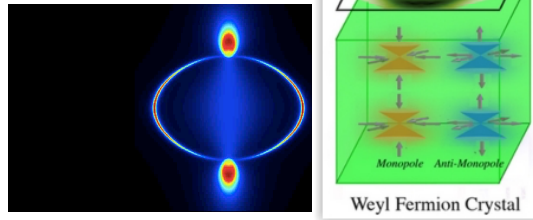
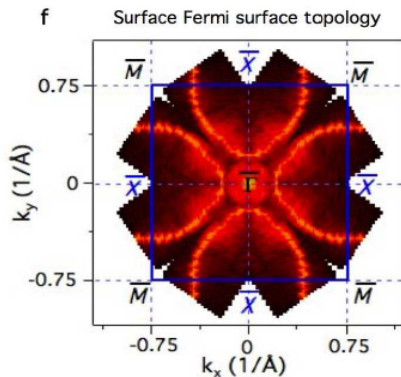
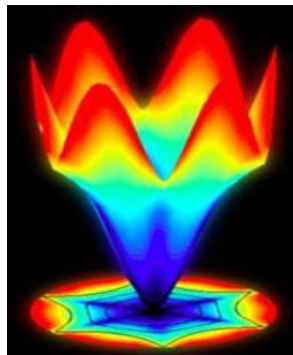
Topo. Supercond.



Fermi-Arc Metal

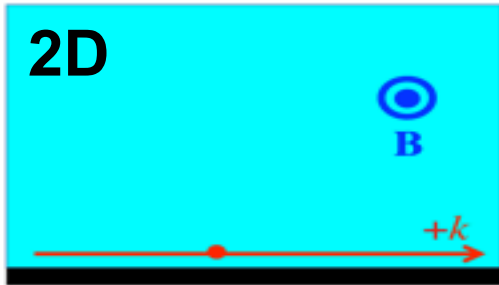


Kondo Insulators



Non-trivial insulators

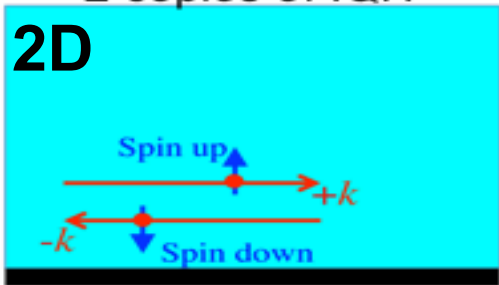
1
Invariant



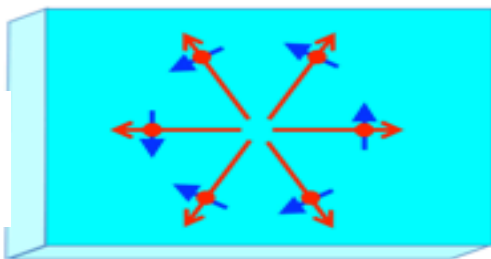
Haldane + spin-orbit

2 copies of IQH

1
Invariant

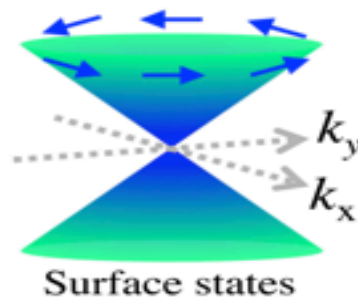
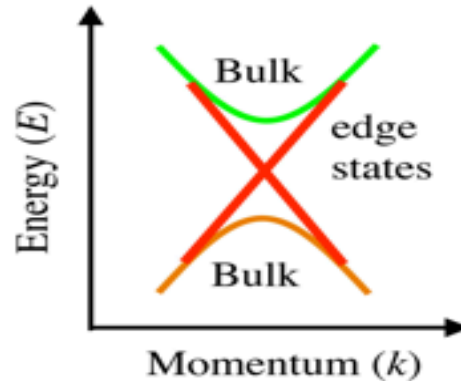
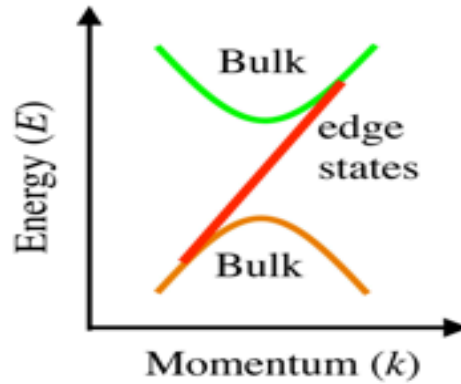


Topological Surface States

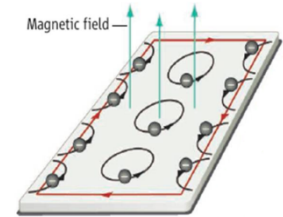


4
Invariant

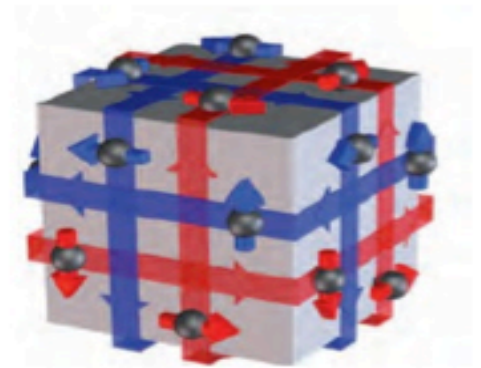
3D TI is a novel topological state
first NON-quantHall-like topological matter



$$\sigma_{xy} = n e^2/h$$



Quant. Hall physics



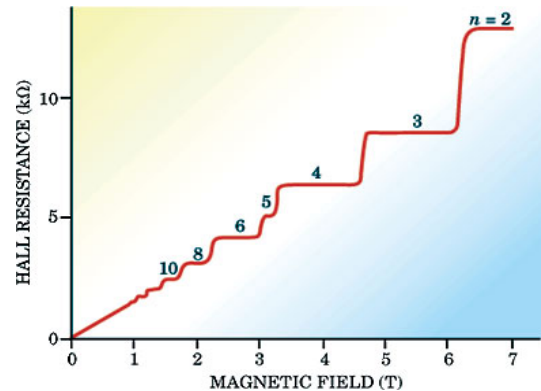
3D Topo. Insulator

QHE phases (2D)

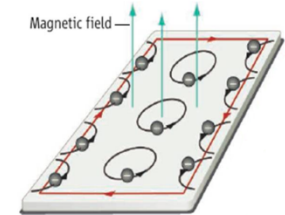
$$\sigma_{xy} = n e^2/h$$

Chern no.

(D. Thouless et.al., M. Berry)



Transport



Topo Insulators

$$\nu_0 = \Theta_{ME}/\pi$$

$\Theta = \pi$ (odd)

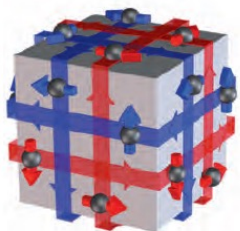
How to experimentally “measure” the topological quantum numbers (ν_i) ?

4 TQNs \rightarrow **15+1** distinct insulators

No quantized transport

via :

$$\{\nu_i\}$$

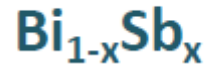


$\{\nu_0, \nu_1, \nu_2, \nu_3\}$
Topological “order parameters!”

Spin-sensitive
Momentum-resolved
Edge vs. Bulk

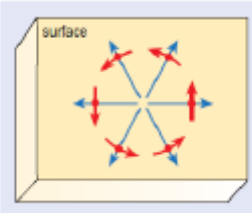
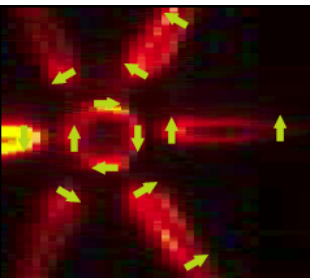
(Bulk-Boundary Correspondence)

Topo. Insulator → Most Researched Topo. Insulator

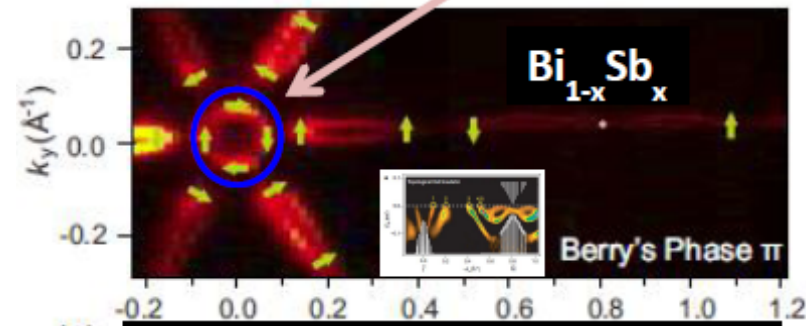


KITP Proceed. (2007)
 Hsieh et.al., NATURE 2008
 Hsieh et.al., SCIENCE 2009
[Physics Today, April-2009](#)

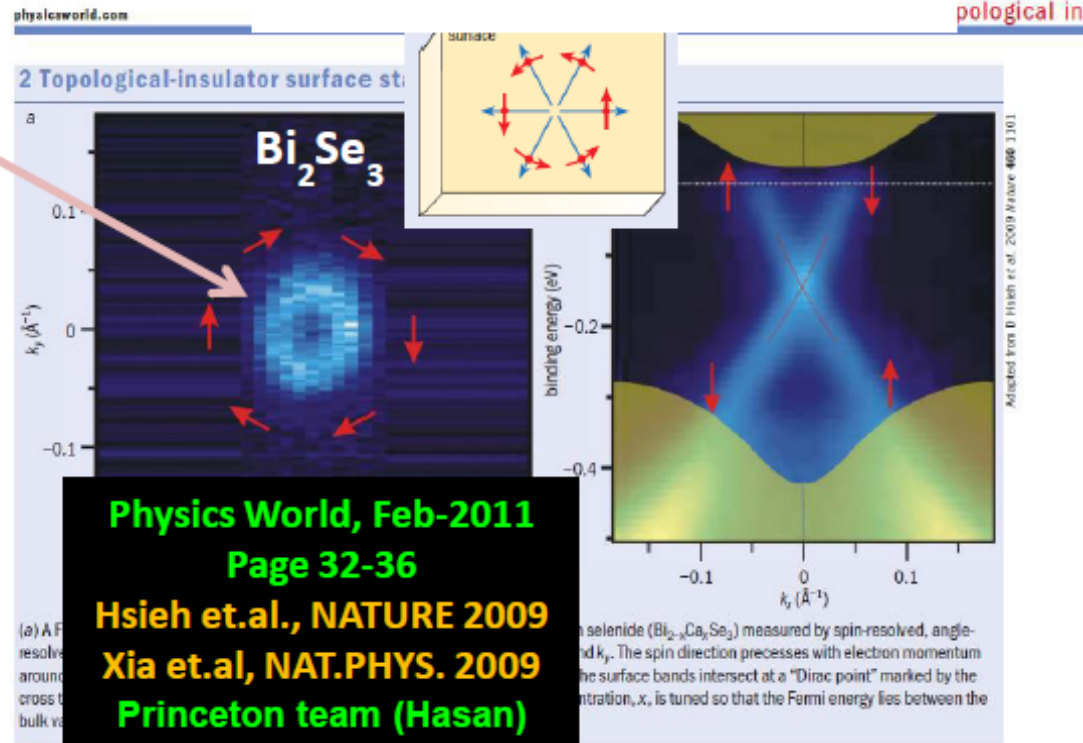
Xia et.al, NAT.PHYS. 2009 (arXiv 2008)
 Hsieh et.al., NATURE 2009
 Zhang et.al, NAT.PHYS. 2009
[Physics World, Feb-2011](#)



Dirac Cone



(a) **Physics Today, April 2009**
 "Search & Discovery" Page 12-13
Topological Insulators ($\text{Bi}_{1-x}\text{Sb}_x$)
Hsieh et.al., NATURE 2008
Princeton team (Hasan)

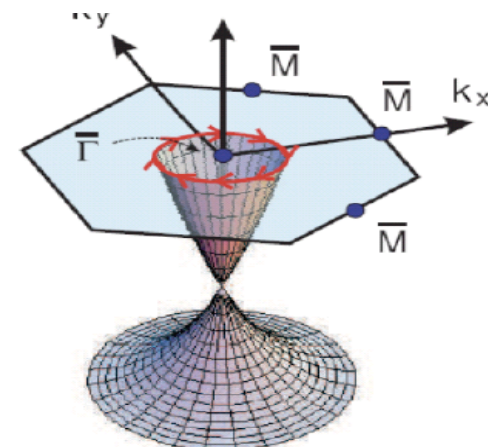
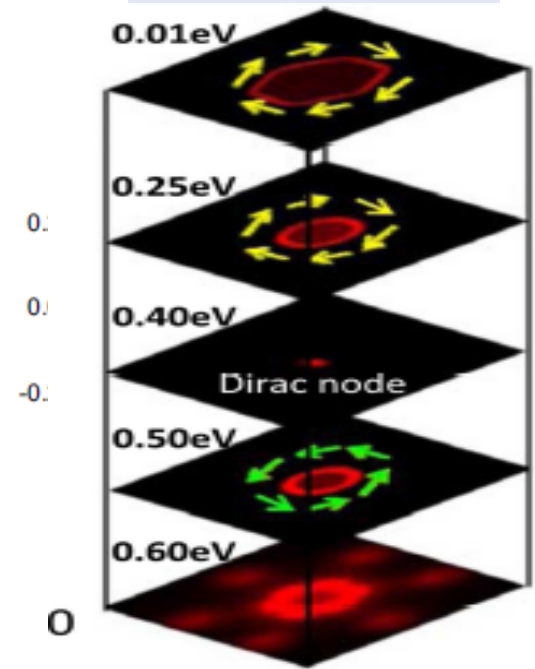
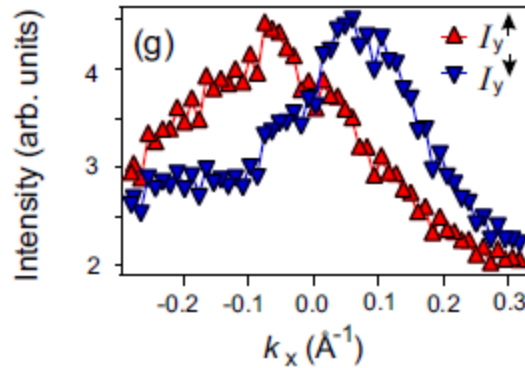
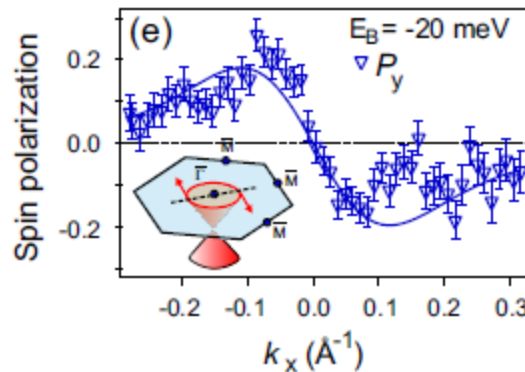
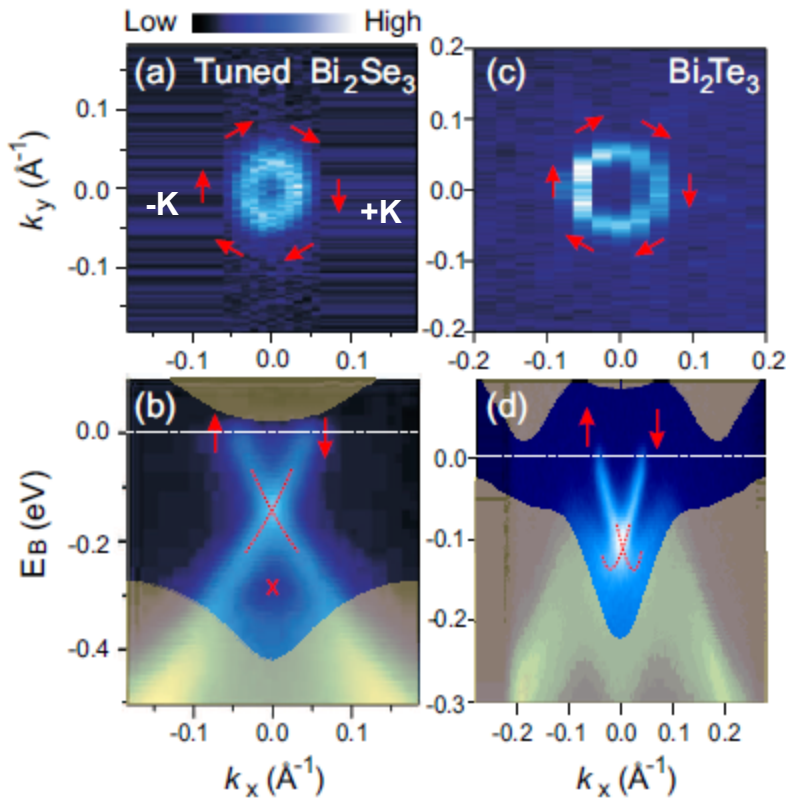
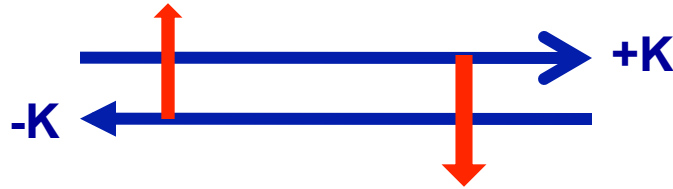
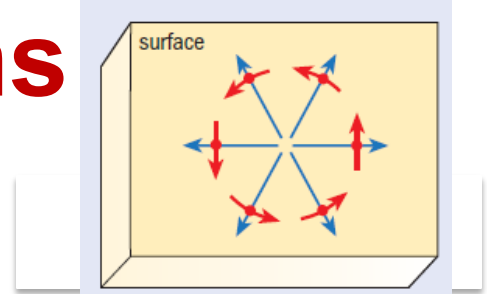
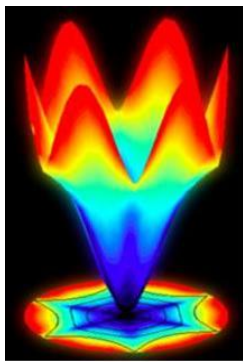


(a) **Physics World, Feb-2011**
 Page 32-36
Hsieh et.al., NATURE 2009
Xia et.al, NAT.PHYS. 2009
Princeton team (Hasan)

3D TI: More than **500** Expt's Papers (arXiv)

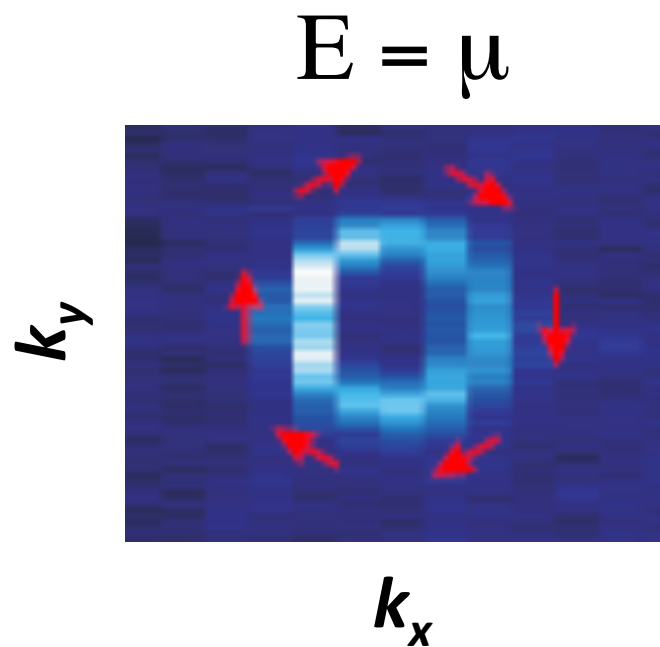
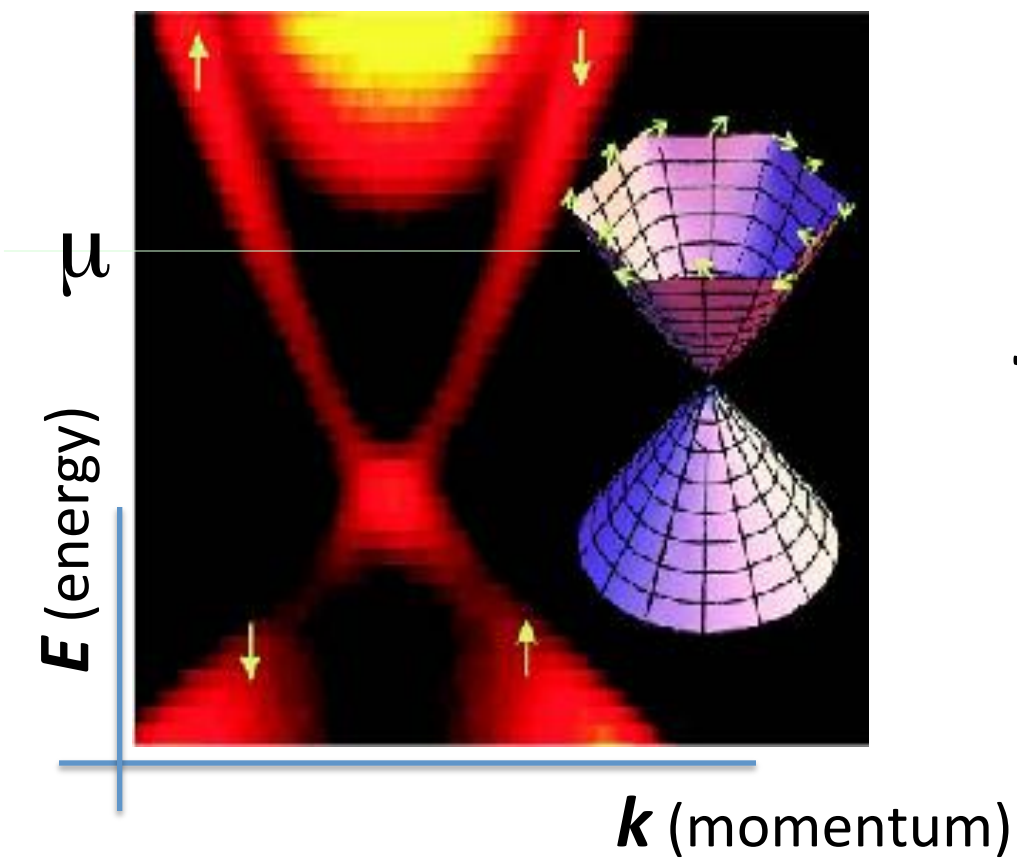
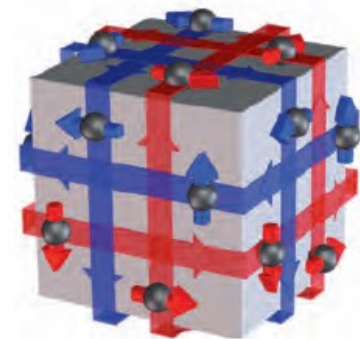
Helical Dirac fermions

One-to-One Spin-LinearMomentum Locking

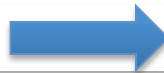


Berry's phase $\theta = \pi$
Invariant = $\theta/\pi = 1$

Helical Dirac fermions

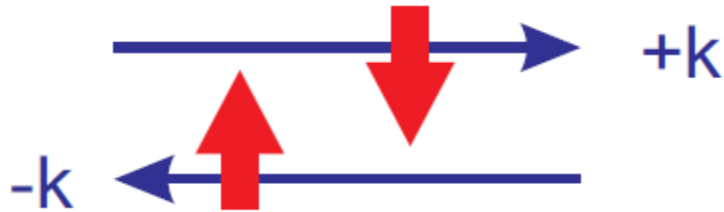


Helical spin texture

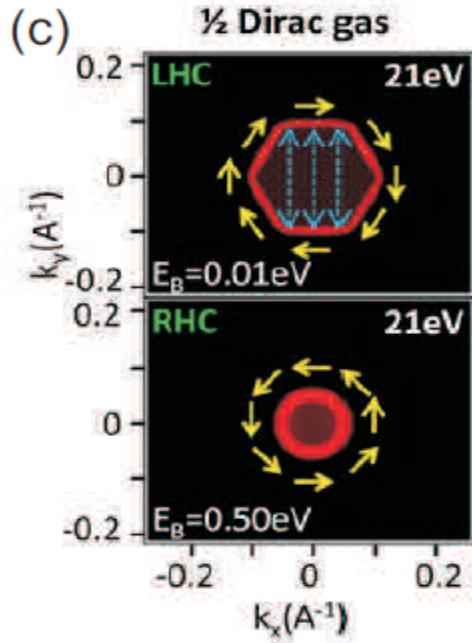
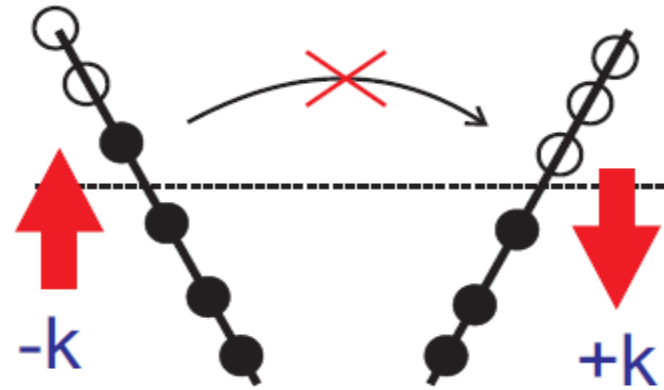


absence of backscattering

Spin-ARPES →



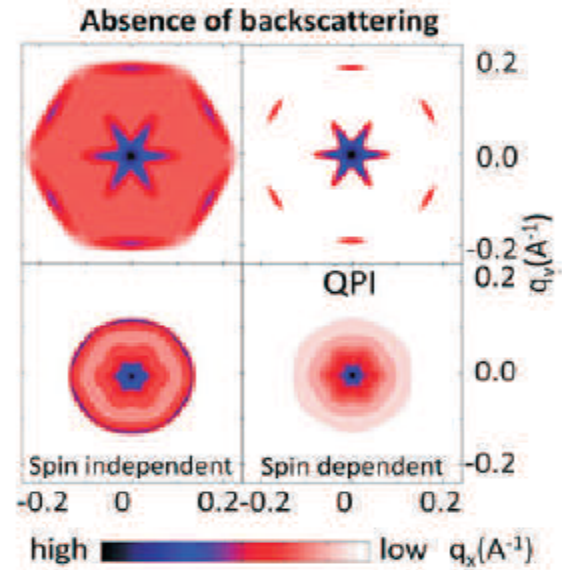
(b)



Directly implies

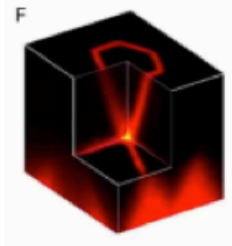
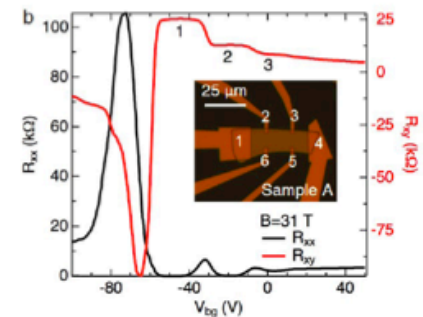
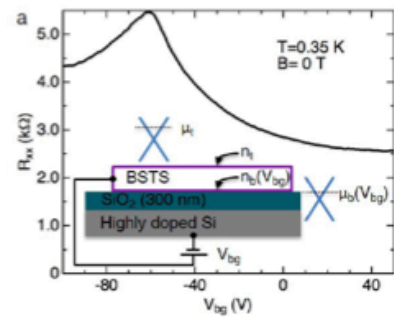
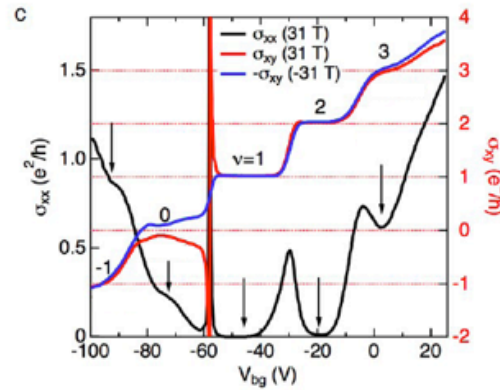
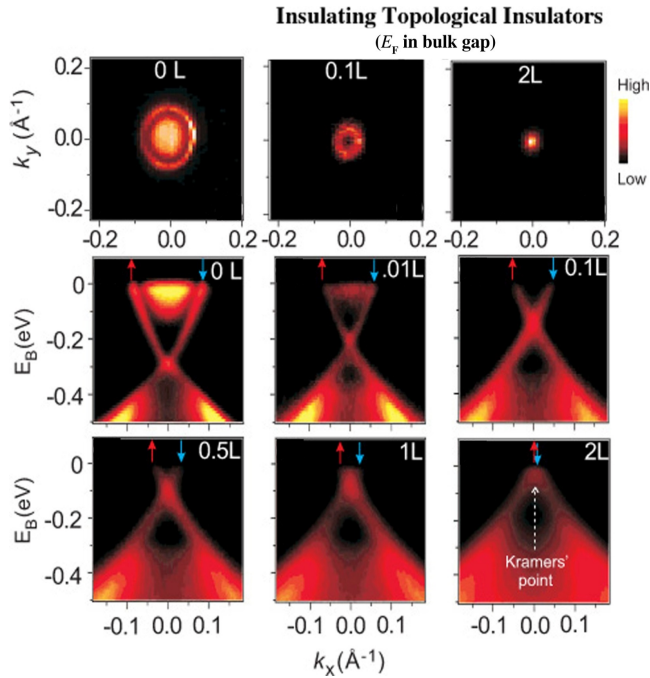


(d)



Calculations

QHE for a 3D Topo. Insulator : Bi(Sb/Te)Se2



Purdue & Princeton
(Xu et.al, Hasan & Chen)
Magnet Lab in Florida

Nature Physics (2014)

TI = 2 surf's (Top + Bot.) of Dirac gas
 $LL = (n_t + 1/2) + (n_b + 1/2) = n_t + n_b + 1$

only Integer QHE !

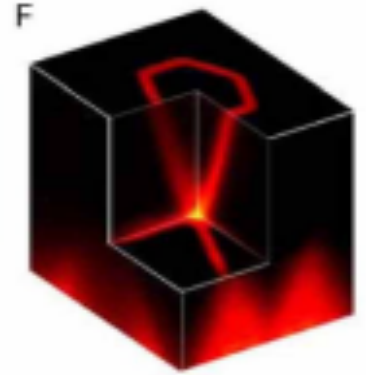
**Bulk insulating (intrinsic)
Topological insulators exist.**

Latest paper : Xu et.al, Nature Physics (2014)

QHE for a 3D Topo. Insulator : Bi(Sb/Te)Se₂

Transport

ARPES+Transport

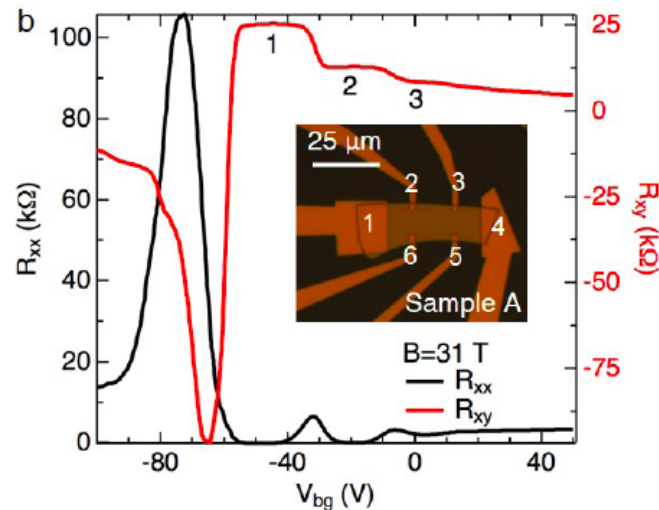
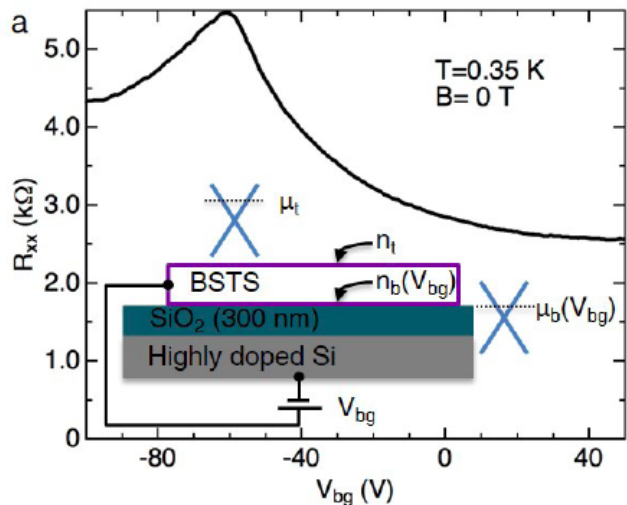
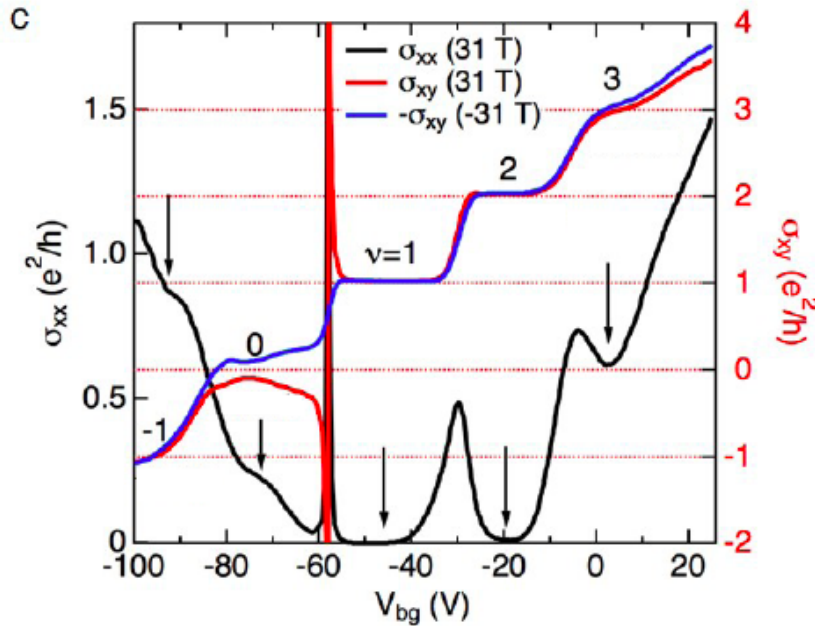


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TI = 2 surf's (Top + Bot.) of Dirac gas
 $LL = (n_t + 1/2) + (n_b + 1/2) = n_t + n_b + 1$

only Integer QHE !



(SPT or Z_2) Topo.Order at Room Temperature

QH-like topological effect at 300K, No magnetic field

Protected Surface States (New 2DEG)

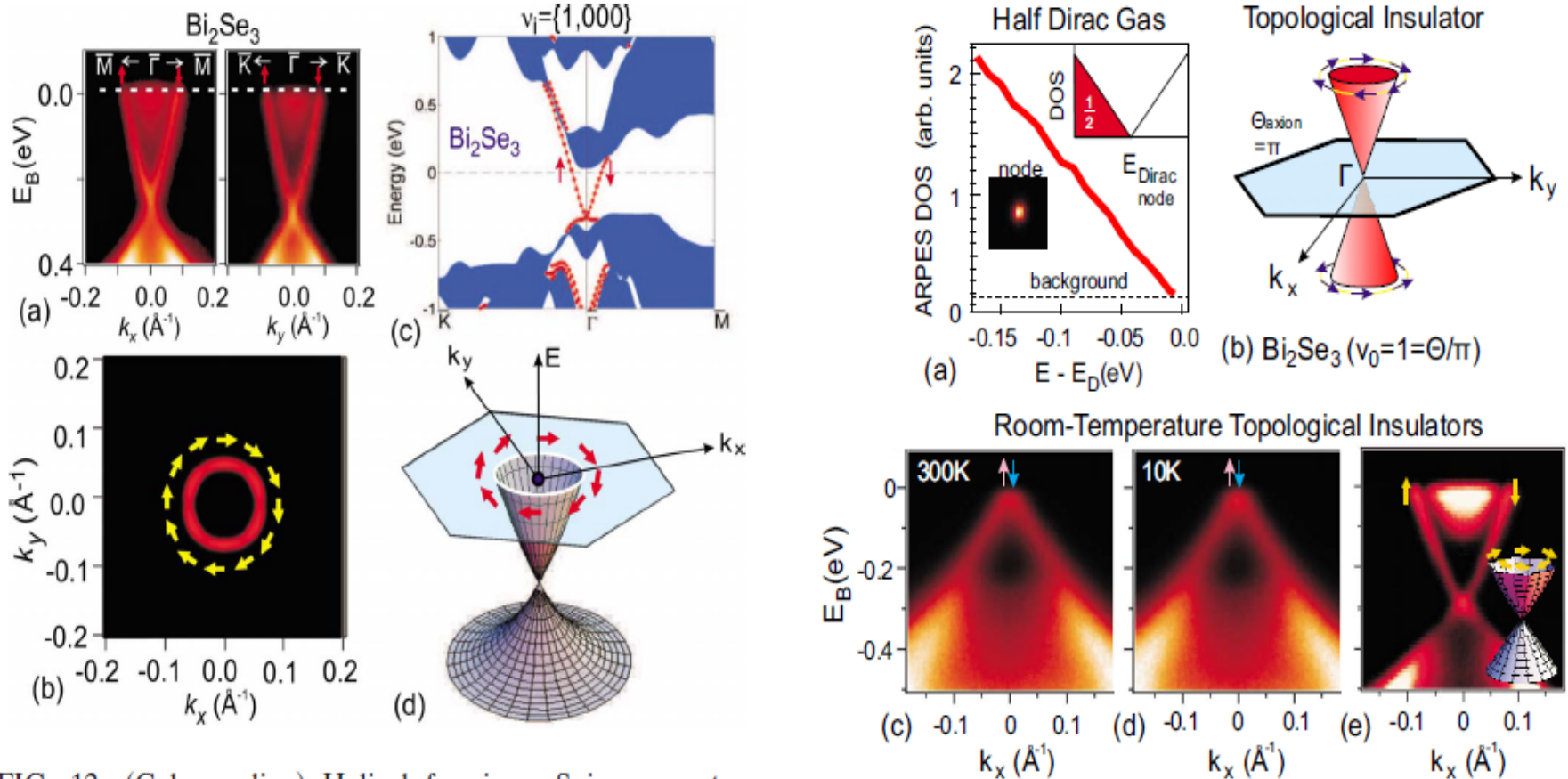


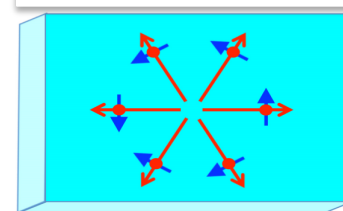
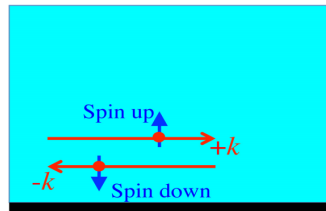
FIG. 12. (Color online) Helical fermions: Spin-momentum

Hsieh, Qian, Wray, Xia et.al., Nature'08, Science'09, Nature'09

3D to 2D Topo. Insulators : $\text{Bi}_2(\text{Se/Te})_3$

MBE growth

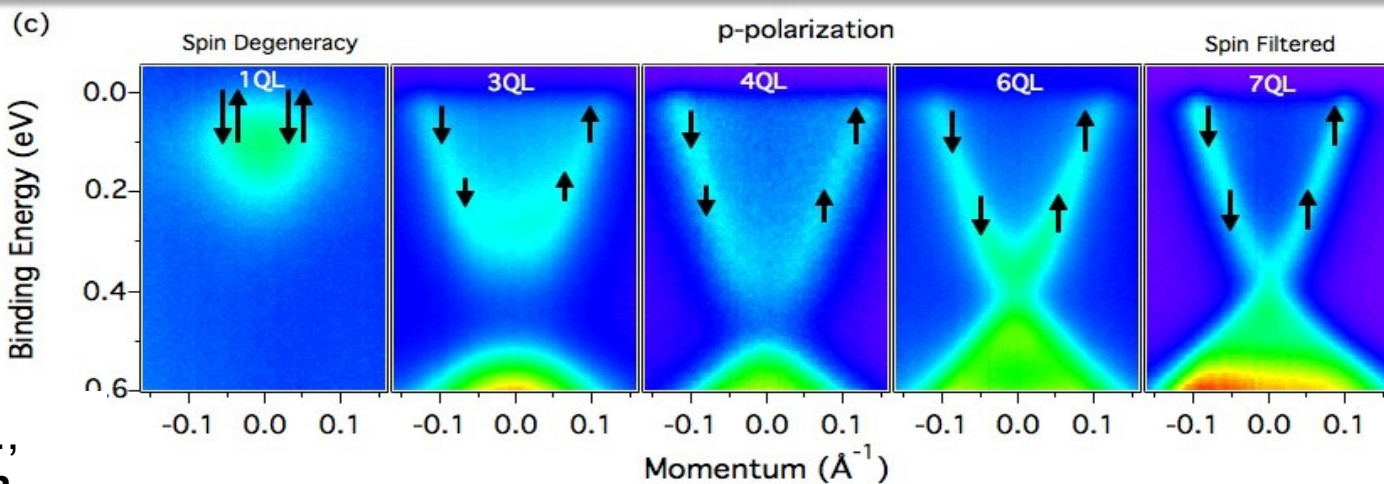
Spin changes
as one 2D \rightarrow 3D
3D \rightarrow 2D (BULK)



2D

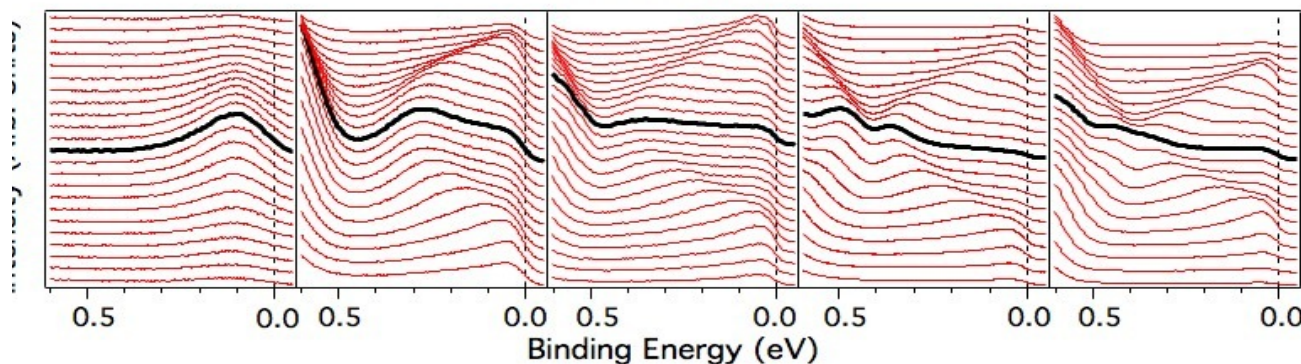


3D



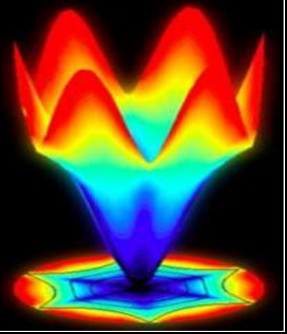
1 QL

7 QL



Neupane et al.,
MZH & Samarth
Nature Commun.
'13 (arXiv)

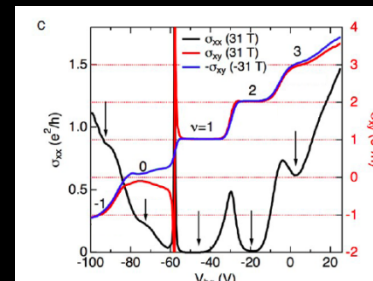
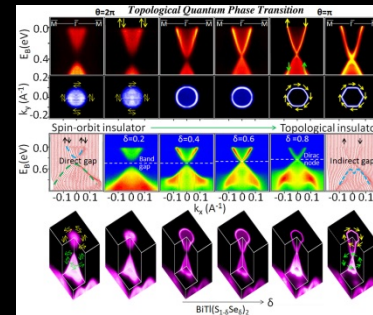
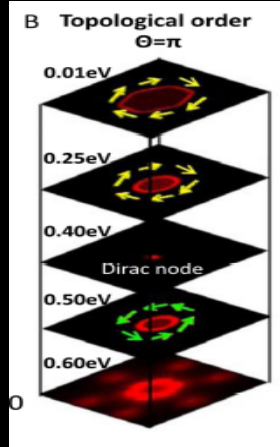
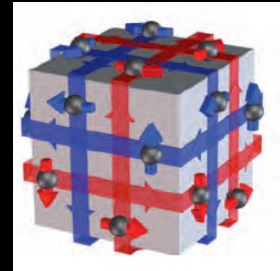
Work by
Xue & Jia groups
'12 (w/out Spin)



Gapped topological states: Topological Insulators

methodology to probe topo.matter.....

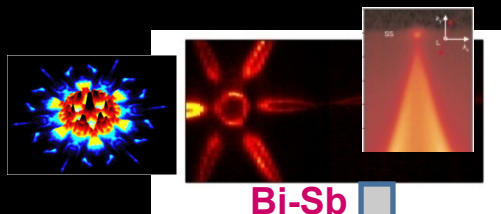
1. Surface States exist and locate inside the bandgap and $\frac{1}{2}$ metallic throughout (**Nature' 08, submit. 2007**)
2. Spin - Momentum Locking (Spin-Texture, Berry's phase) (**Nature' 09, Science' 09**)
3. Topo Phase transition (BI to TI) via spin-orbit tuning (**Nature Physics, Science' 10-11**)
4. Robust up to room temperature (**Nature' 09**)
5. Absence of backscatt. by Spin-Texture (**Nature' 09**)



Experiments on Topo. Insulators (3D)

500+

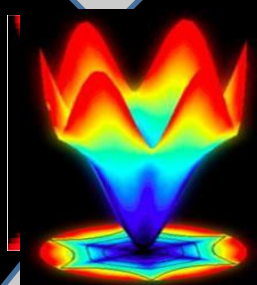
Papers on Bi-based TIs



Hsieh et.al., NATURE 08 (sub. 2007)
Hsieh et.al., SCIENCE 09
Roushan et.al., NATURE 09

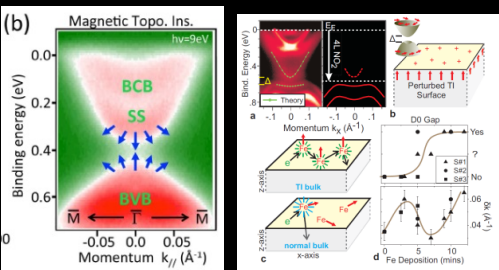
Magnetic TI

Bi_2X_3



Xia et.al, 2008 (arXiv'08, KITP 08)
Xia et.al, 2009 (Nature Phys.) and
Hsieh et.al., Nature 2009
Chen et.al, Sci '09, Zhang et. NatP '09

Superconductivity



Xia et.al, arXiv. 2008

Wray et.al., Nat.Ph'10

Chen et.al, Science '10

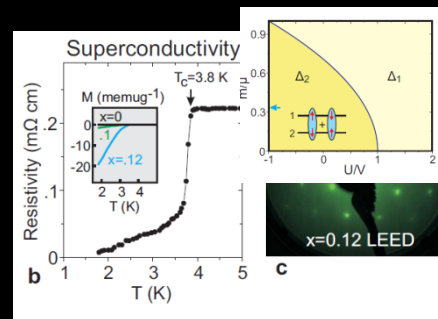
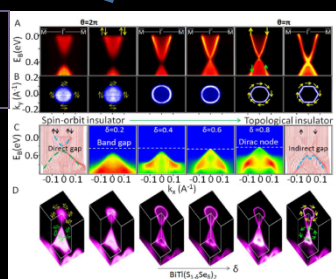
Quantum Hall effect

STM Landau quantization

Xue et.al., PRL 2010

Analytis et.al, NatPhys '10

Xiong et.al., arXiv'11



Hor et.al., PRL 2008

Wray et.al., Nph 2009

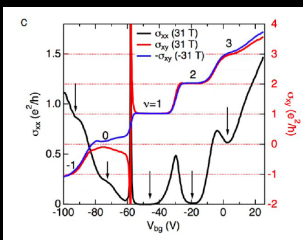
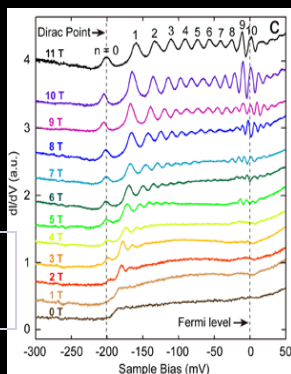
Ando et.al, PRL 2008

Topo. Q. Phase Transition

S.-Y. Xu et.al., 2011
Science '11, arXiv'11

Topo. Kondo Insulators

QAHE

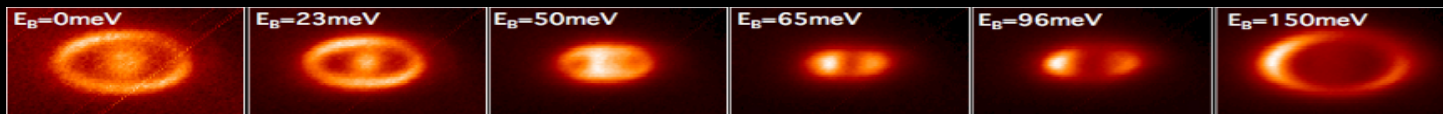
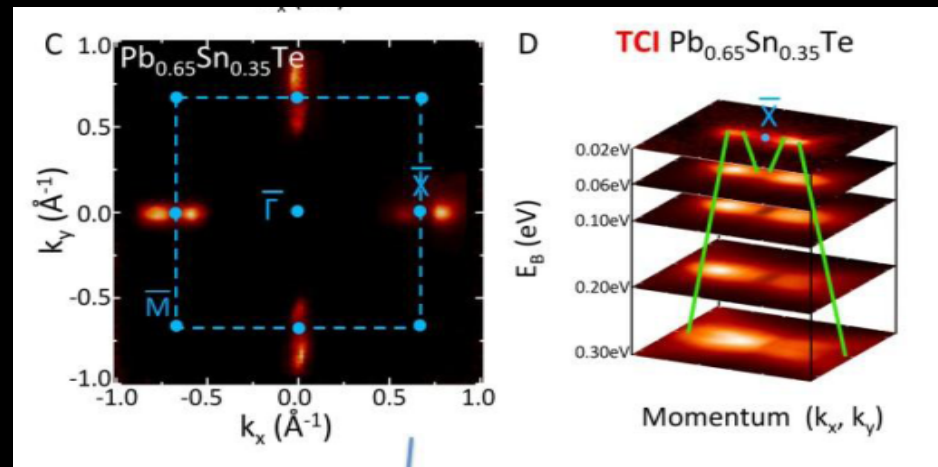


Topo Insulators beyond Z_2 or TRI

TR invariance \leftrightarrow SG symmetry (TCI)

PbSnTe and theory : Fu-Kane '07; Fu '11, Lin-Bansil-Fu et.al., '12
PbSnTe

Mirror Chern no. measured in Bi-Sb;
Hsieh, Xia, et.al., (Kane & Hasan) SCIENCE' 09

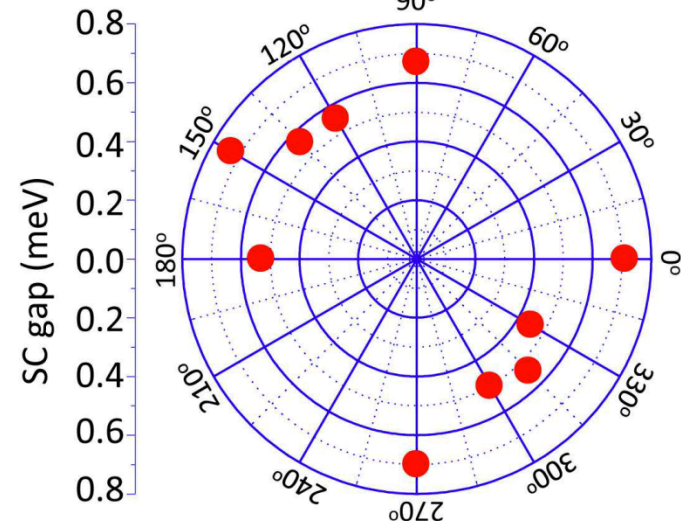
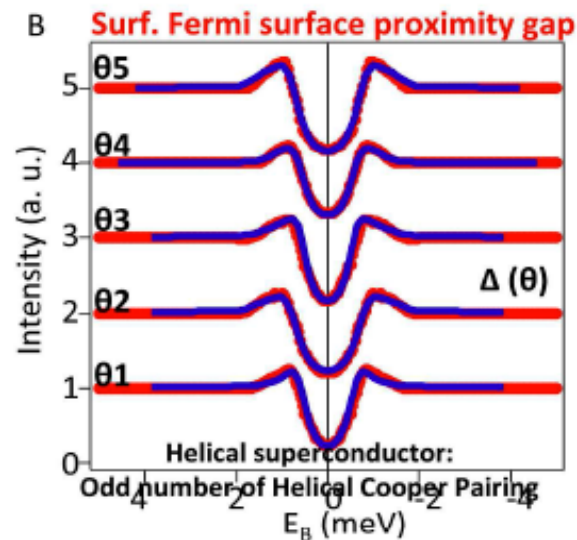
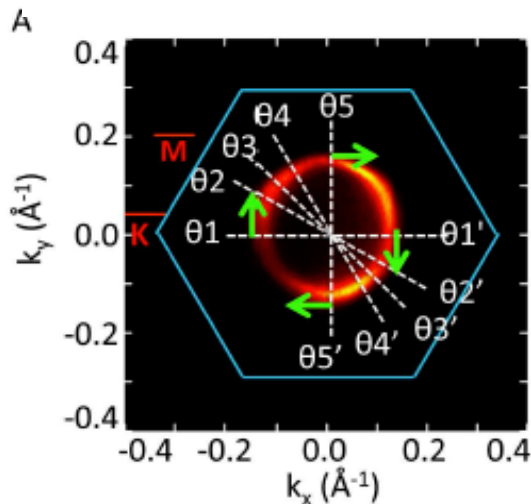
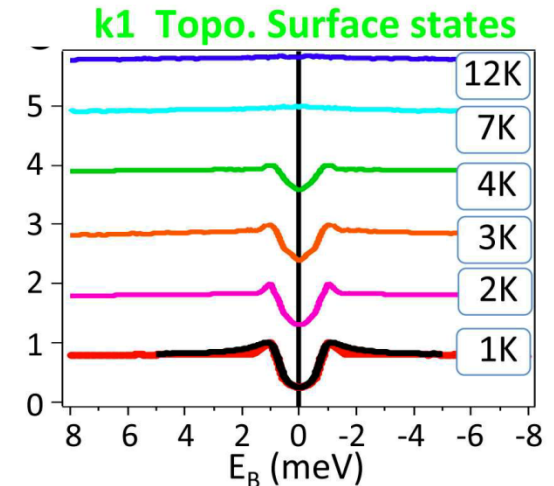
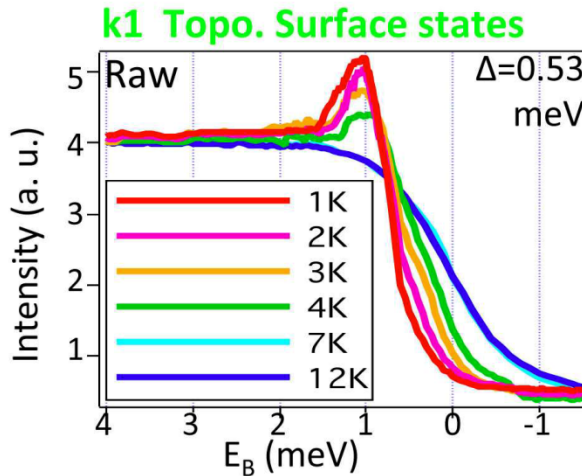
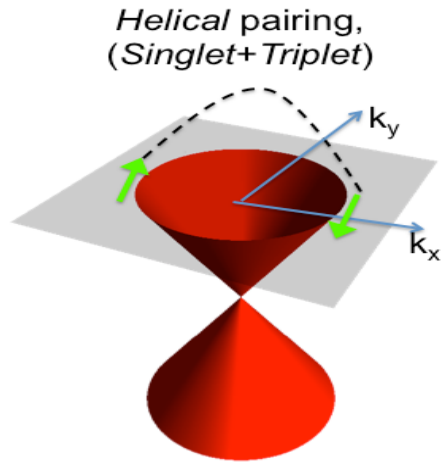


More Gapped topological states:

ARPES \longleftrightarrow MBE Growth

Feedback Loop

2D Topo. (Helical) Superconductor

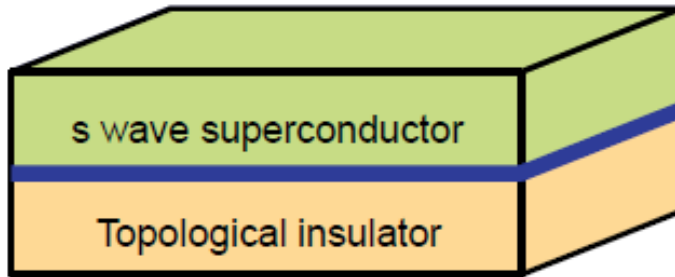


S. Xu, C. Liu et.al., (MZH) Nature Phys (2014)

Majorana Platform

Superconducting Proximity Effect

Fu, Kane PRL 08



Surface states acquire superconducting gap Δ due to Cooper pair tunneling

BCS Superconductor :

$$\langle c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger \rangle \propto \Delta e^{i\varphi}$$

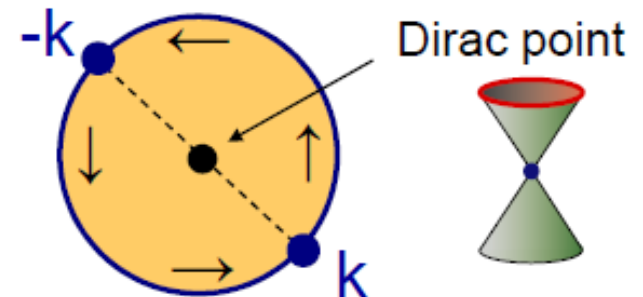
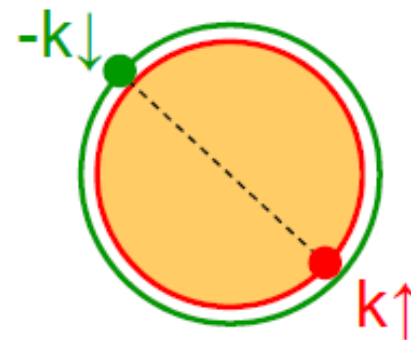
(s-wave, singlet pairing)

Superconducting surface states

$$\langle c_k^\dagger c_{-k}^\dagger \rangle \propto \Delta_{\text{surface}} e^{i\varphi}$$

(s-wave, singlet pairing)

Half an ordinary superconductor
Highly nontrivial ground state

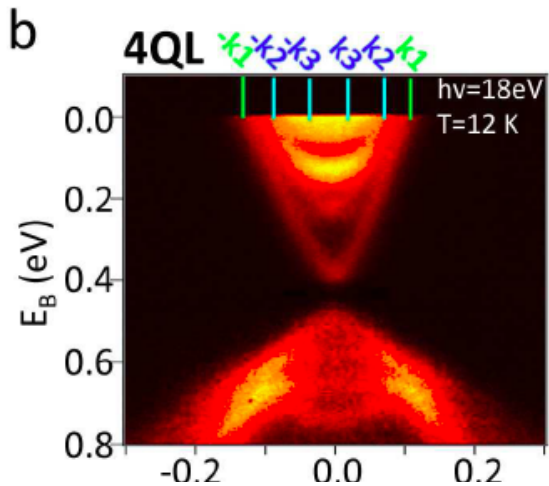


Slide from C. Kane

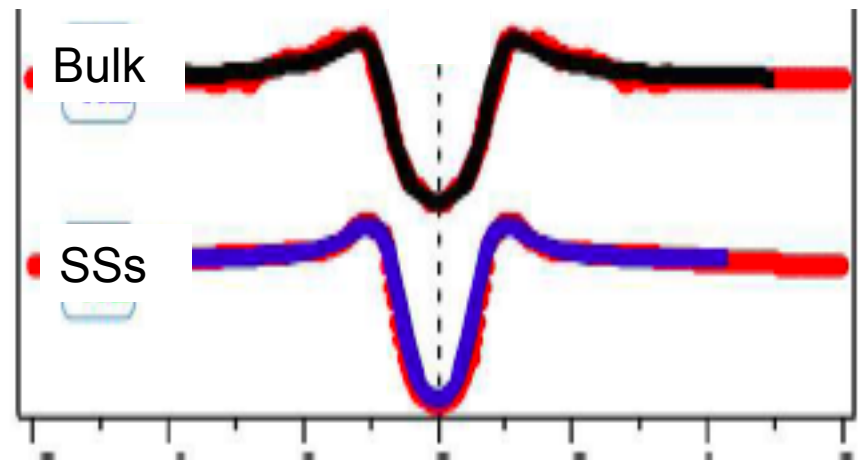
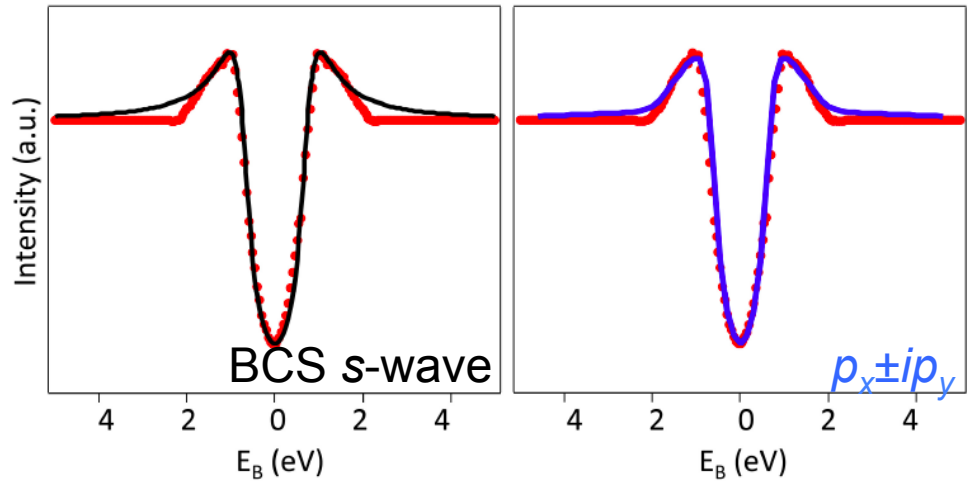
SC gap fitting

Surface $p_x \pm ip_y$; Bulk band: s-wave

Surface state gap fitting



Surface vs bulk gap fitting

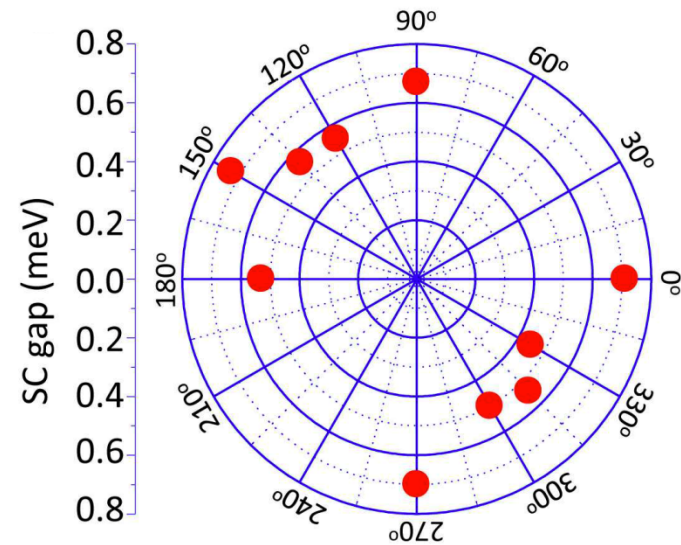
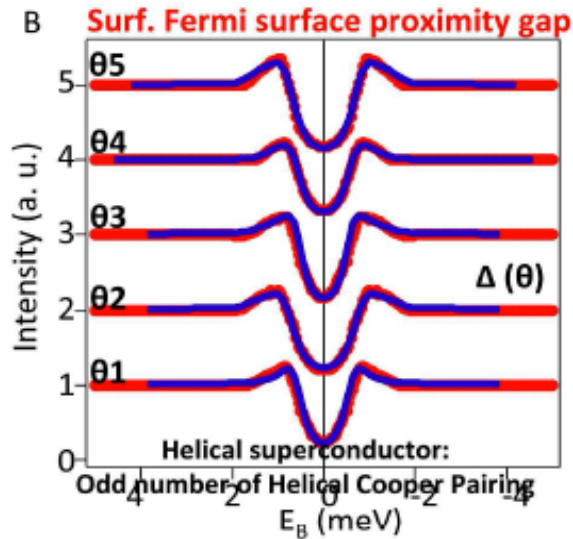
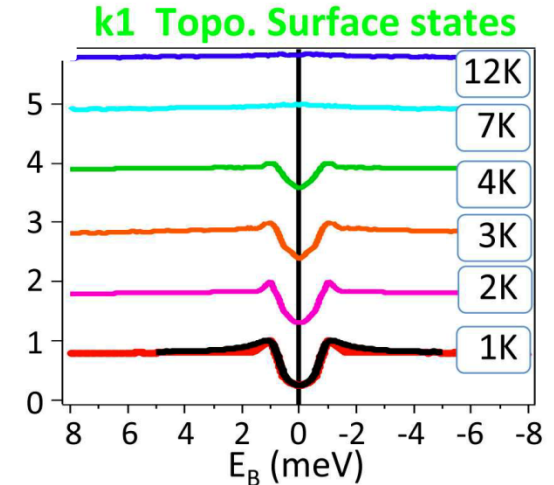
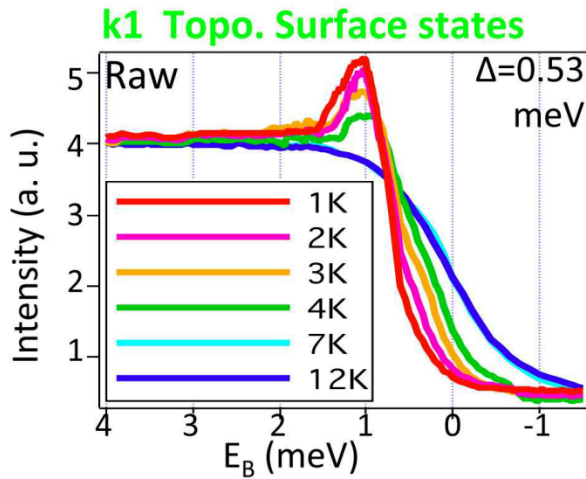
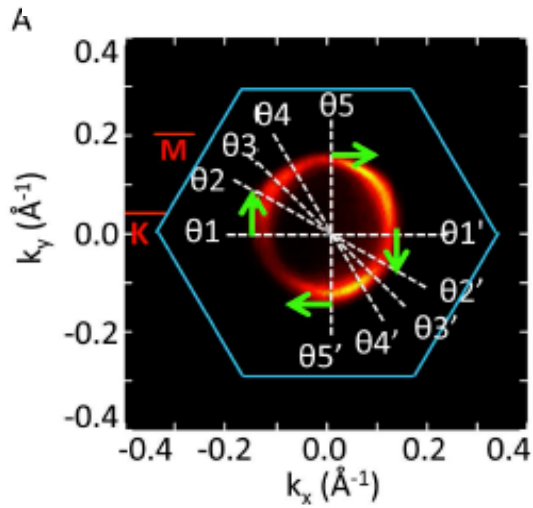
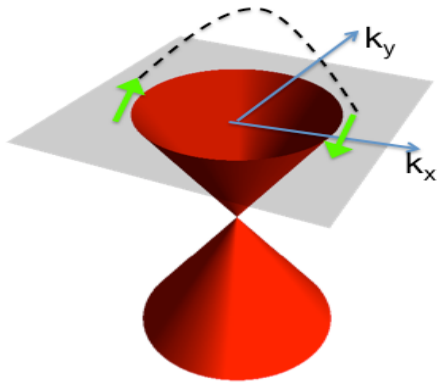


2D Topo. Superconductor

ARPES \longleftrightarrow MBE Growth

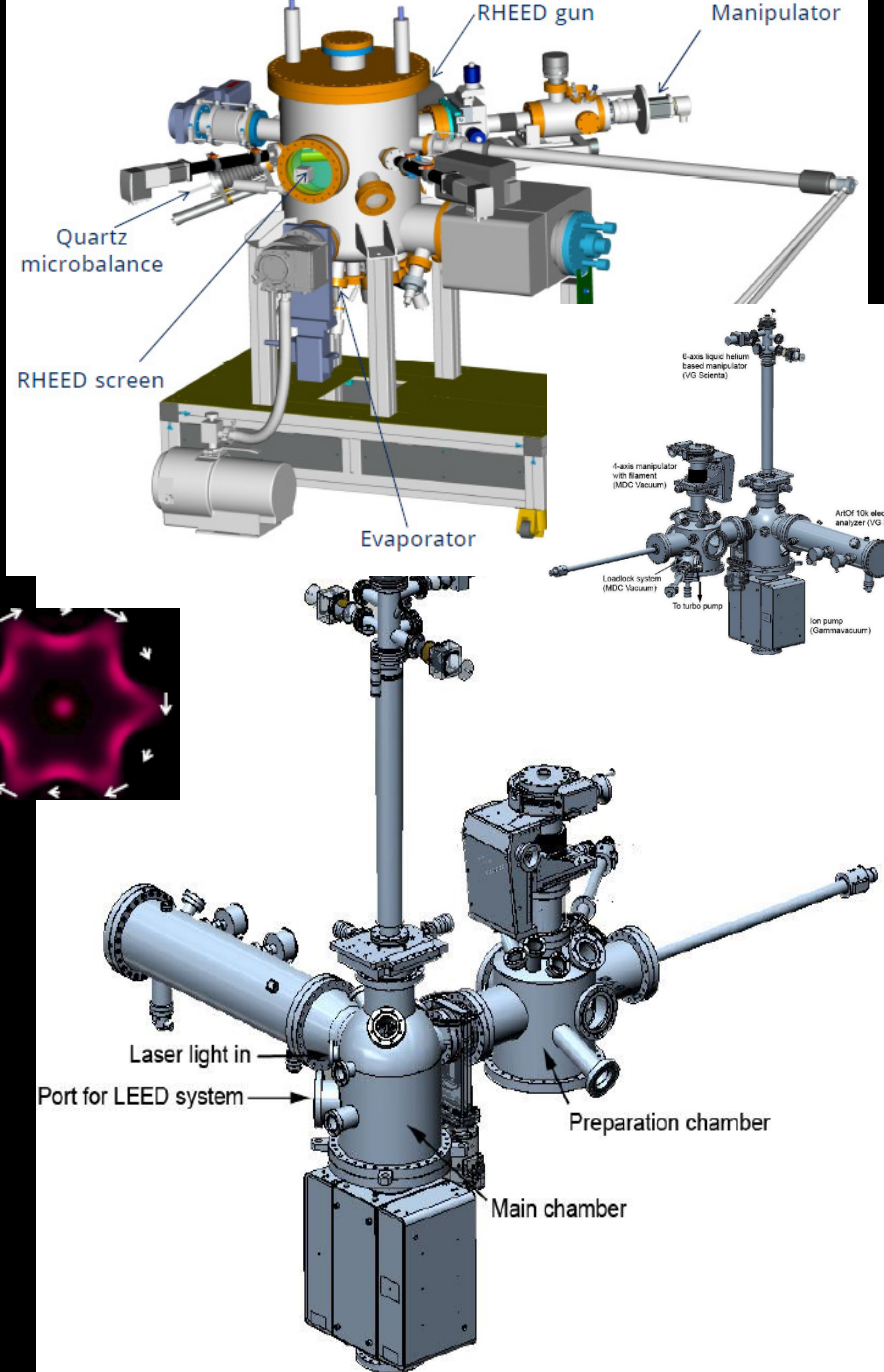
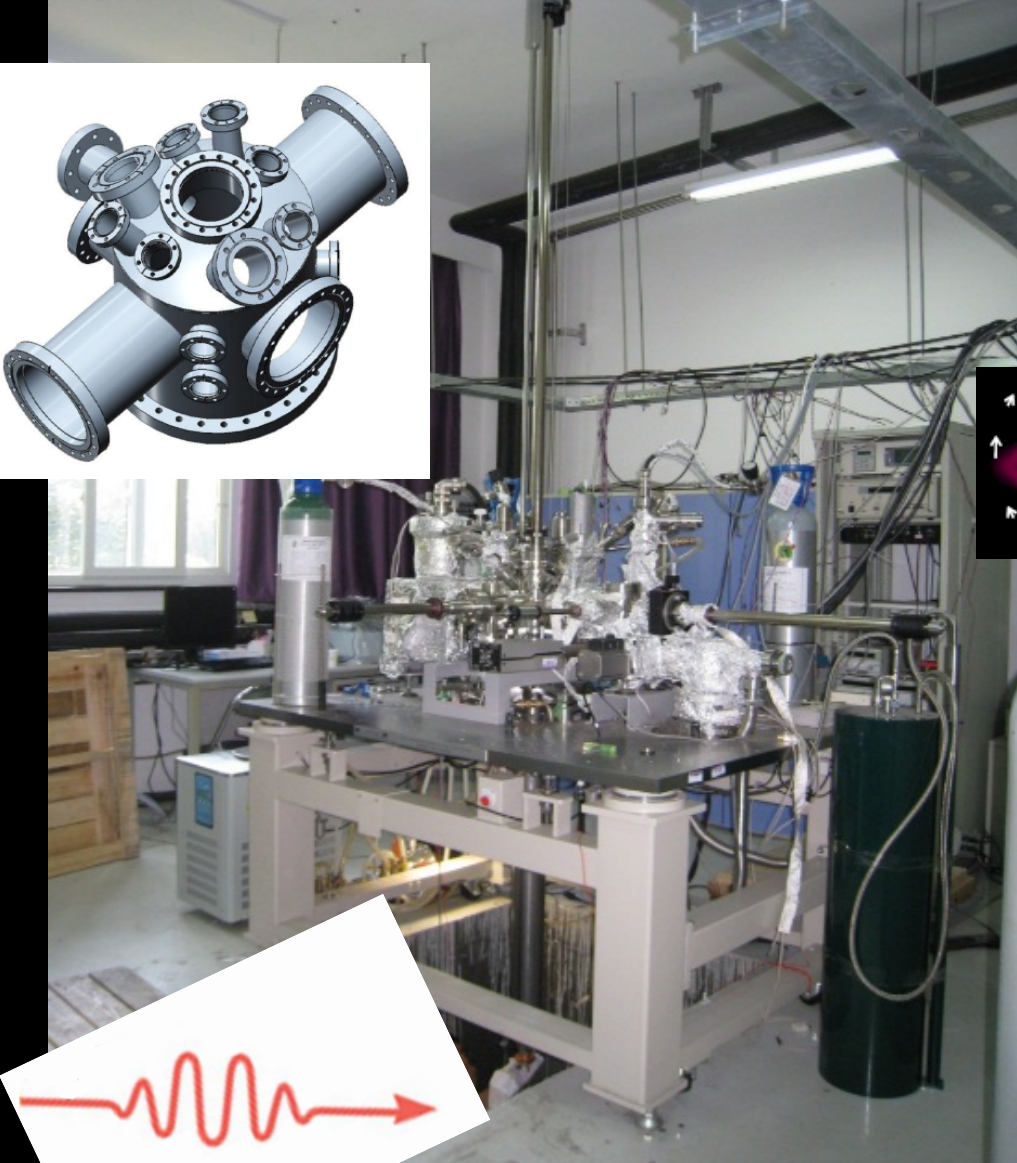
Feedback Loop

Helical pairing,
(Singlet+Triplet)



S. Xu, C. Liu et.al., (MZH) Nature Phys (2014)

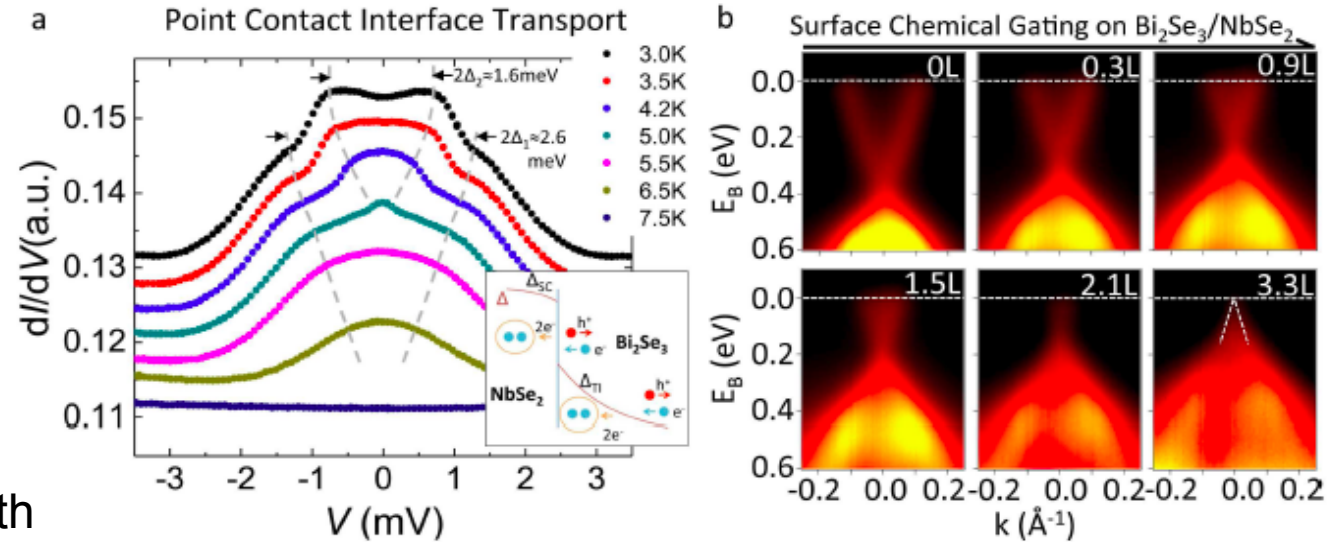
MBE-STM (+ HR ARPES) Under construction



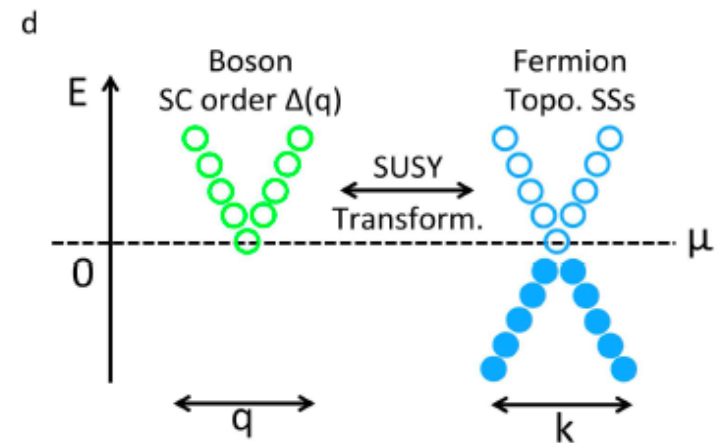
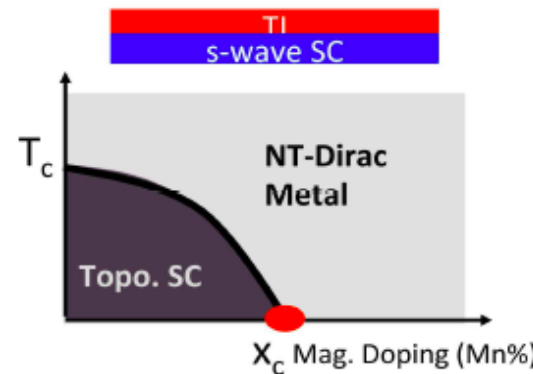
Samples can be driven near a Critical Point

(Emergent SuperSymmetry in theory)

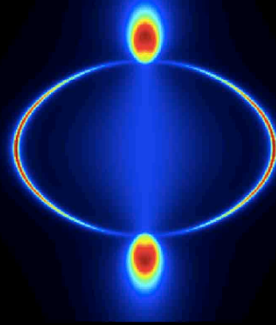
see prediction by Grover, Vishwanath et.al., Science'14



ARPES \longleftrightarrow Growth
Feedback Loop



S. Xu, et.al., (MZH) Nature Phys (2014)

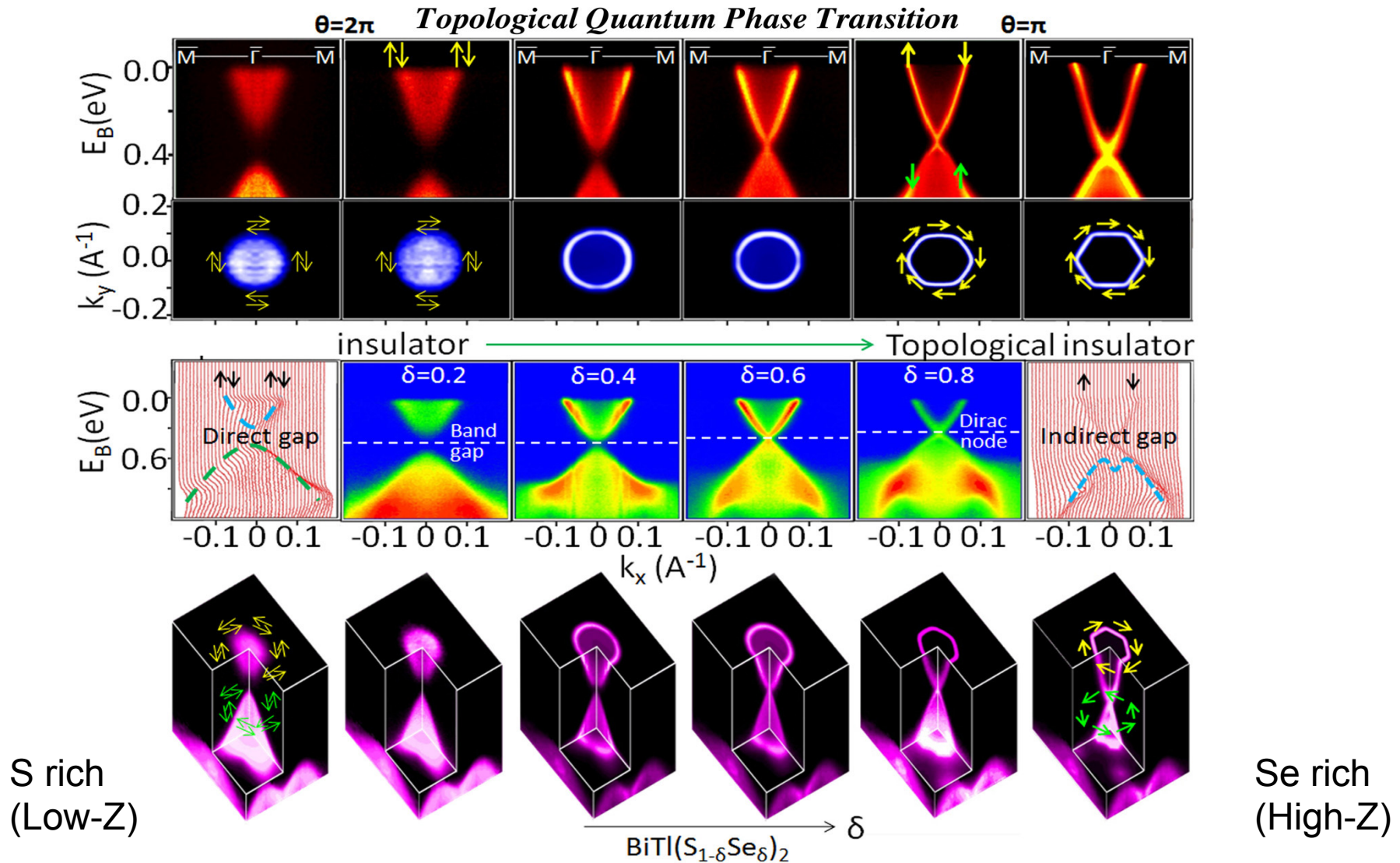


Can gapless systs be topological?

bulk Gapless *but* protected surface sates

3+1 D

Imaging a Topo. Insulator being born out of a Bloch Insulator as SOC is tuned



S.Y. Xu, Y. Xia, L. Wray *et.al.*, (MZH) Science '11

Elektron und Gravitation. I.

Von Hermann Weyl in Princeton, N. J.

(Eingegangen am 8. Mai 1929).

Einleitung. Verhältnis der allgemeinen Relativitätstheorie zu den quantentheoretischen Feldgleichungen des spinnenden Elektrons: Masse, Eichinvarianz, Fernparallelismus. Zu erwartende Modifikationen der Diracschen Theorie. —

5, 1937

PHYSICAL REVIEW

VOLUME

first Solid-State Weyl

Accidental Degeneracy in the Energy Bands of Crystals

CONYERS HERRING

Princeton University, Princeton, New Jersey

(Received June 16, 1937)

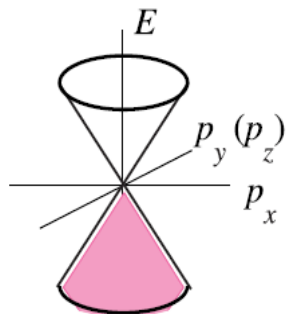
$$N_3 = \frac{1}{8\pi} \epsilon_{ijk} \int_{\text{over 2D surface around Fermi point}} dS^i \hat{\mathbf{g}} \cdot (\partial^j \hat{\mathbf{g}} \times \partial^k \hat{\mathbf{g}})$$

Topological classification
(Volovik, Wan et.al., others...)

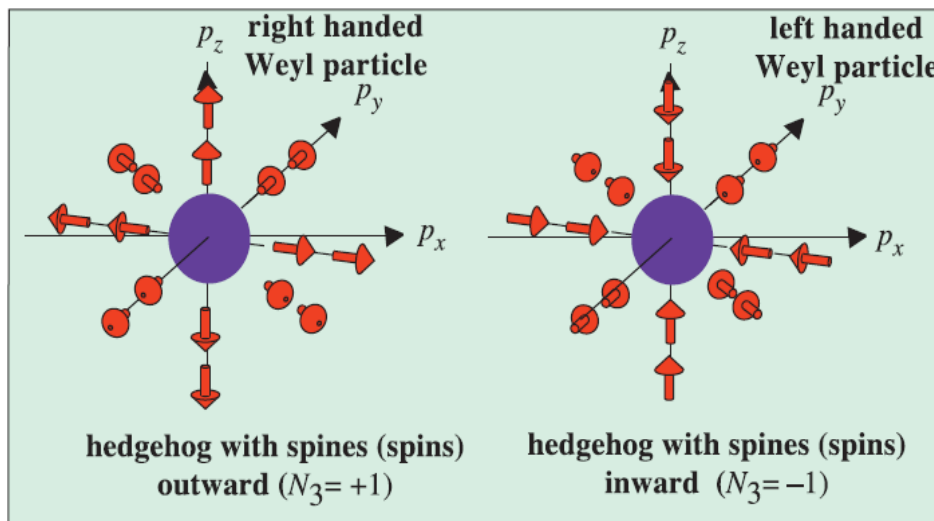
The circumstances are investigated under which two wave functions occurring in the Hartree-Fock solution for a crystal can have the same reduced wave vector and the same energy. It is found that coincidence of the energies of wave functions with the same symmetry properties, as well as those with different symmetries, is often to be expected. Some qualitative features

Weyl Fermions and Topo. Invariants

Weyl particles in Standard Model - hedgehogs in p-space



Weyl point:
conical (diabolical)
crossing point
in fermionic spectrum
in momentum space



$$H = +c \sigma \cdot \mathbf{p}$$

$$\mathbf{g}(\mathbf{p}) = +c\mathbf{p}$$

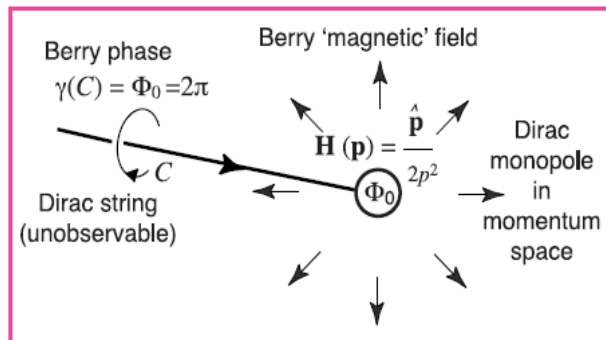
$$H = \sigma \cdot \mathbf{g}(\mathbf{p})$$

$$H = -c \sigma \cdot \mathbf{p}$$

$$\mathbf{g}(\mathbf{p}) = -c\mathbf{p}$$

$$N_3 = \frac{1}{8\pi} \epsilon_{ijk} \int_{\text{over 2D surface around Fermi point}} dS^i \hat{\mathbf{g}} \cdot (\partial^j \hat{\mathbf{g}} \times \partial^k \hat{\mathbf{g}})$$

**p-space topological invariant
for Weyl particles**



Weyl point: Berry-Dirac monopole in p-space

All 3 Pauli Matrices
are used up in 3D
So gap opening is
not possible

Weyl (1929), Herring (1937), Nielsen-Ninomiya (1980s), Volovik (1987, 2003);

Weyl fermion in materials

$$\sigma^\mu \partial_\mu \psi = 0$$

Solid State quasiparticle Weyl

... in Crystals/SSP (1937-):
C. Herring (1937) [Princeton Univ.]
Abrikosov & Benelavsky (1971)
Nielsen-Ninomiya (1983)
Volovik (2003)

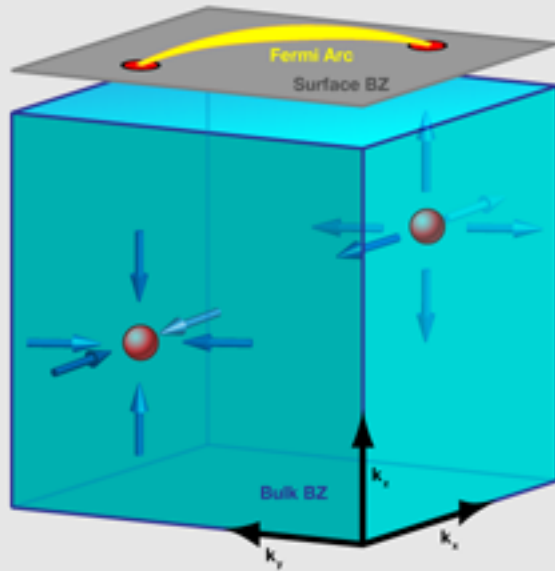
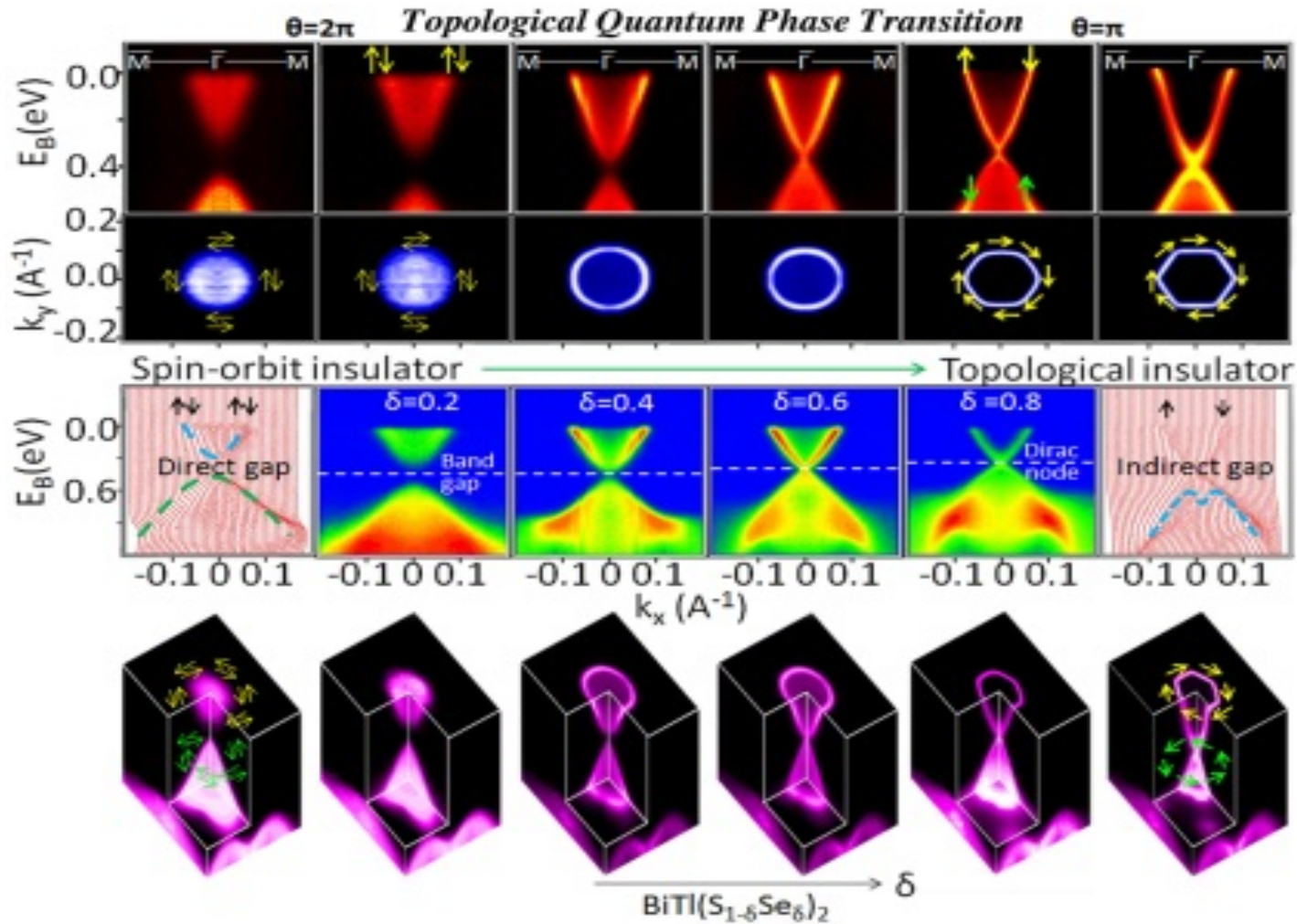


Image: Burkov & Balents (2011)

Murakami (2007), **Topo. Insulator connection...**
Wan, Turner, Vishwanath, Savrasov 2011 PRB
Y. Ran's group (boston) 2011 PRB
Iridate – spc. magnetic order etc.
Burkov, Balents et.al., 2011 PRL
TI/NI multilayers – fine tuning, magnetic order
Fang, Dai (also magnetic Hg-Cr-Se) 2012
Many more proposals on **magnetic compounds**
by many groups but all T-breaking
But
no expt'l realization of these predictions

Early on I was interested in /-breaking Weyl
Singh et.al. (Lin, MZH & Bansil), **PRB 2012**



Wray:

Neupane & Sankar:

Suyang Xu & Ilya: to search in the database to find I-broken materials

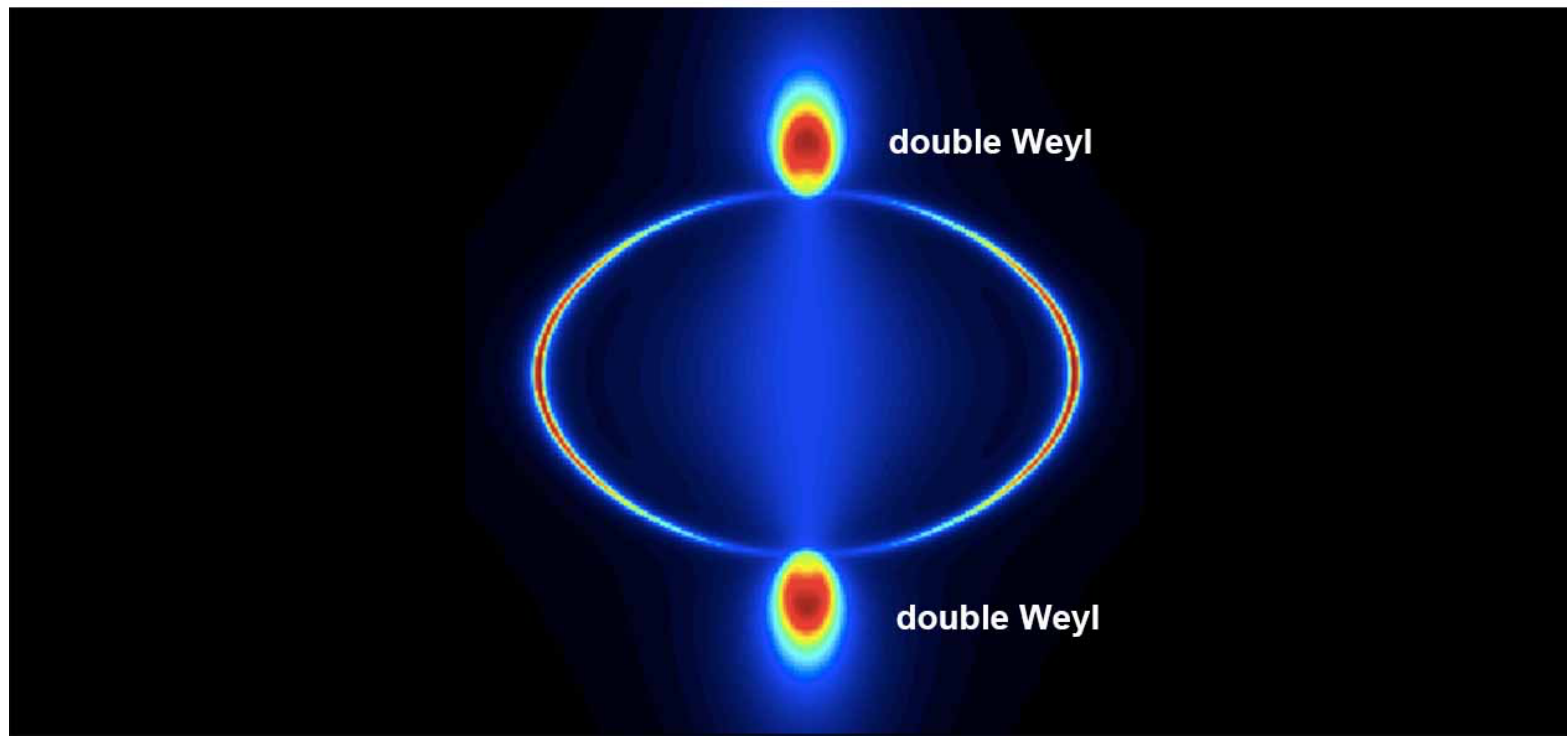
to magnetize the Dirac critical point

to magnetize Bi-Sb, Cd-As

Observation of Fermi arc surface states in a topological metal

Publication date: December 18, 2014

Su-Yang Xu,^{1,2*} Chang Liu,^{1*} Satya K. Kushwaha,³ Raman Sankar,⁴ Jason W. Krizan,³ Ilya Belopolski,¹ Madhab Neupane,¹ Guang Bian,¹ Nasser Alidoust,¹ Tay-Rong Chang,⁵ Horng-Tay Jeng,^{5,6} Cheng-Yi Huang,⁷ Wei-Feng Tsai,⁷ Hsin Lin,⁸ Pavel P. Shibayev,¹ Fangcheng Chou,⁴ Robert J. Cava,³ M. Zahid Hasan^{1,2†}



Searching for compounds

Results: List View								# of Hits: 882	
Select All	Deselect All	Show Detailed View	Show Synoptic View	Export Selected Data			Back to Query		
Coll. Code	HMS	Struct. Form.	Struct. Type	Title	Authors	Reference			
<input type="checkbox"/>	22347	P 1 21 1	Li2 (S O4) (H2 O)	Li2SO4H2O	Crystal structure of the monohydrate of lithium sulfate, Li2 S O4 H2 O	Rannev, N.V.; Datt, I.D.; Tovbis, A.B.; Ozerov, R.P.	Kristallografiya (1965) 10, p914-p915		
<input type="checkbox"/>	23017	P 1 1 21	Li4 Zn (P O4)2		Crystal structure of lithium zinc orthophosphate Li4 Zn (P O4)2	Sandomirskii, P.A.; Simonov, M.A.; Belov, N.V.	Doklady Akademii Nauk SSSR (1976) 228, p344-p347		
<input type="checkbox"/>	23021	P 1 1 21	Na.55 Cd2.45 P2 O7.45 (O H).55		Crystal Structure of Na, Cd- Phosphate Na1-x, Cdx Cd2 (P O4) (P O3+x (O H)1-x)	Ivanov, Yu.A.; Simonov, M.A.; Belov, N.V.	Doklady Akademii Nauk SSSR (1976) 228, p600-p602		
<input type="checkbox"/>	23022	P 1 1 2	Ba3 Ge9 O20 (O H)2		Crystal structure of Ba3 Ge9 O20 (O H)2	Malinovskii, Yu.A.; Pobedimskaya, E.A.; Belov, N.V.	Doklady Akademii Nauk SSSR (1976) 227, p1350-p1353		
<input type="checkbox"/>	23150	P 1 21 1	H Br (H2 O)4		Hydrogen-Bond Studies. XXX. The Crystal Structure of Hydrogen Bromide Tetrahydrate, (H7O3)+ (H9O4)+ 2Br- .(H2O) (H2 O)	Lundgren, J.O.; Olovsson, I.	Journal of Chemical Physics (1968) 49, p1068-p1074		
<input type="checkbox"/>	23841	P 1 21 1	P4 S5	P4S5	Refinement of the crystal structures of some phosphorus sulphides	Vos, A.; Olthof, R.; van Bolhuis, F.; Botterweg, R.	Acta Crystallographica (1,1948-23,1967) (1965) 19, p864-p867		
<input type="checkbox"/>	23974	P 1 21 1	S3 N2 Cl2		The Crystal Structure of Chlorothiodiazyl Chloride, S3 N2 Cl2	Zalkin, A.; Hopkins, T.E.; Templeton, D.H.	Inorganic Chemistry (1966) 5, p1767-p1770		
<input type="checkbox"/>	24848	P 1 21 1	N3 P3 Cl4 (Fe (C O)4)2		Synthesis of a Di-iron-spirocyclotriphazene and a Tri-iron-cluster-cyclotriphosphazene	Suszko, P.R.; Whittle, R.R.; Allcock, H.R.	Journal of the Chemical Society. Chemical Communications (1972-) (1982) 1982, p1344-p1344		
<input type="checkbox"/>	25702	P 1 21 1	N H4 (P O S (N H2)2)		Die Kristallstruktur von Ammonium-diamidothiophosphat	Mootz, D.; Look, W.; Sassmannshauer G.	Zeitschrift fuer Anorganische und Allgemeine Chemie (1950) (DE) (1968) 358, p282-p295		
<input type="checkbox"/>	26010	P 1 1 21	Ca2 (Nb2 O7)	La2Ti2O7(mP44	Compounds with perovskite-type slabs. III. The structure of a monoclinic modification of Ca2 Nb2 O7	Ishizawa, N.; Marumo, F.; Iwai, S.I.; Kimura, M.; Kawamura, T.	Acta Crystallographica B (24,1968-38,1982) (1980) 36, p763-p766		

Challenges in finding an I-breaking Weyl semimetal

- **>1000** I-breaking compounds entries (based on crystallographic library).
- **So many compounds have negative MR, transport does not help!!**
- **Weyl nodes at arbitrary k points**
- **Where is the Fermi level ?**
- **What is the cleaved surface potential?**
- **How to separate surface and bulk?**

Calculation/Prediction can NOT tell us that it will work

Experimentally! So many people predicted so many Weyl compounds

Searching for compounds

Results: List View # of Hits: 882

[Select All](#)
[Deselect All](#)
[Show Detailed View](#)
[Show Synoptic View](#)
[Export Selected Data](#)
[Back to Query](#)

Coll. Code	HMS	Struct. Form.	Struct. Type	Title	Authors	Reference		
<input type="checkbox"/>	22347	P 1 21 1	Li2 (S O4) (H2 O)	Li2SO4H2O	Crystal structure of the monohydrate of lithium sulfate, Li2 S O4 H2 O	Rannev, N.V.; Datt, I.D.; Tovbis, A.B.; Ozerov, R.P.	Kristallografiya (1965) 10, p914-p915	
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<input type="checkbox"/>	23021	P 1 1 21	Na.55 Cd2.45 P2 O7.45 (O H).55		Crystal Structure of Na, Cd- Phosphate Na1-x, Cdx Cd2 (P O4) (P O3+x (O H)1-x)	Ivanov, Yu.A.; Simonov, M.A.; Belov, N.V.	Doklady Akademii Nauk SSSR (1976) 228, p600-p602	
<input type="checkbox"/>	23022	P 1 1 2	Ba3 Ge9 O20 (O H)2		Crystal Structure of Ba3 Ge9 O20 (O H)2	Malinovskii, Yu.A.; Pobedimskaya, E.A.; Belov, N.V.	Doklady Akademii Nauk SSSR (1976) 227, p1350-p1353	
<input type="checkbox"/>	23150	P 1 21 1	H Br (H2 O)4		Hydrogen-Bond Studies. XXX. The Crystal Structure of Hydrogen Bromide Tetrahydrate, (H7O3)+ (H9O4)+ 2Br- .(H2O) (H2 O)	Lundgren, J.O.; Olovsson, I.	Journal of Chemical Physics (1968) 49, p1068-p1074	
<input type="checkbox"/>	23841	P 1 21 1	P4 S5	P4S5	Refinement of the crystal structures of some phosphorus sulphides	Vos, A.; Olthof, R.; van Bolhuis, F.; Botterweg, R.	Acta Crystallographica (1,1948-23,1967) (1965) 19, p864-p867	
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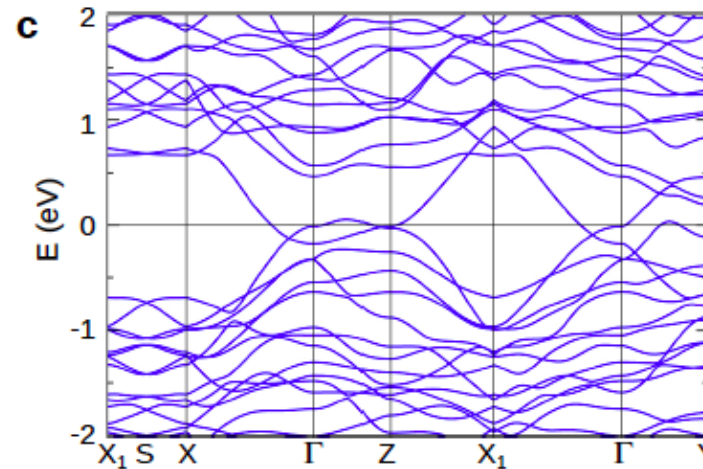
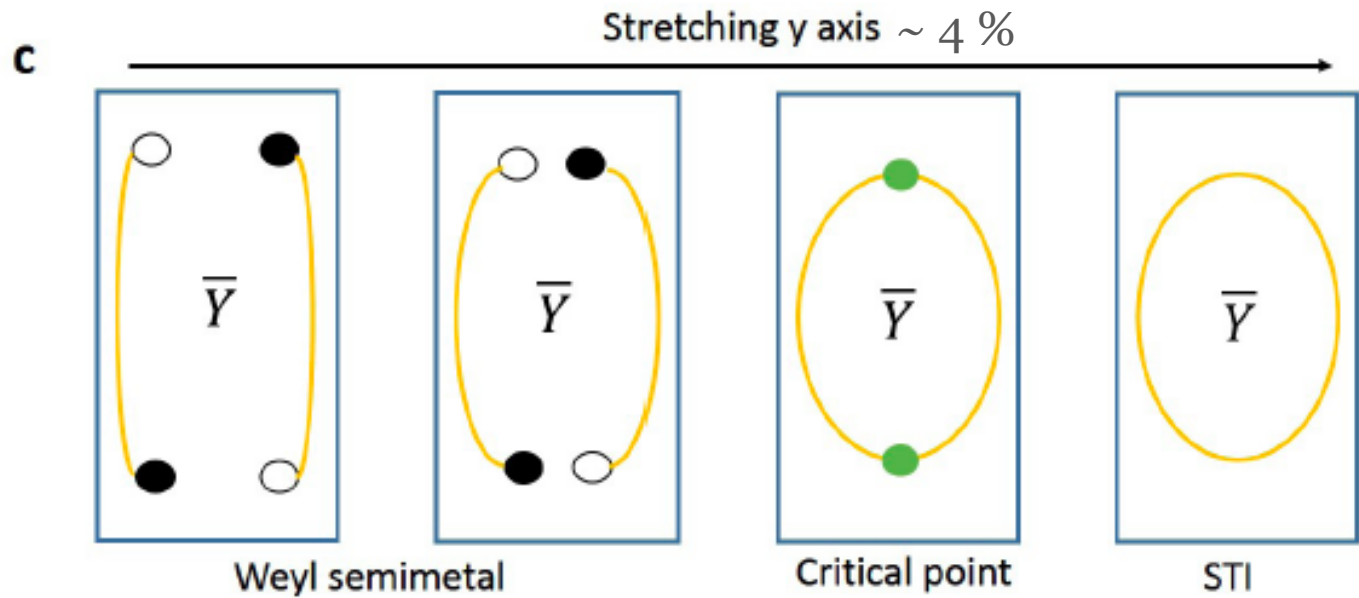
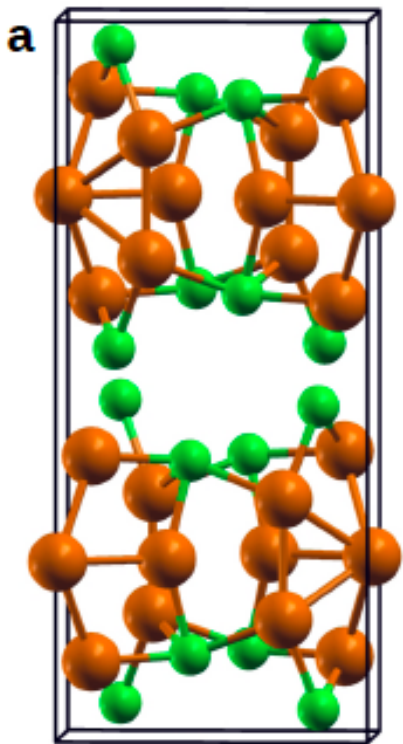
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Conducted by
Suyang Xu
& Ilya Belopolski

We found the
TaAs, Ta3S2,
Ta-Se-I class

Ta₃S₂ – Topo. Weyl to Insulator Transition

G. Chang*, S.-Y. Xu* et al. <http://arxiv.org/abs/1512.08781> (2015)

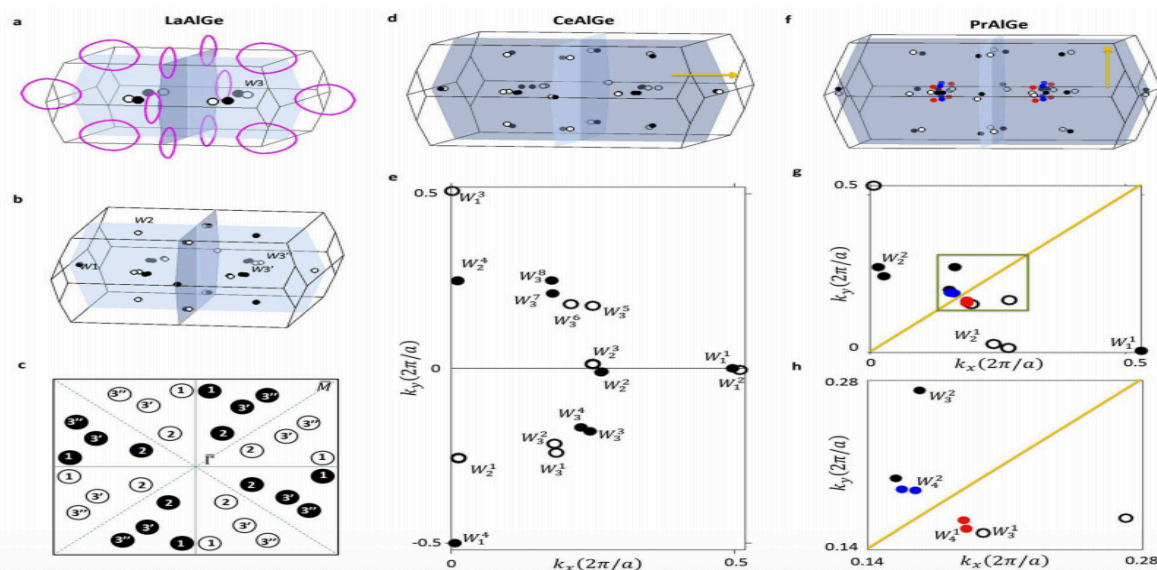


Theoretical prediction of magnetic and noncentrosymmetric Weyl fermion semimetal states in the R-Al-X family of compounds (R=rare earth, Al=aluminium, X=Si, Ge)

Guoqing Chang, Bahadur Singh, Su-Yang Xu, Guang Bian, Shin-Ming Huang, Chuang-Han Hsu, Ilya Belopolski, Nasser Alidoust, Daniel S. Sanchez, Hao Zheng, Hong Lu, Xiao Zhang, Yi Bian, Tay-Rong Chang, Horng-Tay Jeng, Arun Bansil, Han Hsu, Shuang Jia, Titus Neupert, Hsin Lin, M. Zahid Hasan

(Submitted on 7 Apr 2016 (v1), last revised 12 Apr 2016 (this version, v3))

Weyl semimetals are novel topological conductors that host Weyl fermions as emergent quasiparticles. While the Weyl fermions in high-energy physics are strictly defined as the massless solution of the Dirac equation and uniquely fixed by Lorentz symmetry, there is no such constraint for a topological metal in general. Specifically, the Weyl quasiparticles can arise by breaking either the space-inversion (\mathcal{I}) or time-reversal (\mathcal{T}) symmetry. They can either respect Lorentz symmetry (type-I) or strongly violate it (type-II). To date, different types of Weyl fermions have been predicted to occur only in different classes of materials. In this paper, we present a significant materials breakthrough by identifying a large class of Weyl materials in the RAIX (R=Rare earth, Al, X=Ge, Si) family that can realize all different types of emergent Weyl fermions (\mathcal{I} -breaking, \mathcal{T} -breaking, type-I or type-II), depending on a suitable choice of the rare earth elements. Specifically, RAIX can be ferromagnetic, nonmagnetic or antiferromagnetic and the electronic band topology and topological nature of the Weyl fermions can be tuned. The unparalleled tunability and the large number of compounds make the RAIX family of compounds a unique Weyl semimetal class for exploring the wide-ranging topological phenomena associated with different types of emergent Weyl fermions in transport, spectroscopic and device-based experiments.



Some examples of Weyl materials candidates :

SrSi₂: Huang, S.-Y. Xu, Belopolski *et al.* *PNAS* **113**, 1180 (2015)

(Quadratic double Weyl)

Ta₃S₂: Chang, Xu, Belopolski *et.al.*, <http://arxiv.org/abs/1512.08781> (2015)

(Type II Weyl)

Co₂TiX (X=Si, Ge, and Sn):

Chang, Xu, Belopolski *et.al.*, <http://arxiv.org/abs/1603.01255> (Magnetic Weyl)

MoxW_{1-x}Te/Se₂: Chang, Xu, Belopolski *et.al.*, *Nature Commun.* **7**, 10639 (2016)

More theoretical predictions forthcoming from our group..

Searching for inversion-symm. breaking WSM

TaAs FP: Huang, S. Xu,(Lin & MZH) **Nat. Commun. 2015** (subm. Nov 2014)

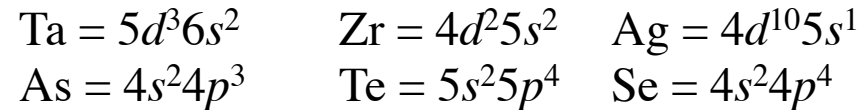
See also: FP: Weng et al., (Fang, IOP group) **PRX 2015** (subm. Jan 2015)



nature
COMMUNICATIONS

Similar cases: ZrTe, Ag₂Se

(November 2014)



ARTICLE

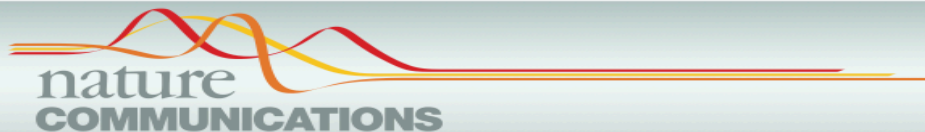
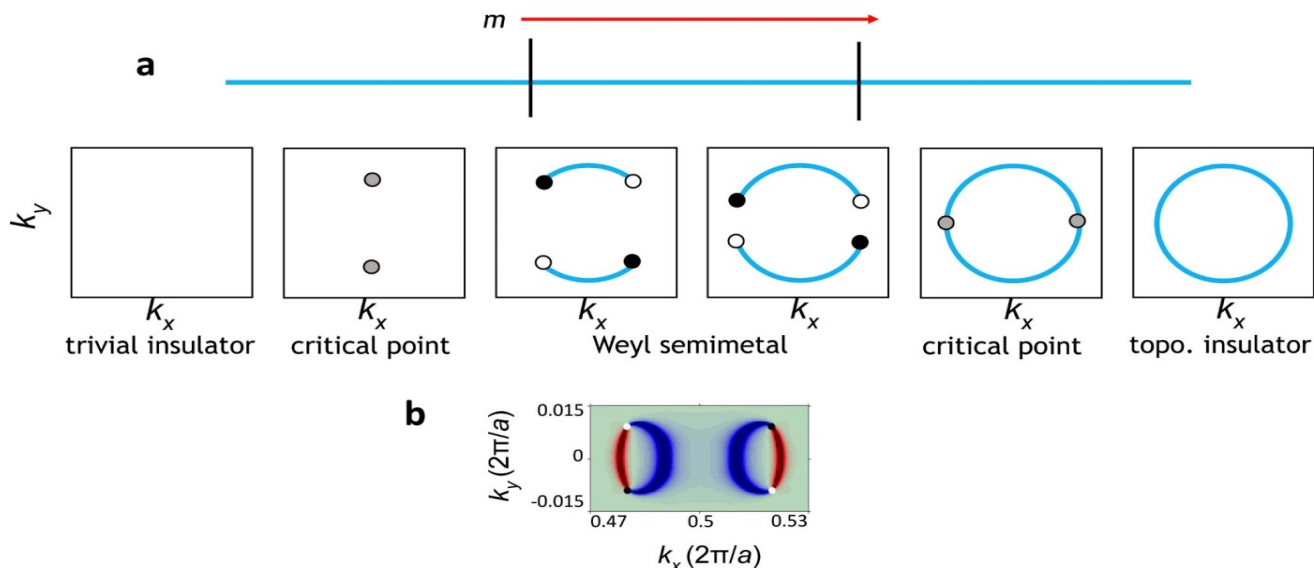
Received 24 Nov 2014 | Accepted 30 Apr 2015 | Published 12 Jun 2015

DOI: 10.1038/ncomms8373

OPEN

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

Shin-Ming Huang^{1,2,*}, Su-Yang Xu^{3,4,*}, Ilya Belopolski^{3,4,*}, Chi-Cheng Lee^{1,2}, Guoqing Chang^{1,2}, BaoKai Wang^{1,2,5}, Nasser Alidoust^{3,4}, Guang Bian³, Madhab Neupane^{3,4,6}, Chenglong Zhang⁷, Shuang Jia^{7,8}, Arun Bansil⁵, Hsin Lin^{1,2} & M. Zahid Hasan^{3,4,9}



November 2014

Materials algorithm for finding Weyl

ARTICLE

Received 24 Nov 2014 | Accepted 30 Apr 2015 | Published 12 Jun 2015

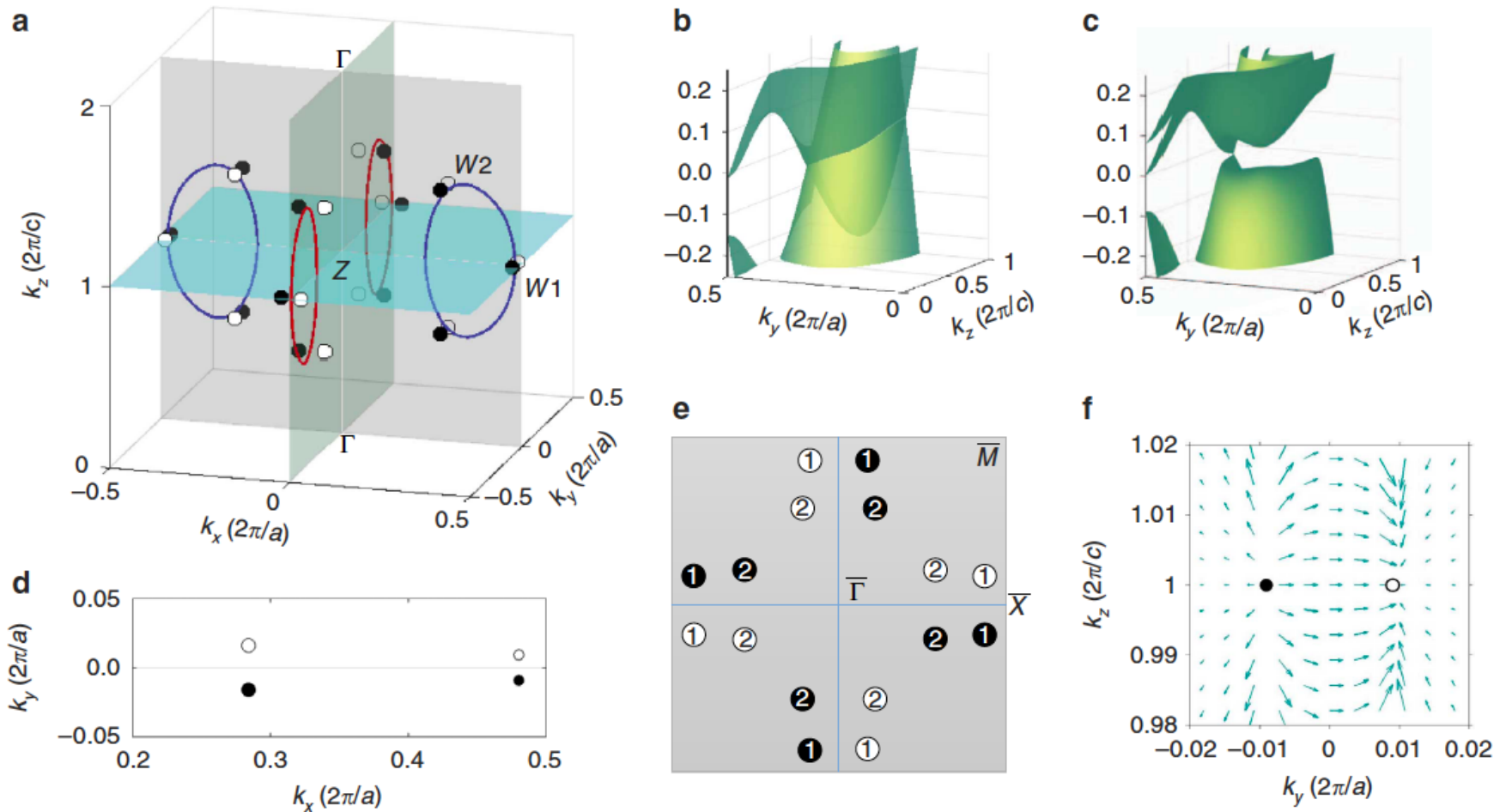
DOI: 10.1038/ncomms8373

OPEN

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

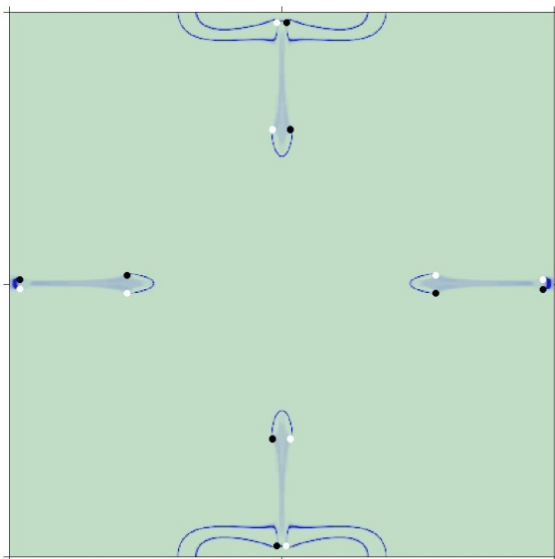
Shin-Ming Huang^{1,2,*}, Su-Yang Xu^{3,4,*}, Ilya Belopolski^{3,4,*}, Chi-Cheng Lee^{1,2}, Guoqing Chang^{1,2}, BaoKai Wang^{1,2,5}, Nasser Alidoust^{3,4}, Guang Bian³, Madhab Neupane^{3,4,6}, Chenglong Zhang⁷, Shuang Jia^{7,8}, Arun Bansil⁵, Hsin Lin^{1,2} & M. Zahid Hasan^{3,4,9}

24 Weyl nodes in the bulk of TaAs, NbAs

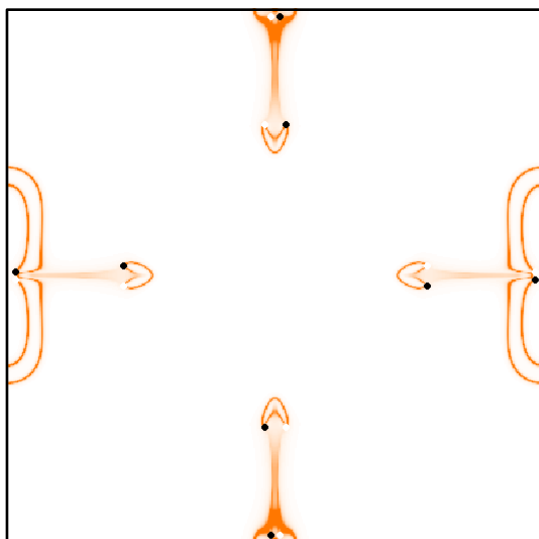


Theory FIGURES from
 S. Huang, Suyang Xu, Belopolski et.al., Nature Commun. 2015

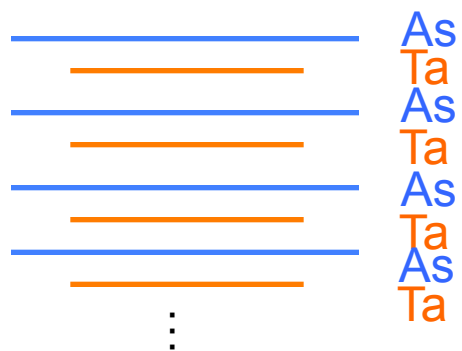
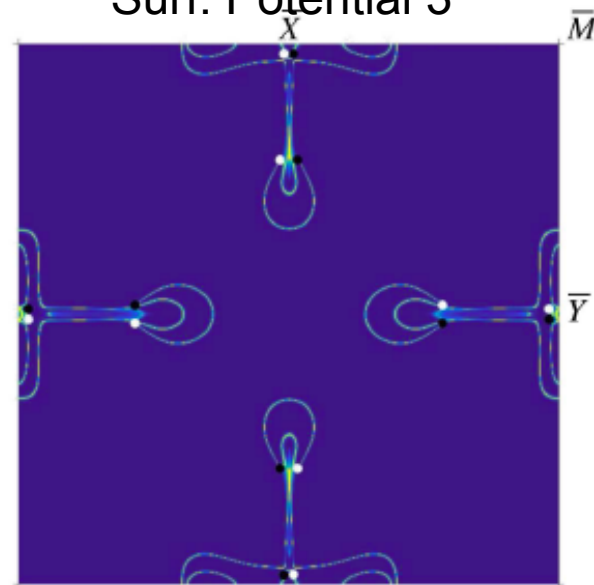
Surf. Potential 1



Surf. Potential 2

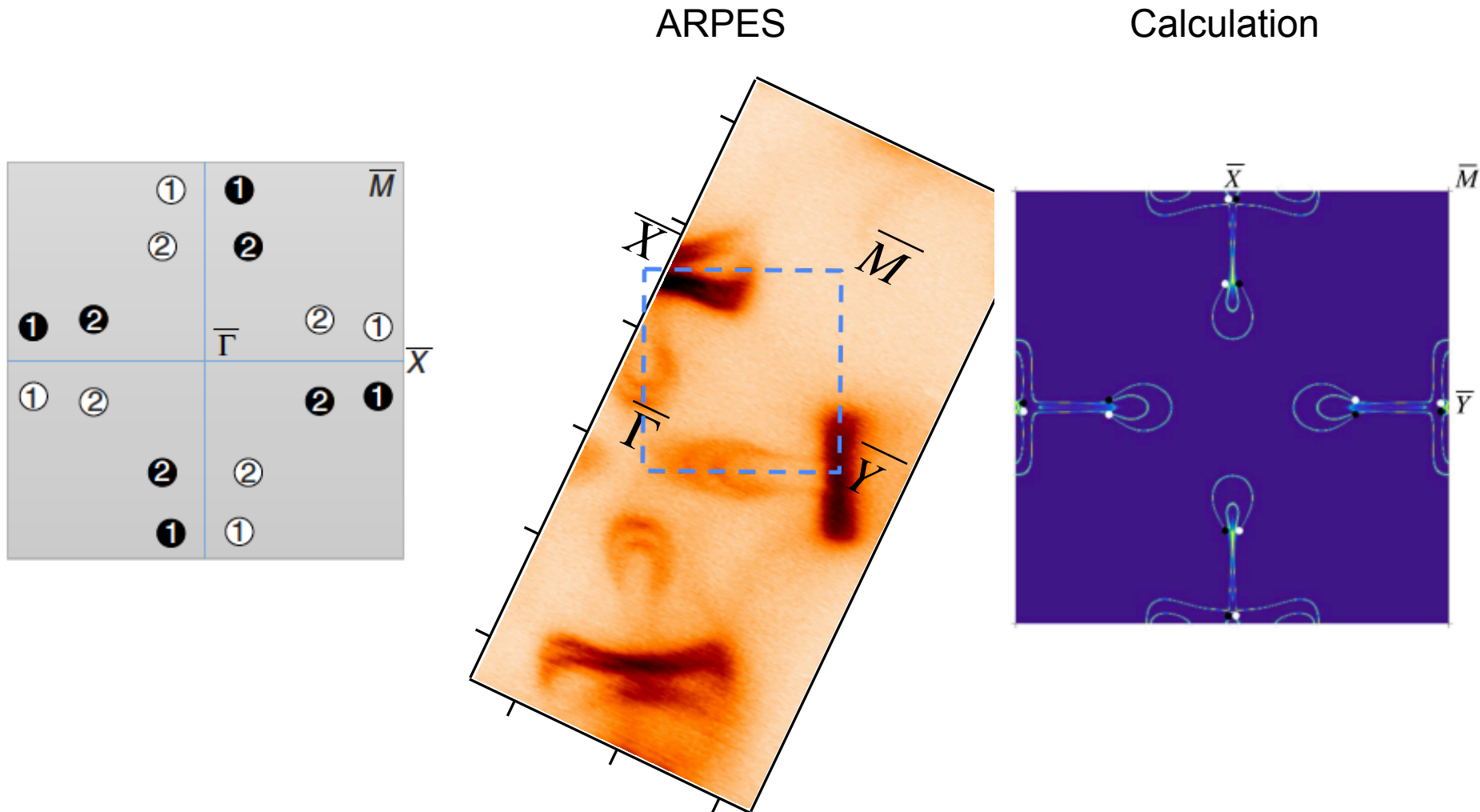


Surf. Potential 3



Ta 5s 5d, As 4s, 4p

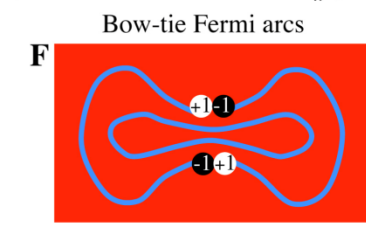
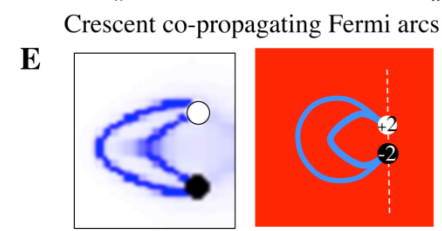
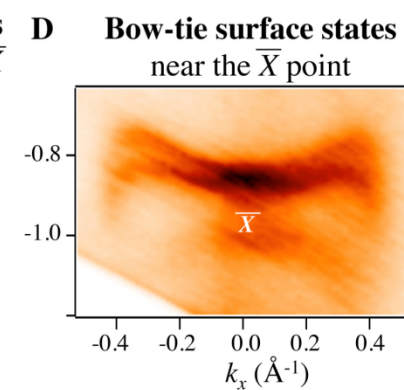
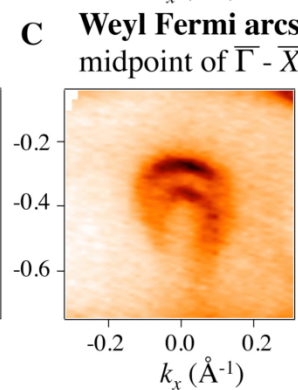
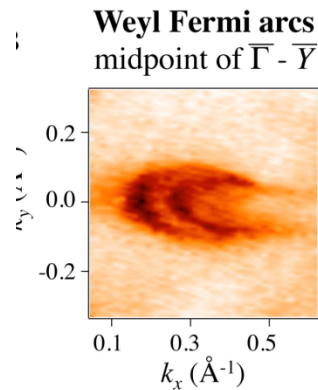
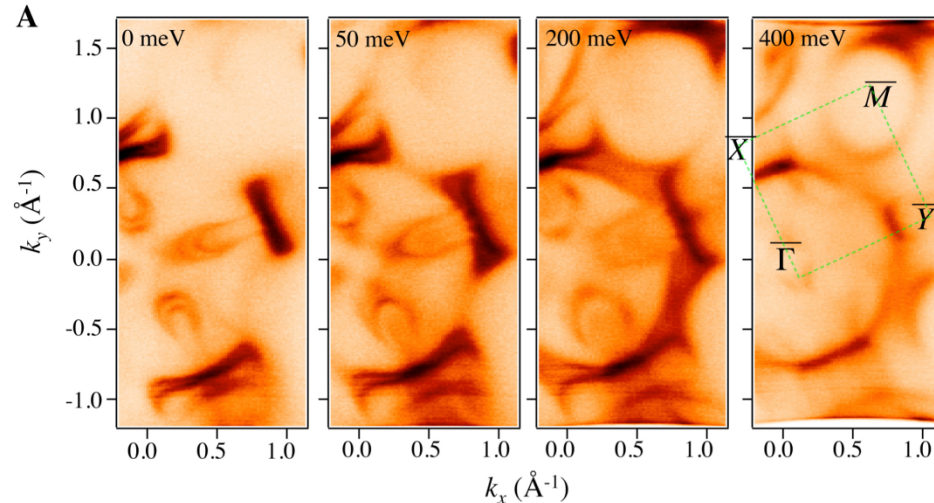
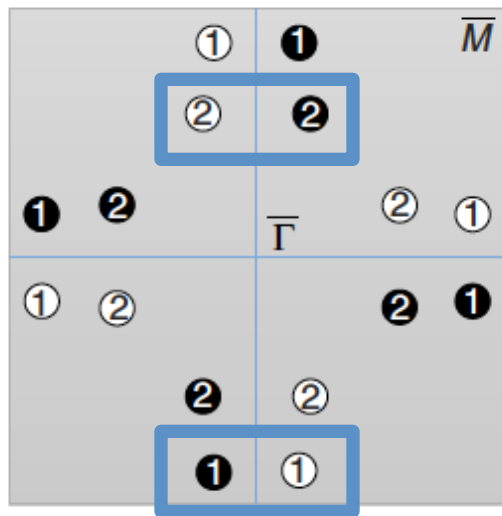
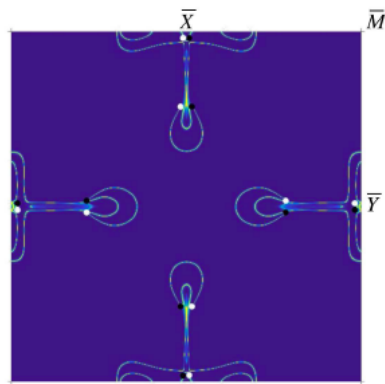
ARPES-1 (low photon energies)



Weyl SM Data : Xu, Belopolski, et.al., Science, 349, 613 (2015)

Fermi arc Methods : Xu, Liu, Belopolski, et.al., Science, 347, 294 (2014) AOP

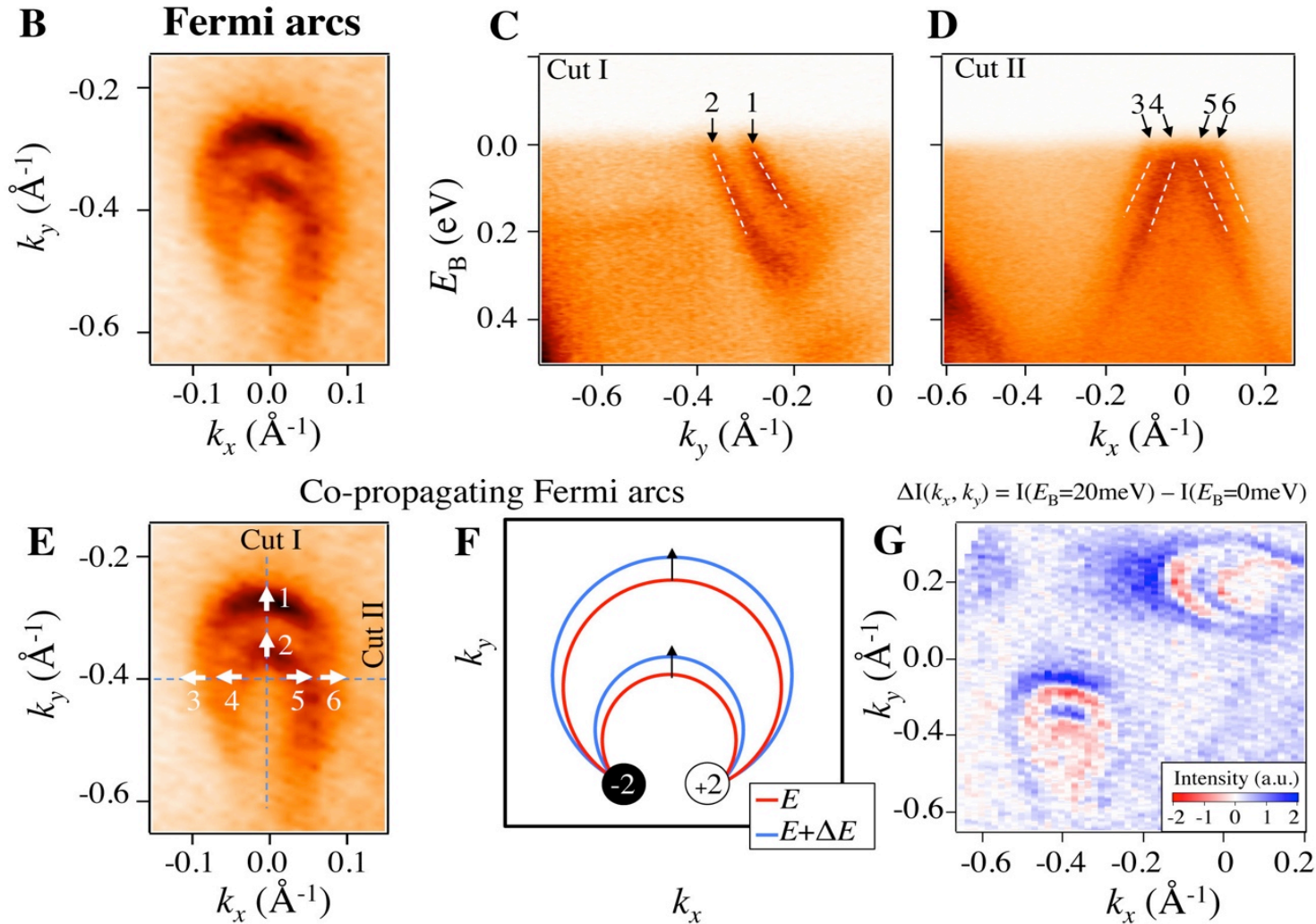
ARPES-1: Surface states



Weyl SM Data : Xu, Belopolski, et.al., Science, 349, 613 (2015)
 Fermi arc Methods : Xu, Liu, Belopolski, et.al., Science, 347, 294 (2014) AOP

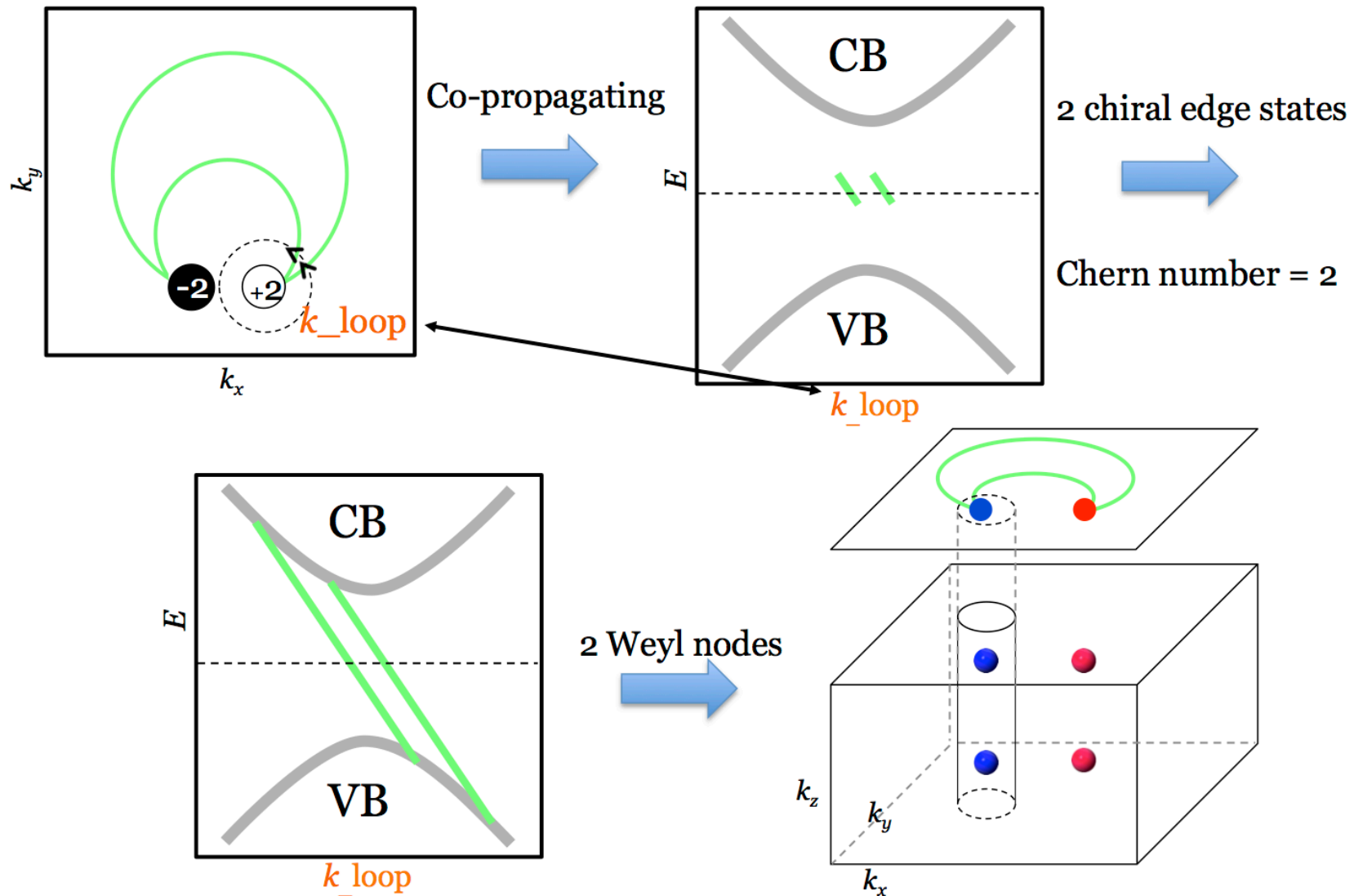
ARPES-1: Weyl Fermi surfaces

Co-propagating



Weyl SM Data : Xu, Belopolski, et.al., Science, 349, 613 (2015)
 Fermi arc Methods : Xu, Liu, Belopolski, et.al., Science, 347, 294 (2014) AOP

Weyl Fermi arcs – *Copropagating!*

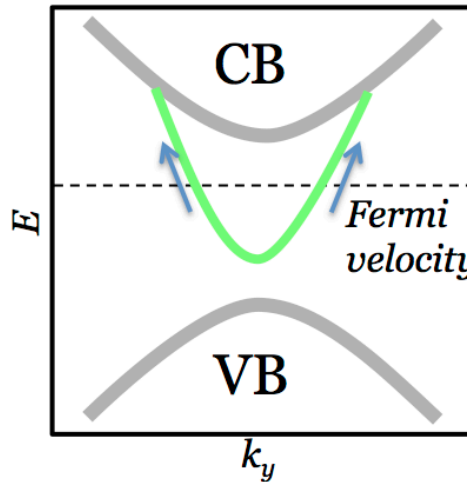
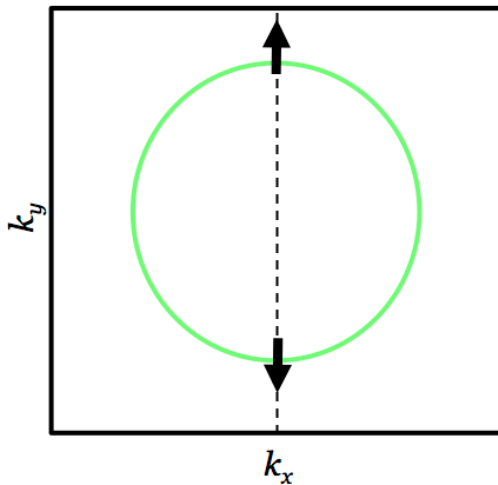


Weyl SM Data : Xu, Belopolski, et.al.,

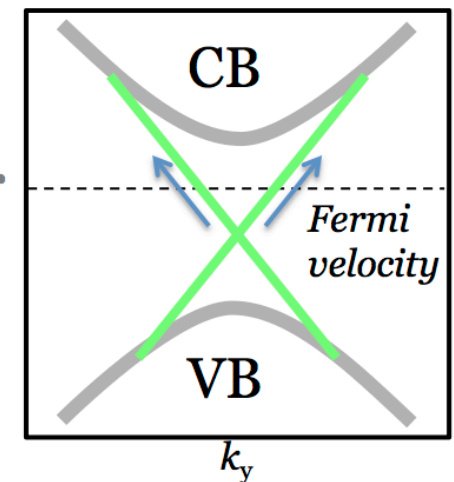
Science, 349, 613 (2015)

Weyl Fermi arcs – **Copropagating!**

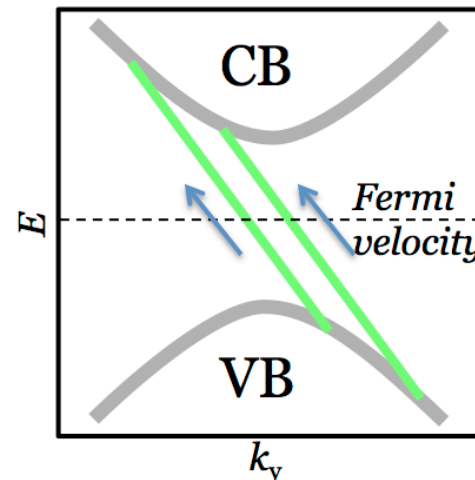
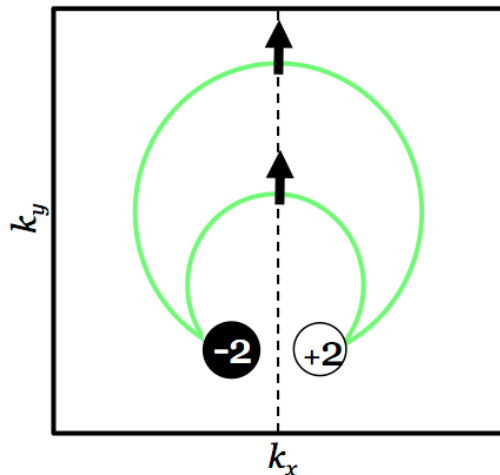
Counter-propagating (opposite slopes) → Closed contour



Or



Co-propagating (same slope) → Fermi arcs

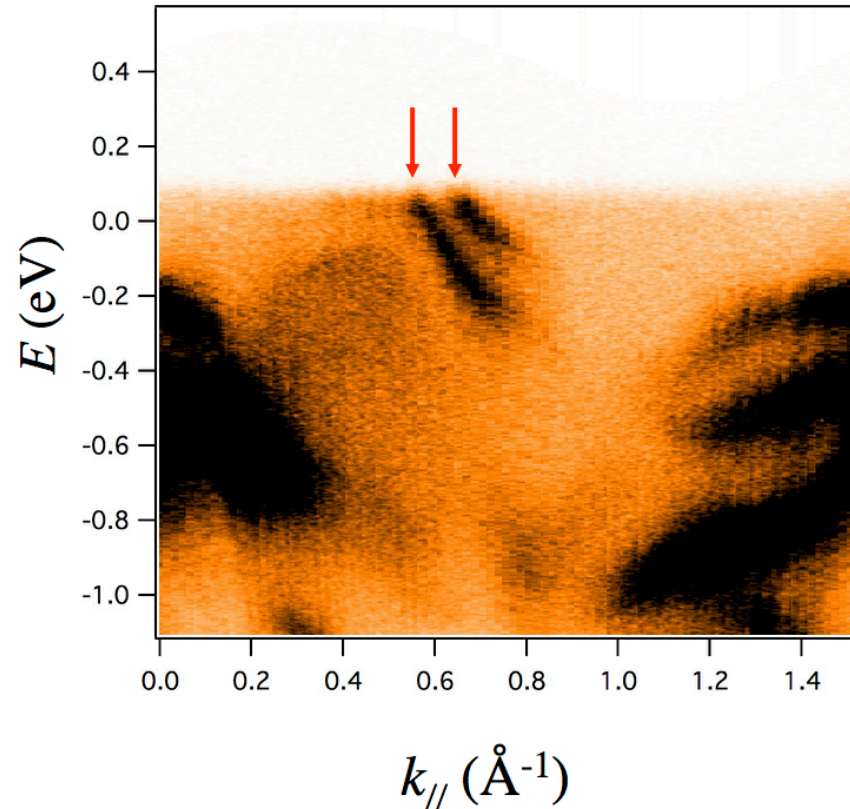
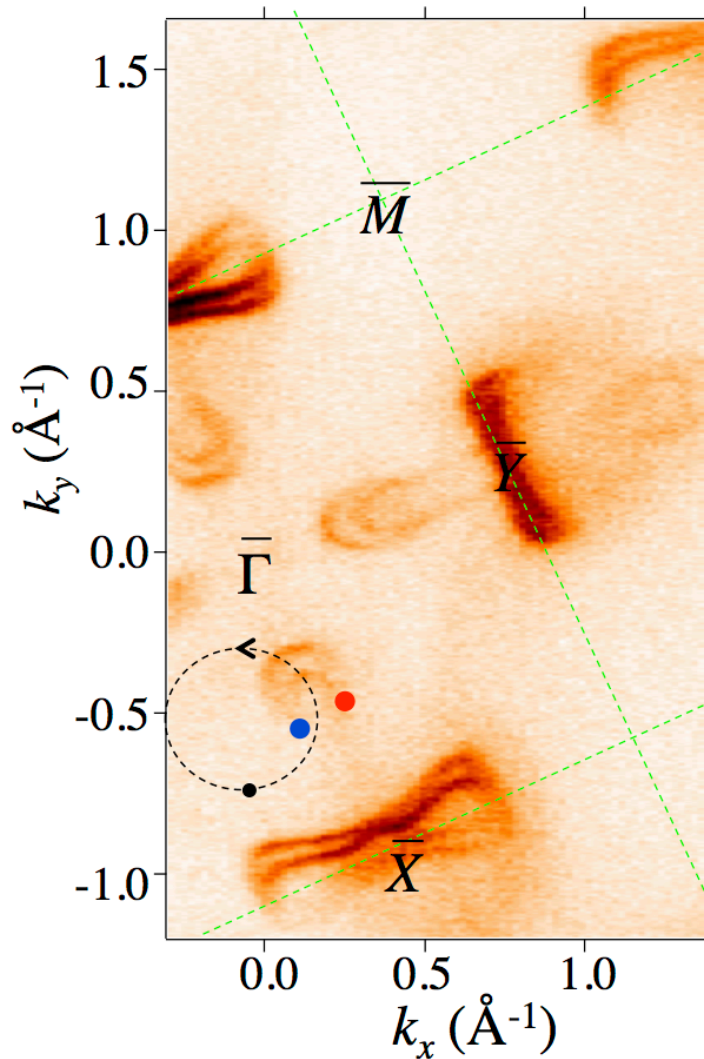


Weyl SM Data : Xu, Belopolski, et.al.,

Science, 349, 613 (2015)

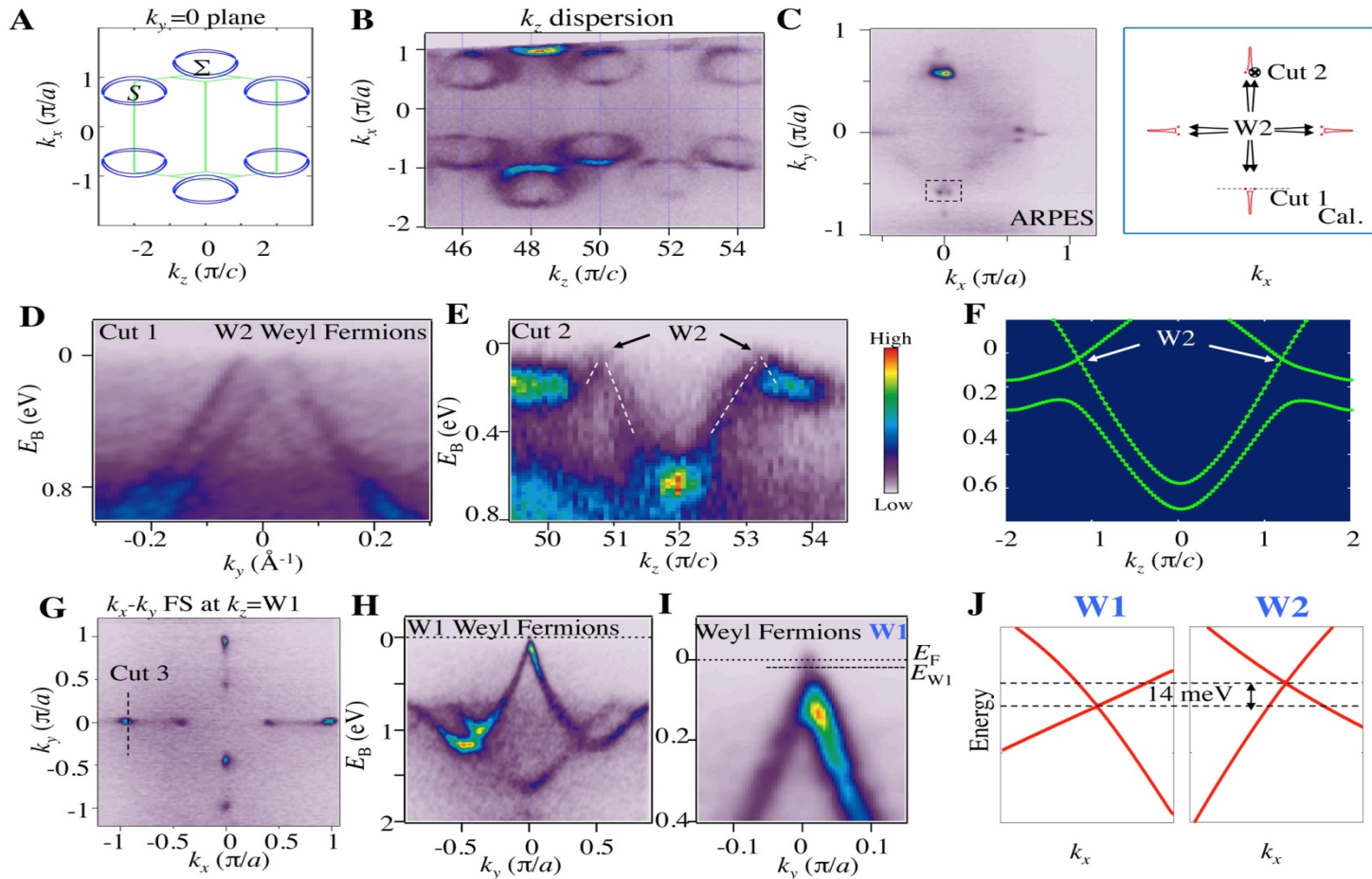
Fermi arc Methods : Xu, Liu, Belopolski, et.al., **Science, 347, 294 (2014)** AOP

Weyl Fermi arcs – *Copropagating!*



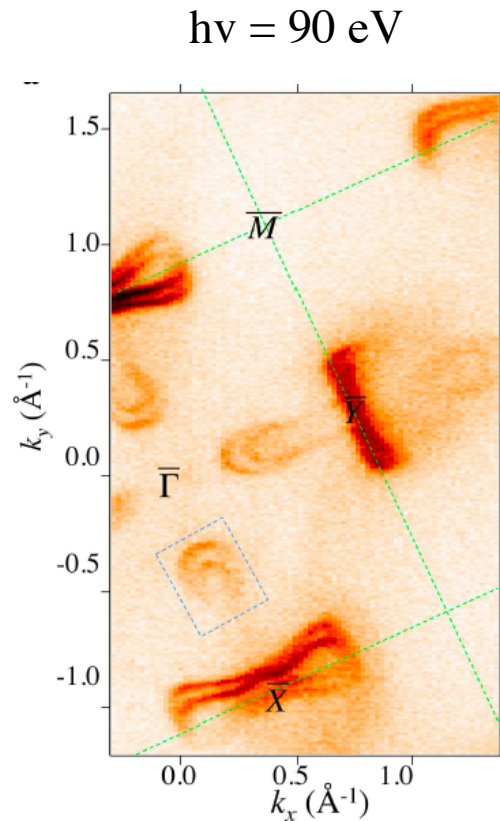
Weyl SM Data : Xu, Belopolski, et.al., **Science, 349, 613 (2015)**
Fermi arc Methods : Xu, Liu, Belopolski, et.al., **Science, 347, 294 (2014)** AOP

ARPES-2: Bulk fermions

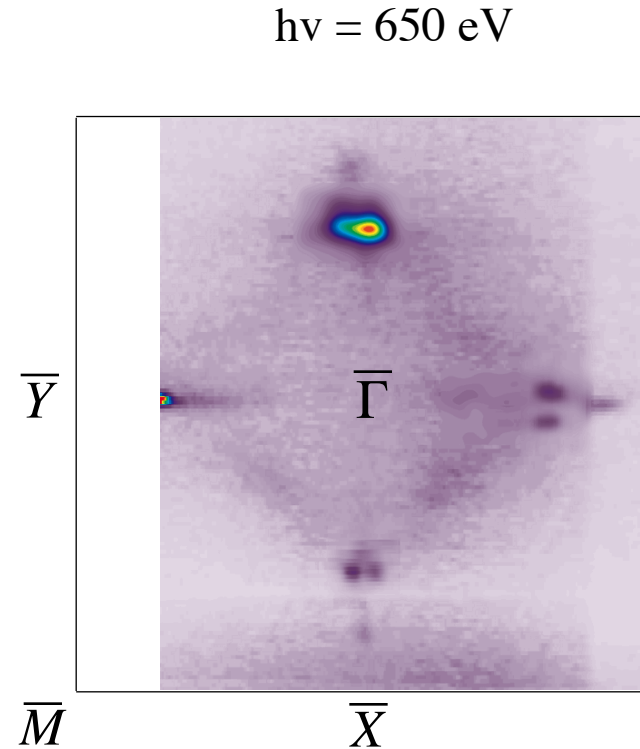


Weyl SM Data : Xu, Belopolski, et.al., Science, 349, 613 (2015)
 Fermi arc Methods : Xu, Liu, Belopolski, et.al., Science, 347, 294 (2014) AOP

ARPES: Surface vs. Bulk



Low Photon Energy
(**surface** sensitive)

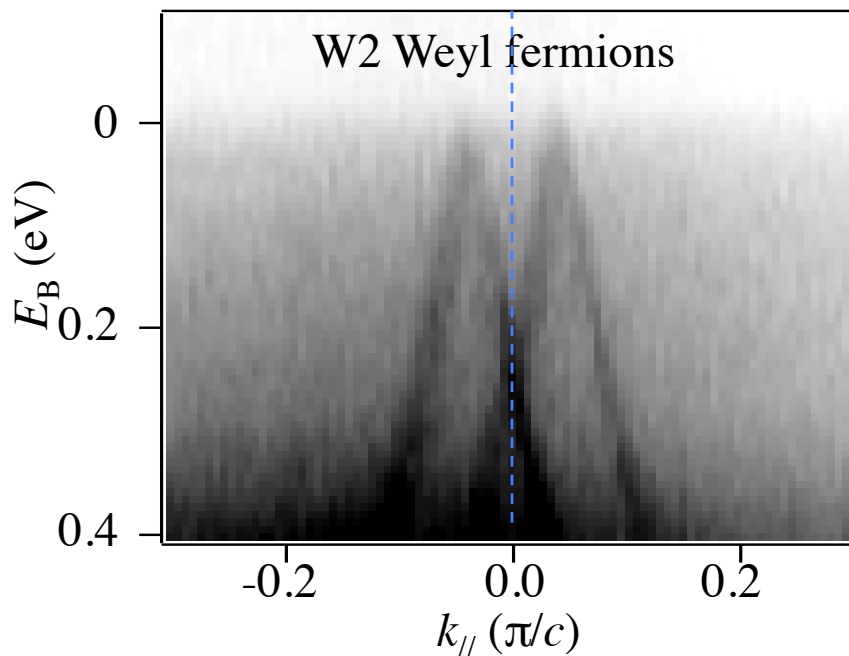
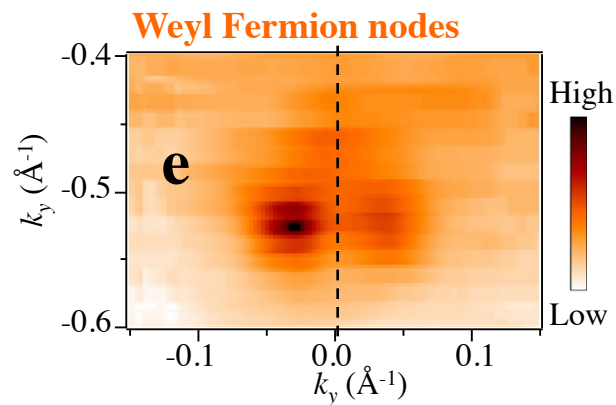
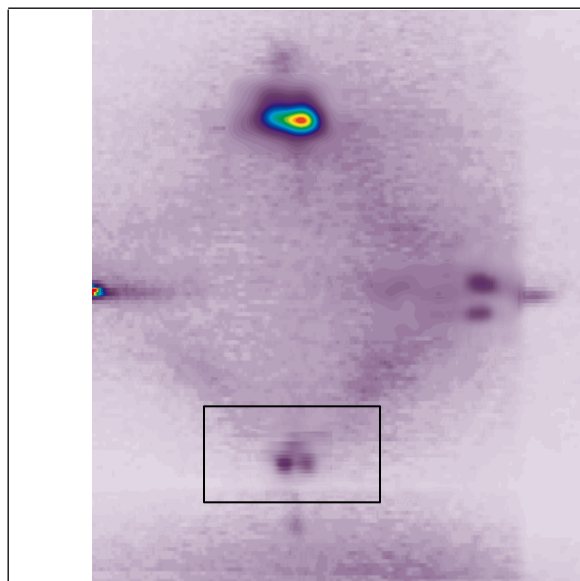


High Photon Energy
(**Bulk** sensitive)

Weyl SM Data : Xu, Belopolski, et.al., **Science, 349, 613 (2015)**
Fermi arc Methods : Xu, Liu, Belopolski, et.al., **Science, 347, 294 (2014)** AOP

ARPES-2: Bulk Weyl fermions

Away from Kramers points or rotational axes

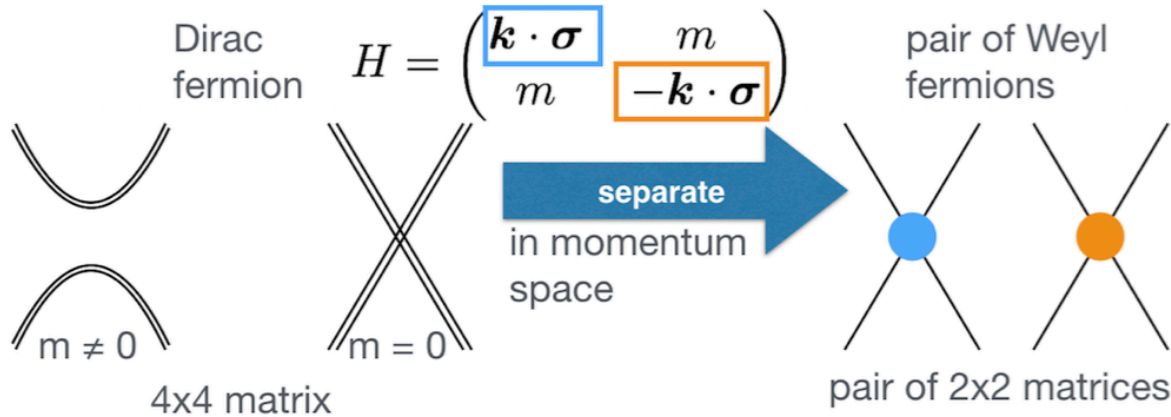


Weyl SM Data : Xu, Belopolski, et.al., Science, 349, 613 (2015)

Fermi arc Methods : Xu, Liu, Belopolski, et.al., Science, 347, 294 (2014) AOP

“Half” Fermions

Two ways to decompose a Dirac fermion



H.Weyl 1929

electron \sim 2 Majoranas

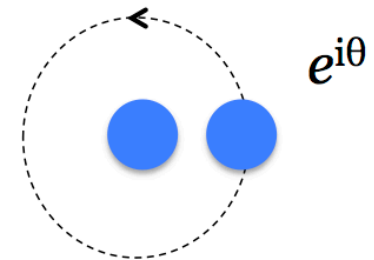
$$c = (\gamma + i\gamma')/2$$

$$c^\dagger = (\gamma - i\gamma')/2$$

Majorana = anti-Majorana

$$\gamma = \gamma^\dagger$$

2 Majoranas \sim 2-level system

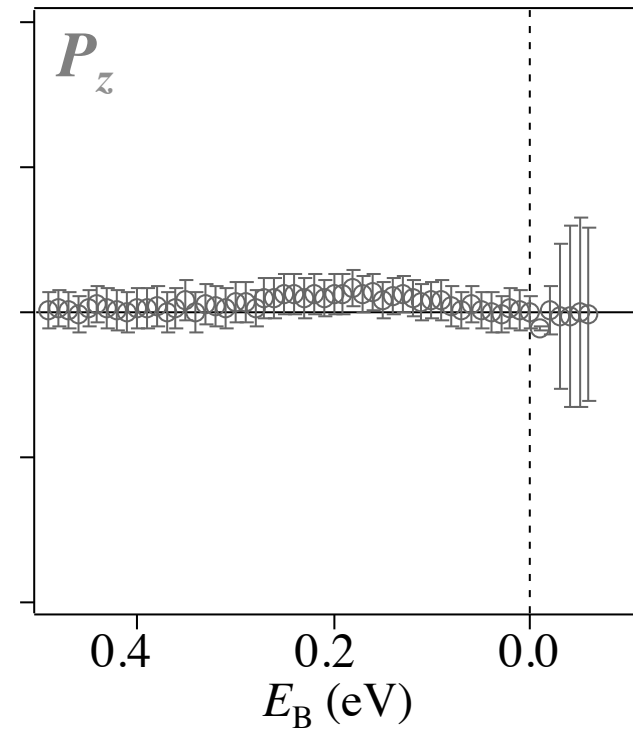
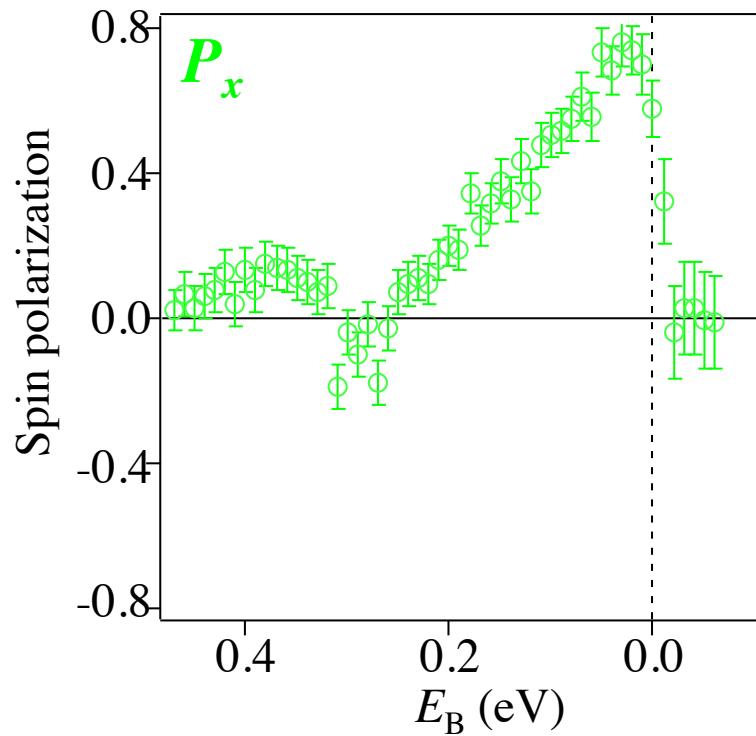
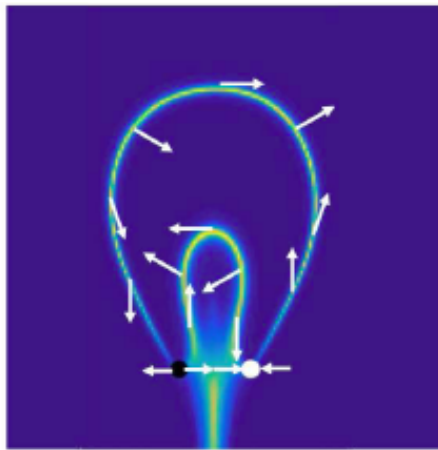


Ettore Majorana 1937

Spin polarization in TaAs

> 80%

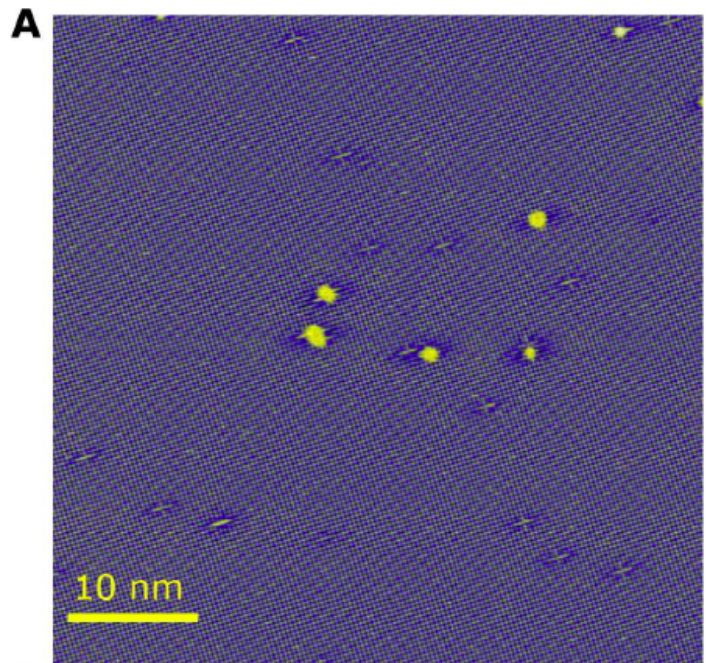
Measured spin texture



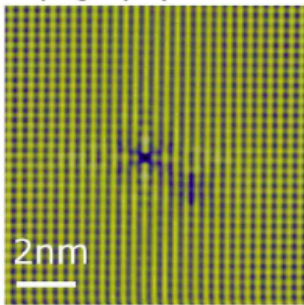
- Singly degenerate
- Spin pol. > 80%
- $P_z = 0$ (C_2T)

First STM images on Weyl

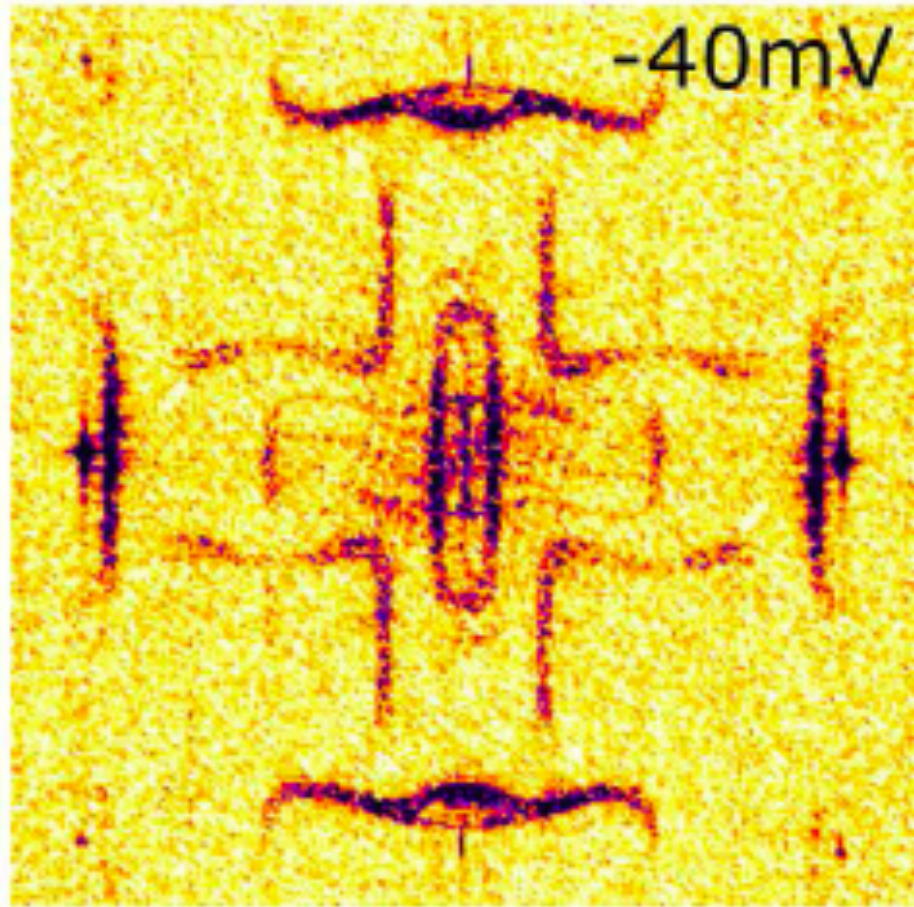
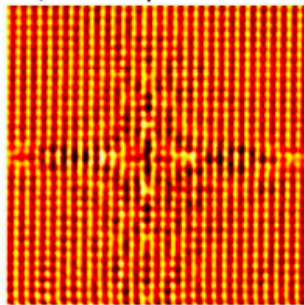
atomic resolution view of the surface



B Topography



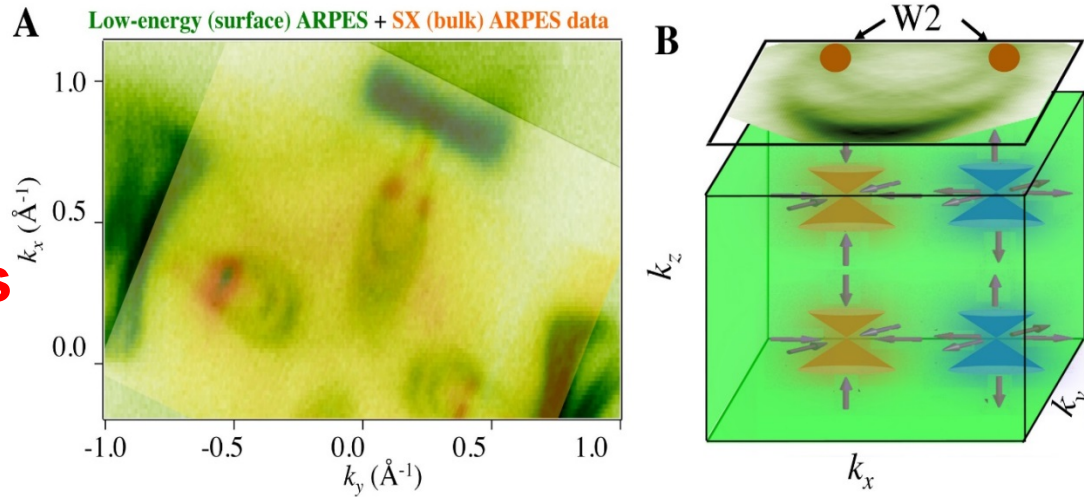
C dI/dV map



H. Zheng, S.-Y. Xu, *et al.*, (MZH) (2015)
ACS Nano

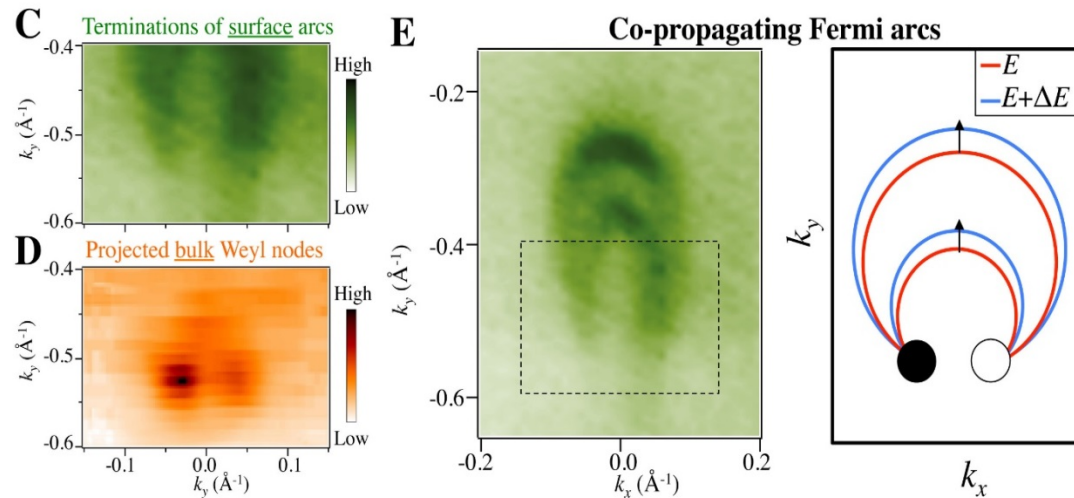
Weyl quasiparticles & Topological Fermi arcs

Weyl nodes and Fermi arcs in TaAs



**Weyl
Semimetals**

**K-space:
Monopole
- Anti MP**

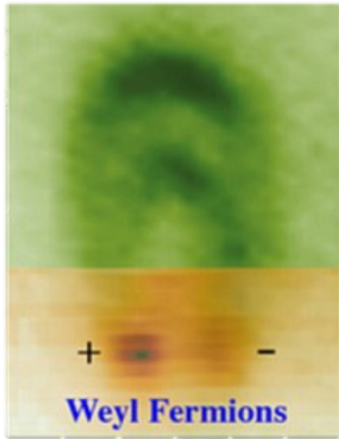


**Weyl
Fermions**

**Fermi
Arcs**

Weyl SM Data : Xu, Belopolski, et.al., Science, 349, 613 (2015)

Fermi arc Methods : Xu, Liu, Belopolski, et.al., Science, 347, 294 (2014) AOP



Discovery of a Weyl Fermion semimetal and topological Fermi arcs

16th July, 2015

Su-Yang Xu,^{1,2*} Ilya Belopolski,^{1*} Nasser Alidoust,^{1,2*} Madhab Neupane,^{1,3*} Guang Bian,¹ Chenglong Zhang,⁴ Raman Sankar,⁵ Guoqing Chang,^{6,7} Zhujun Yuan,⁴ Chi-Cheng Lee,^{6,7} Shin-Ming Huang,^{6,7} Hao Zheng,¹ Jie Ma,⁸ Daniel S. Sanchez,¹ BaoKai Wang,^{6,7,9} Arun Bansil,⁹ Fangcheng Chou,⁵ Pavel P. Shibayev,^{1,10} Hsin Lin,^{6,7} Shuang Jia,^{4,11} M. Zahid Hasan^{1,2†}

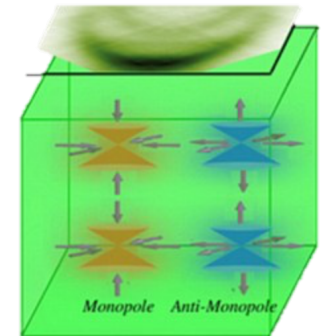
nature
physics

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PUBLISHED ONLINE: XX MONTH XXXX | DOI: 10.1038/NPHYS3437

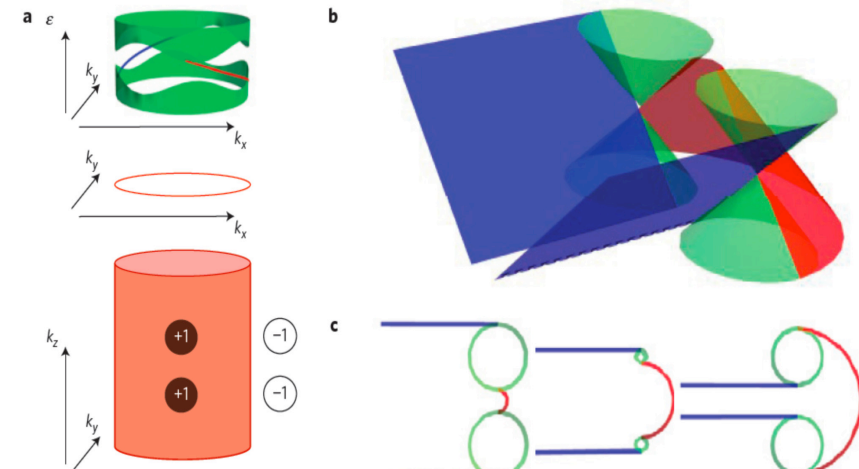
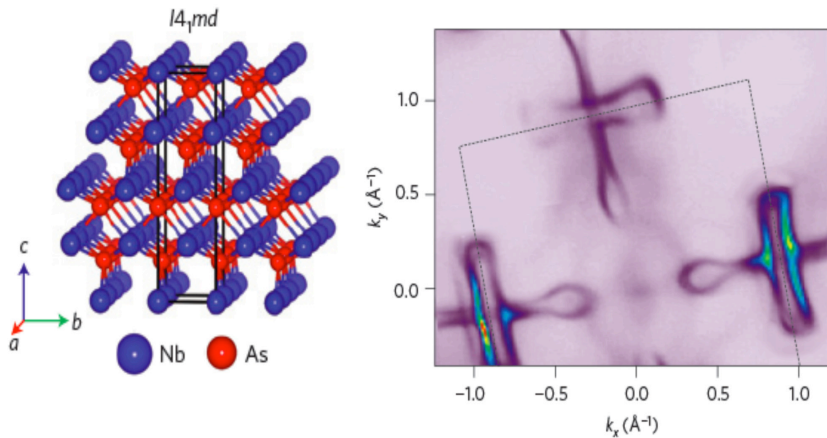
Discovery of a Weyl fermion state with Fermi arcs in niobium arsenide

Su-Yang Xu^{1,2†}, Nasser Alidoust^{1,2†}, Ilya Belopolski^{1,2†}, Zhujun Yuan³, Guang Bian¹, Tay-Rong Chang^{1,4}, Hao Zheng¹, Vladimir N. Strocov⁵, Daniel S. Sanchez¹, Guoqing Chang^{6,7}, Chenglong Zhang³, Daixiang Mou^{8,9}, Yun Wu^{8,9}, Lunan Huang^{8,9}, Chi-Cheng Lee^{6,7}, Shin-Ming Huang^{6,7}, BaoKai Wang^{6,7,10}, Arun Bansil¹⁰, Horng-Tay Jeng^{4,11}, Titus Neupert¹², Adam Kaminski^{8,9}, Hsin Lin^{6,7}, Shuang Jia^{3,13} and M. Zahid Hasan^{1,2*}



Discovery of a Weyl fermion state with Fermi arcs in niobium arsenide

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RESEARCH ARTICLE

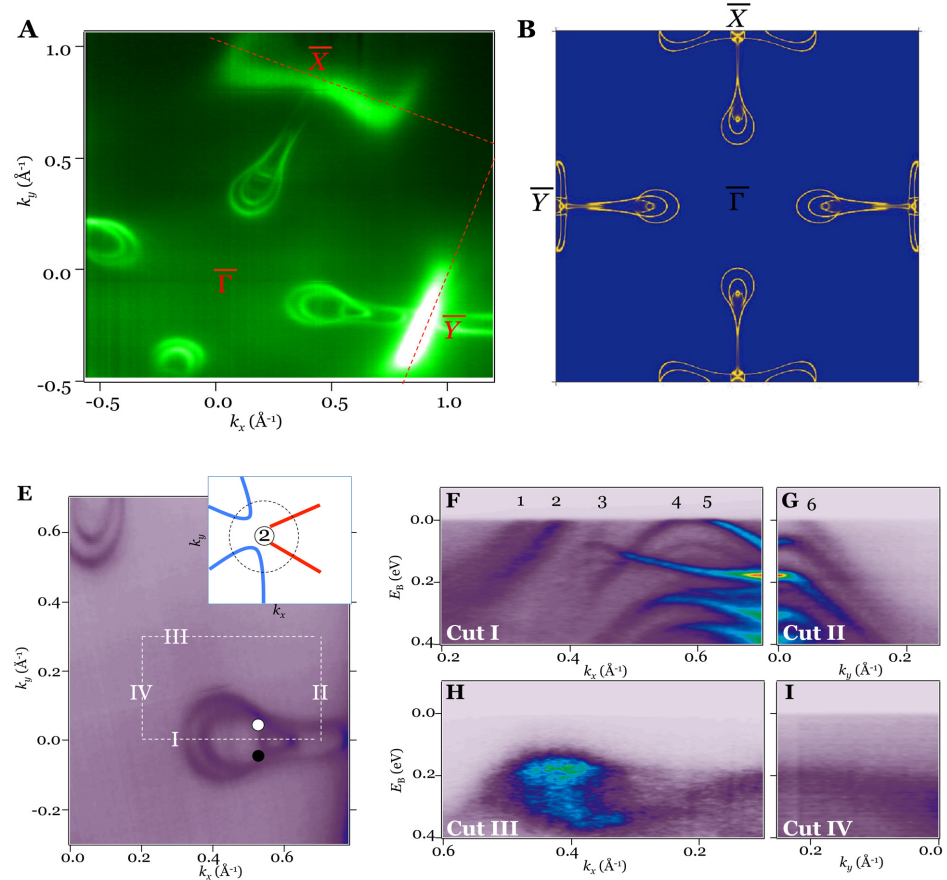
Science Advances

Science advances 1, e1501092 (2015)

PHYSICS

Experimental discovery of a topological Weyl semimetal state in TaP

Su-Yang Xu,^{1,*†} Ilya Belopolski,^{1,*} Daniel S. Sanchez,^{1,*} Chenglong Zhang,² Guoqing Chang,^{3,4} Cheng Guo,² Guang Bian,¹ Zhujun Yuan,² Hong Lu,² Tay-Rong Chang,⁵ Pavel P. Shibayev,¹ Mykhailo L. Prokopovych,⁶ Nasser Alidoust,¹ Hao Zheng,¹ Chi-Cheng Lee,^{3,4} Shin-Ming Huang,^{3,4} Raman Sankar,^{7,8} Fangcheng Chou,⁷ Chuang-Han Hsu,^{3,4} Horng-Tay Jeng,^{5,8} Arun Bansil,⁹ Titus Neupert,¹⁰ Vladimir N. Strocov,⁶ Hsin Lin,^{3,4} Shuang Jia,^{2,11} M. Zahid Hasan^{1,12†}



First Experimental Papers on Weyl physics

1. S. Xu et al (Princeton); *Science* 349, 617 (2015) Weyl fermion with Fermi arc
2. L. Lu et.al., (MIT); *Science* 349, 622 (2015) Weyl photonic (bosonic) crystal
3. B. Lv et al (IOP-China) *Phy. Rev. X* (2015) Fermi arc and now more(including a few from us)

PRL 116, 066802 (2016)

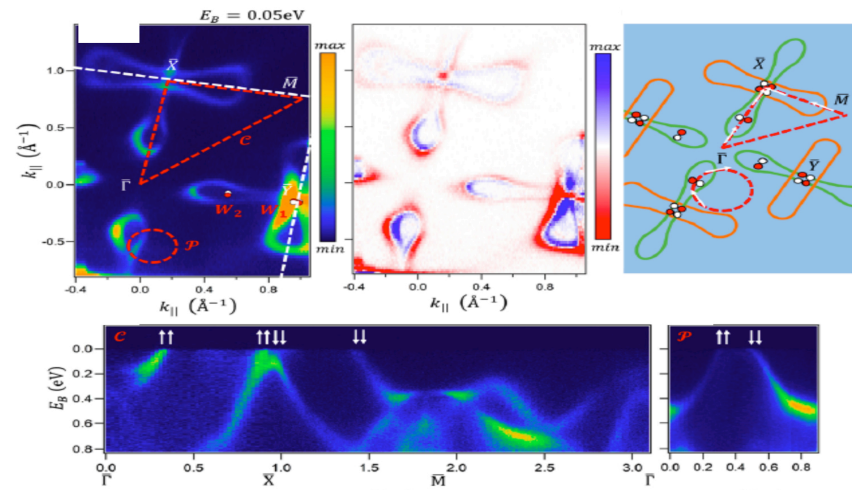
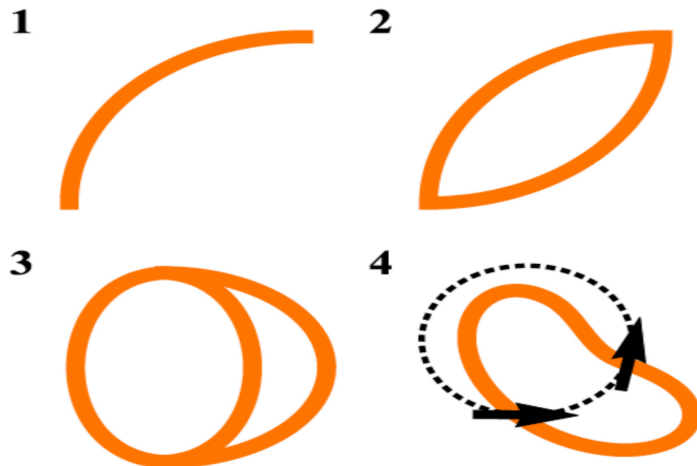
PHYSICAL REVIEW LETTERS

week ending
12 FEBRUARY 2016



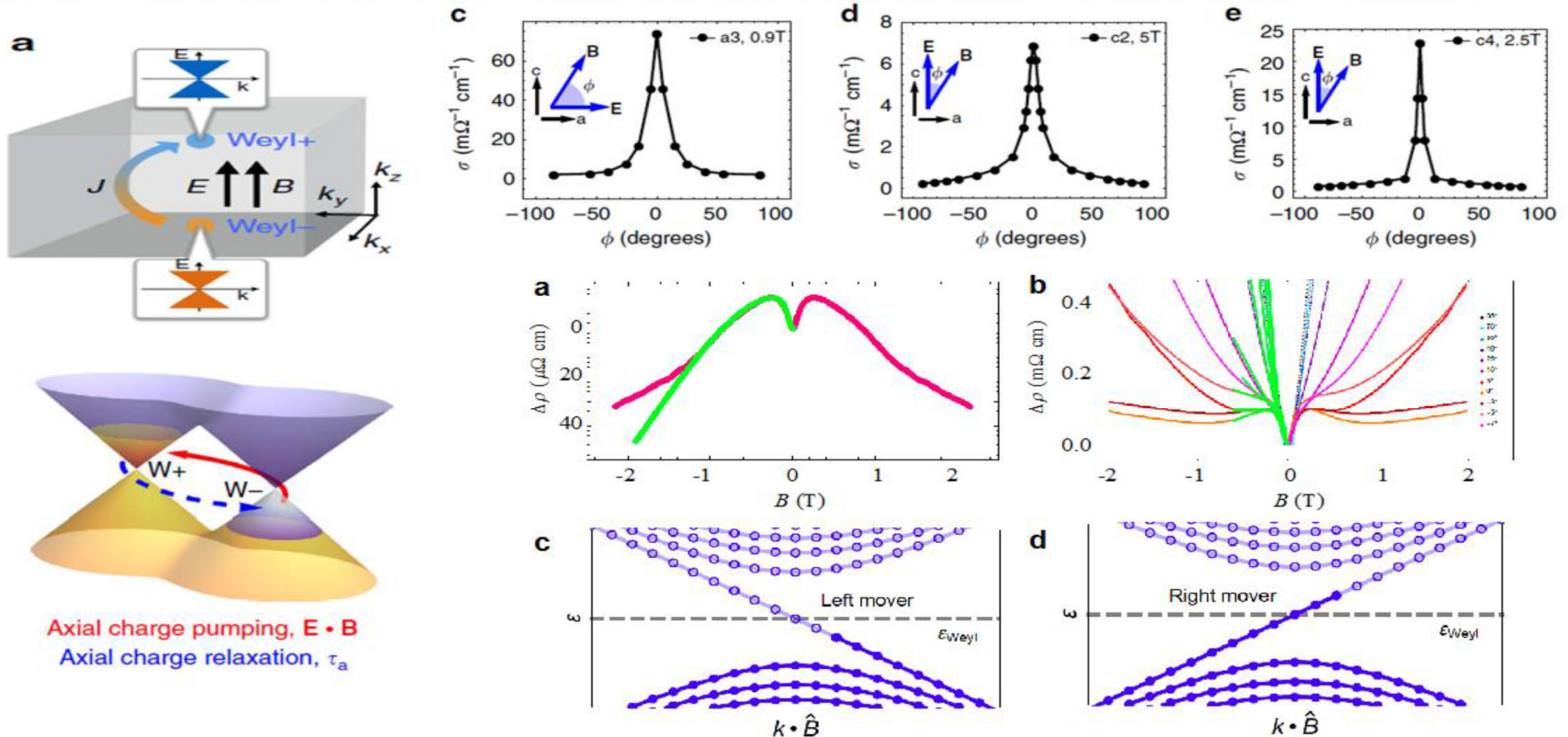
Criteria for Directly Detecting Topological Fermi Arcs in Weyl Semimetals

Ilya Belopolski,^{1,*} Su-Yang Xu,¹ Daniel S. Sanchez,¹ Guoqing Chang,^{2,3} Cheng Guo,⁴ Madhab Neupane,^{5,6}
 Hao Zheng,¹ Chi-Cheng Lee,^{2,3} Shin-Ming Huang,^{2,3} Guang Bian,¹ Nasser Alidoust,¹ Tay-Rong Chang,^{1,7}
 BaoKai Wang,^{2,3,8} Xiao Zhang,⁴ Arun Bansil,⁸ Horng-Tay Jeng,^{7,9} Hsin Lin,^{2,3}
 Shuang Jia,⁴ and M. Zahid Hasan^{1,†}



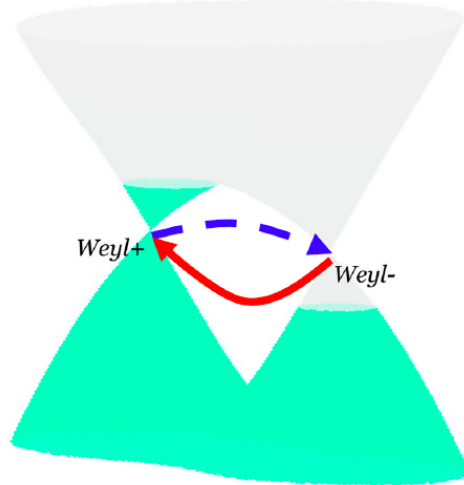
Signatures of the Adler–Bell–Jackiw chiral anomaly in a Weyl fermion semimetal

Cheng-Long Zhang^{1,*}, Su-Yang Xu^{2,*}, Ilya Belopolski^{2,*}, Zhujun Yuan^{1,*}, Ziquan Lin³, Bingbing Tong¹, Guang Bian², Nasser Alidoust², Chi-Cheng Lee^{4,5}, Shin-Ming Huang^{4,5}, Tay-Rong Chang^{2,6}, Guoqing Chang^{4,5}, Chuang-Han Hsu^{4,5}, Horng-Tay Jeng^{6,7}, Madhab Neupane^{2,8,9}, Daniel S. Sanchez², Hao Zheng², Junfeng Wang³, Hsin Lin^{4,5}, Chi Zhang^{1,10}, Hai-Zhou Lu¹¹, Shun-Qing Shen¹², Titus Neupert¹³, M. Zahid Hasan² & Shuang Jia^{1,10}

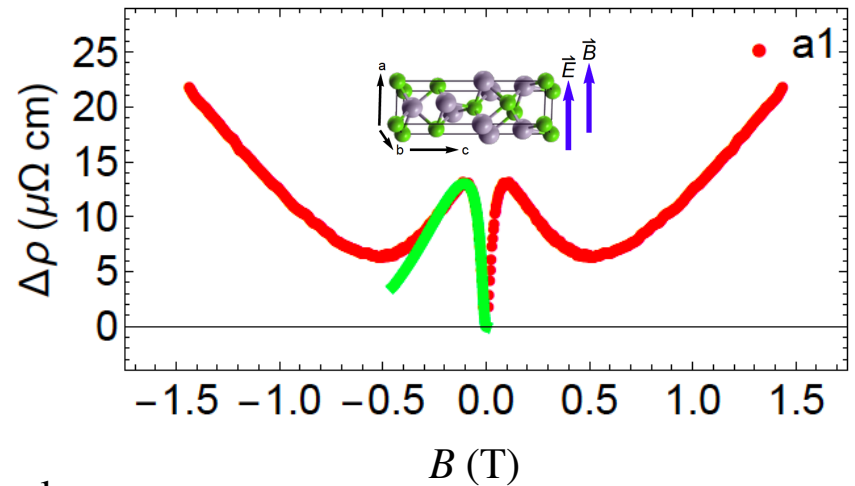
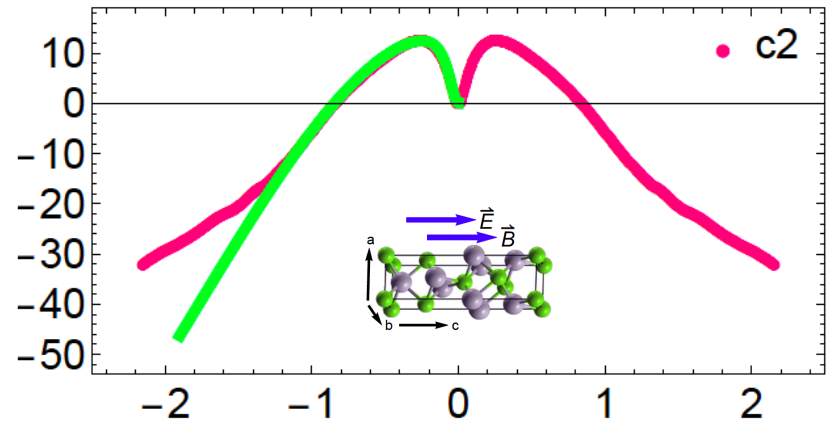
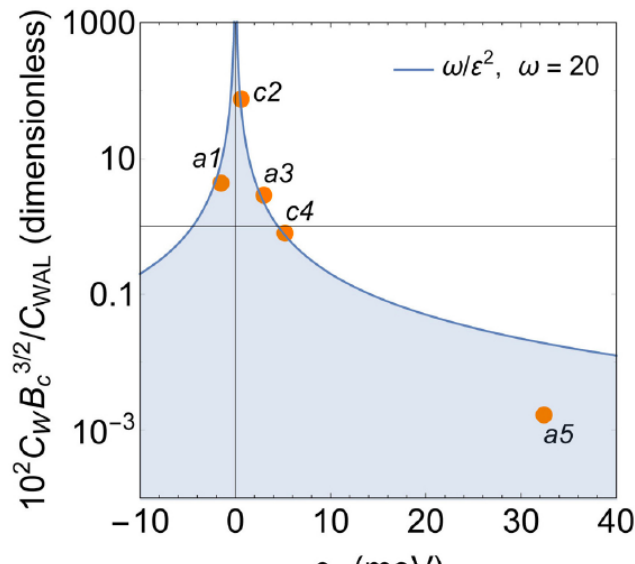


TaAs (WSM) chiral anomaly - $E \cdot B$

C.L. Zhang, Su-Yang Xu, Belopolski, Jia *et al.* arxiv:1503.02630 (2015). **The Chiral Anomaly**

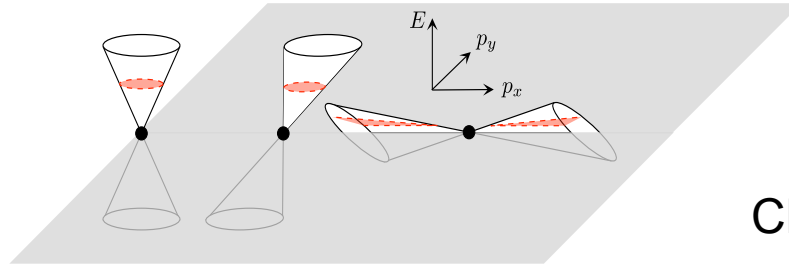


Axial charge pumping, $\vec{E} \cdot \vec{B}$
 Axial charge relaxation, τ_a



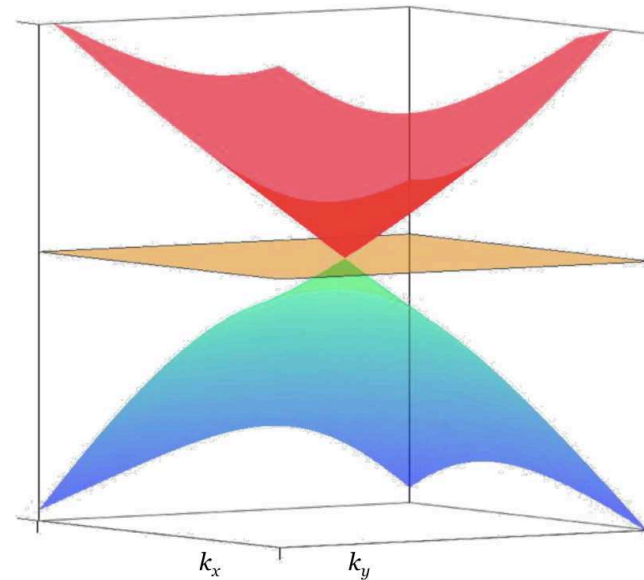
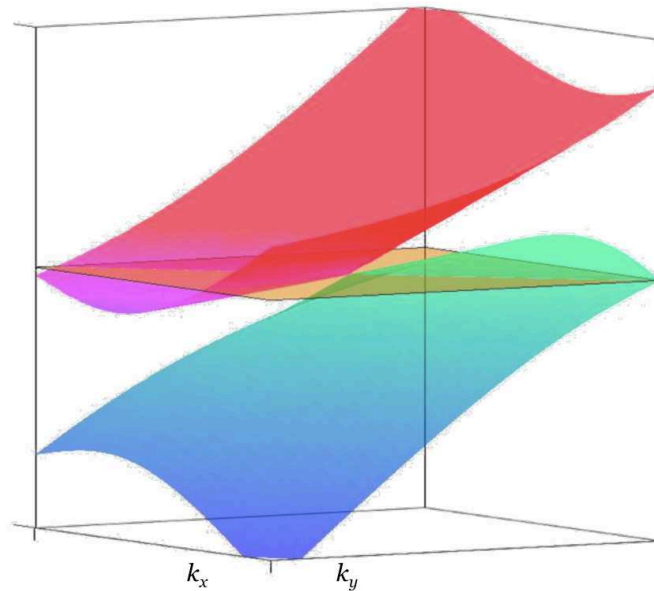
See also
 Huang et al., *Phys. Rev. X* **5**, 031023 (2015)

Tilting the Weyl Cone: Lorentz-violation



CM-JC 2015

Type II Weyl fermions (LaAlGe) **i** Type I Weyl fermions (TaAs)



Lorentz violating tilt in Dirac & Weyl: Many theory papers at least since 1995
Type-II by Soluyanov, Bernevig et.al., (2015) and others

Discovery of Lorentz-violating Weyl fermion semimetal state in LaAlGe materials

Su-Yang Xu*,¹ Nasser Alidoust*,¹ Guoqing Chang*,^{2,3} Hong Lu*,⁴ Bahadur Singh*,² Ilya Belopolski,¹ Daniel S. Sanchez,¹ Xiao Zhang,^{4,3} Guang Bian,¹ et al.,

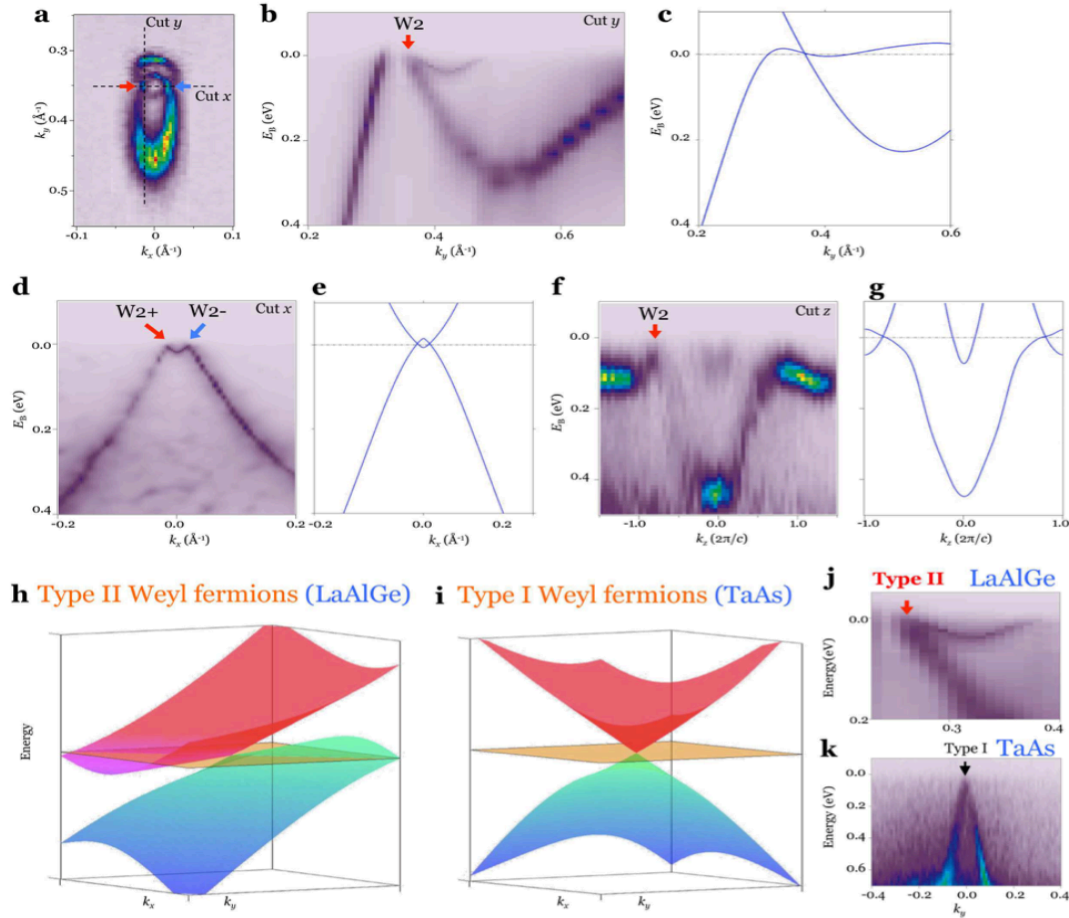
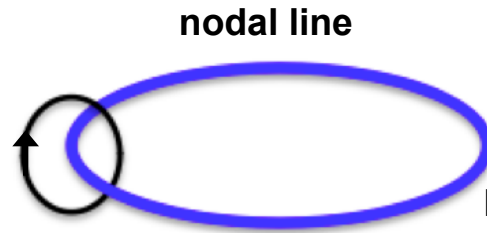
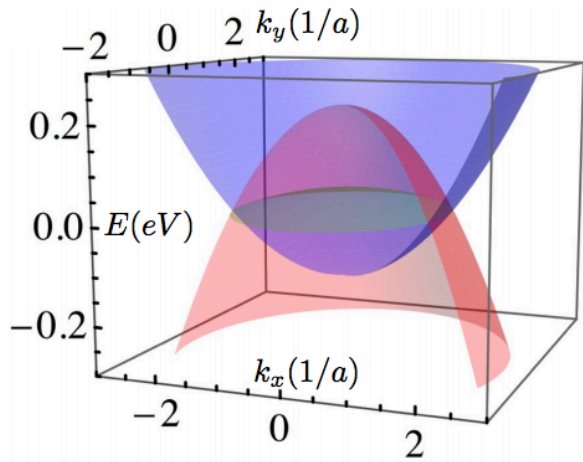


FIG. 3: **Type-II Weyl fermions in LaAlGe.** **a**, SX-ARPES-measured $k_x - k_y$ Fermi surface map in the region marked by the green rectangle in panel c of Fig. 2. **b**, Measured and **c**, calculated

Ta3S2 is also Lorentz-violating

Topological Nodal-Line Semimetals



winding number

$$\gamma/\pi = \pm 1$$

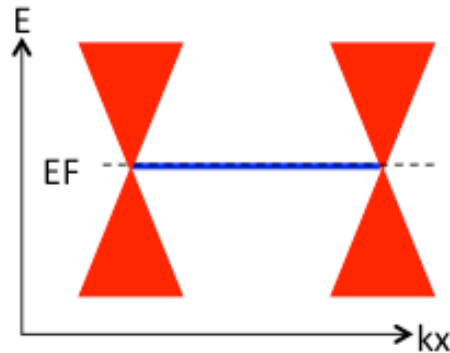
bulk-boundary correspondence

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

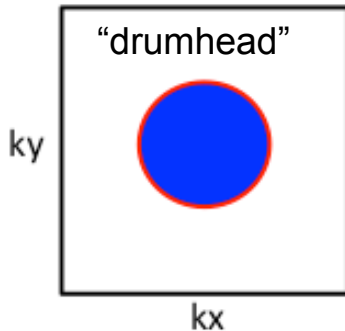
Chan *et al.*, arXiv:1510.02759 (2015)

↓
topo. surface states

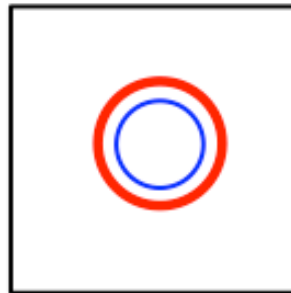
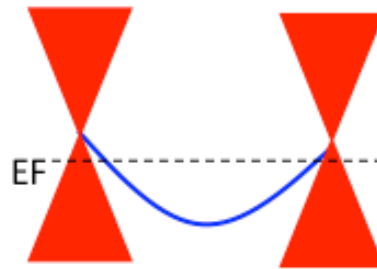
particle-hole symmetry



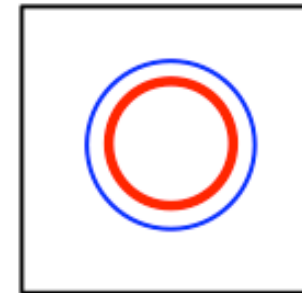
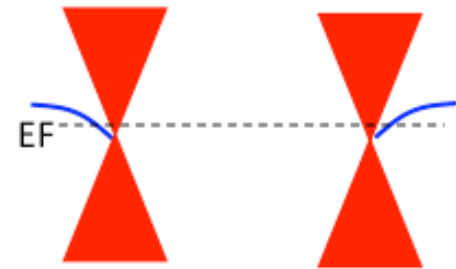
Fermi surface



general case-1



general case-2

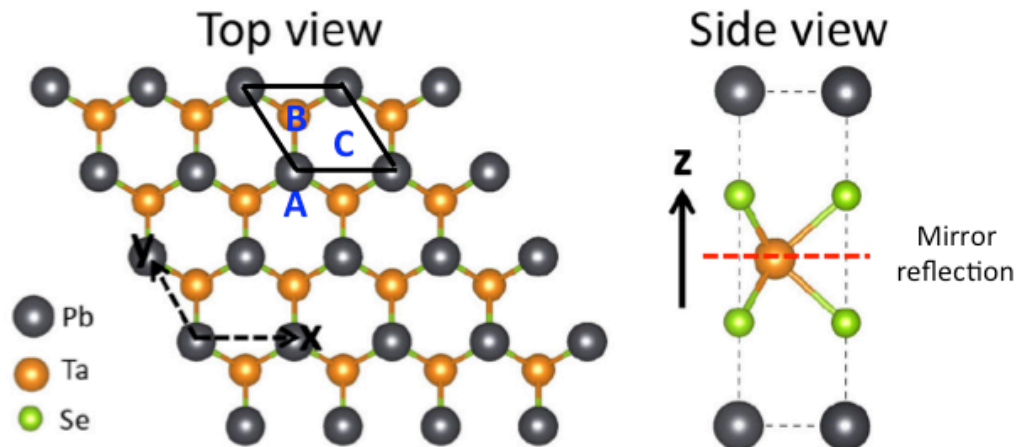


Topological Nodal-Line Semimetals: PbTaSe_2

Theory & Experiments

PbTaSe_2 :

G. Bian, T.-R. Chang, R. Sankar *et al.*, (MZH) *Nature Commun.* 7:10556 (2016)



Space group: $P-6m2$ (# 187)

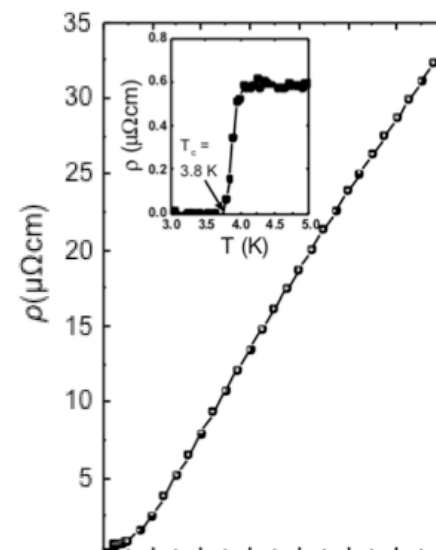
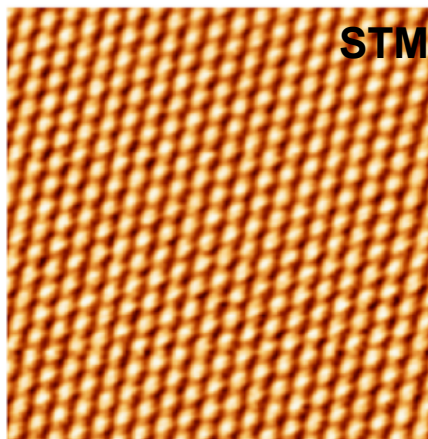
$a=b=3.44 \text{ \AA}$

$c=9.35 \text{ \AA}$

Bond-length

$\text{Pb-Se} = 2.90 \text{ \AA}$

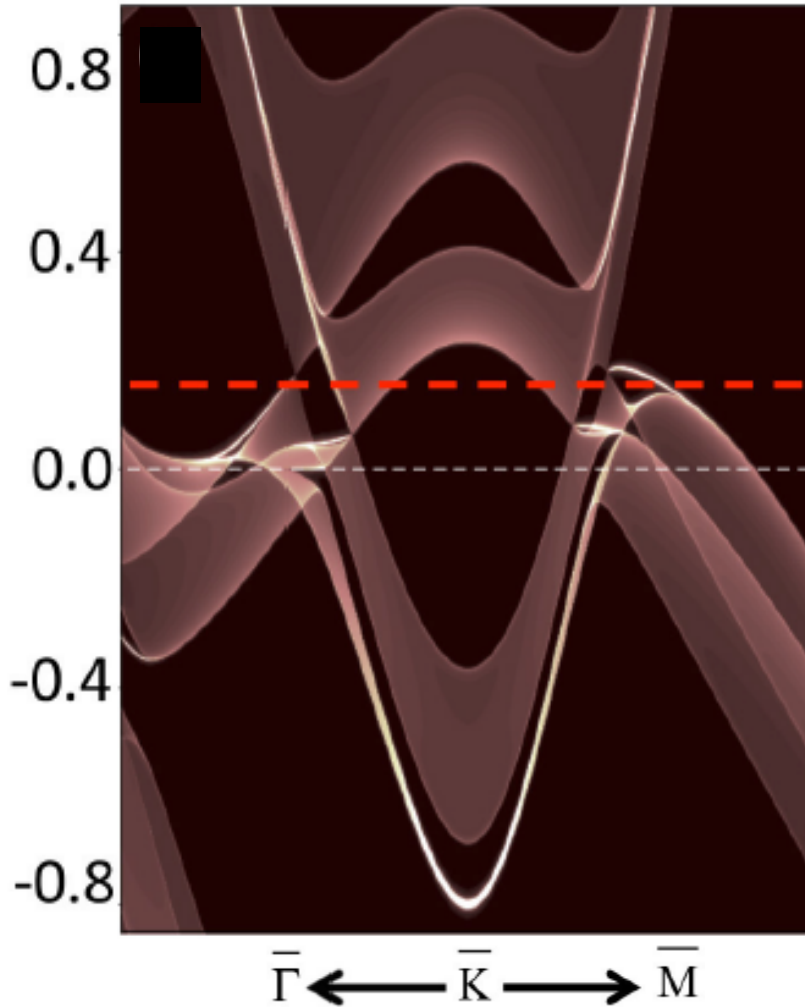
$\text{Ta-Se} = 2.66 \text{ \AA}$



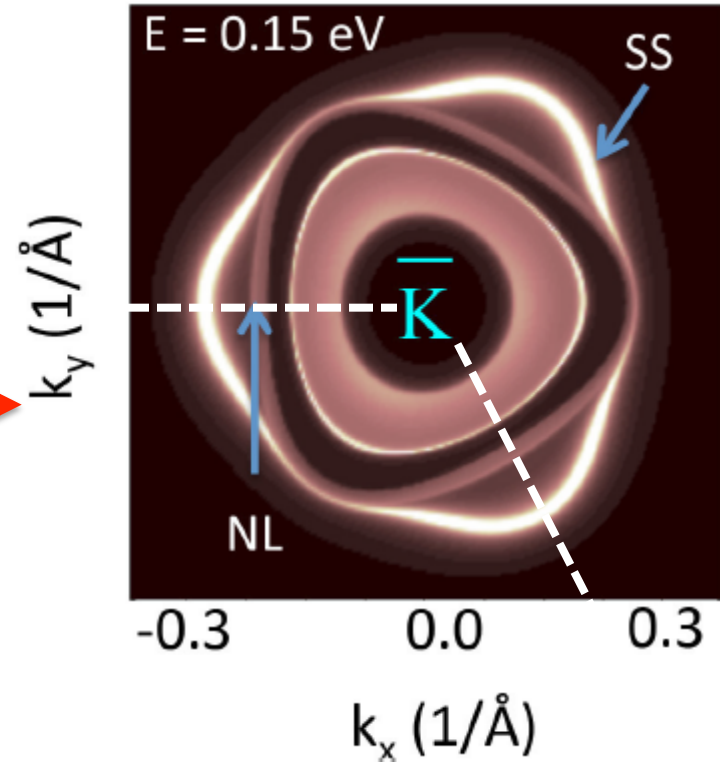
Superconducting!

Topological Nodal-Line Semimetals: PbTaSe_2

Se-terminated surface



Se-termination



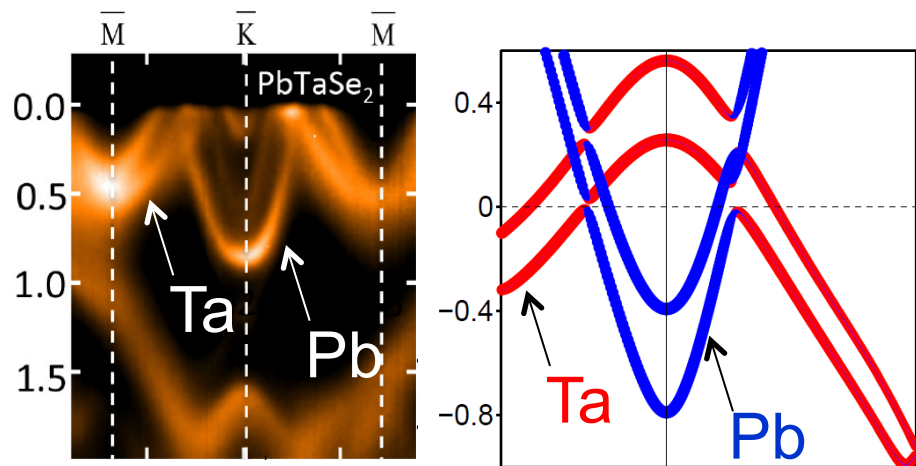
Experimental goals:

- A. Crossing of Pb and Ta bands
- B. Ring-shaped bulk Fermi surface
- C. Surface states

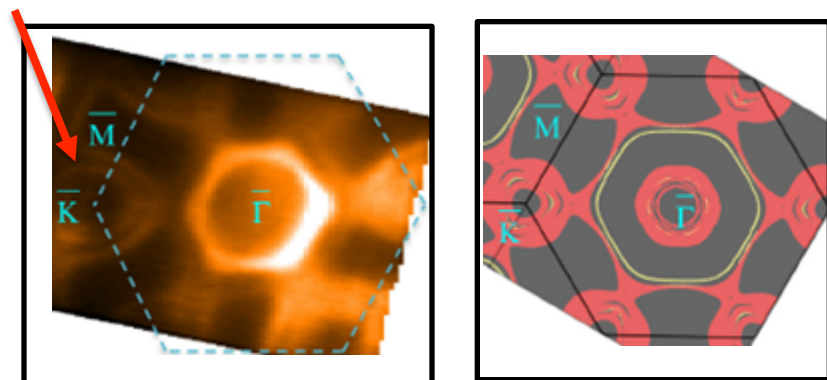
Topological Nodal-Line Semimetals: PbTaSe₂

A

Pb and Ta bands



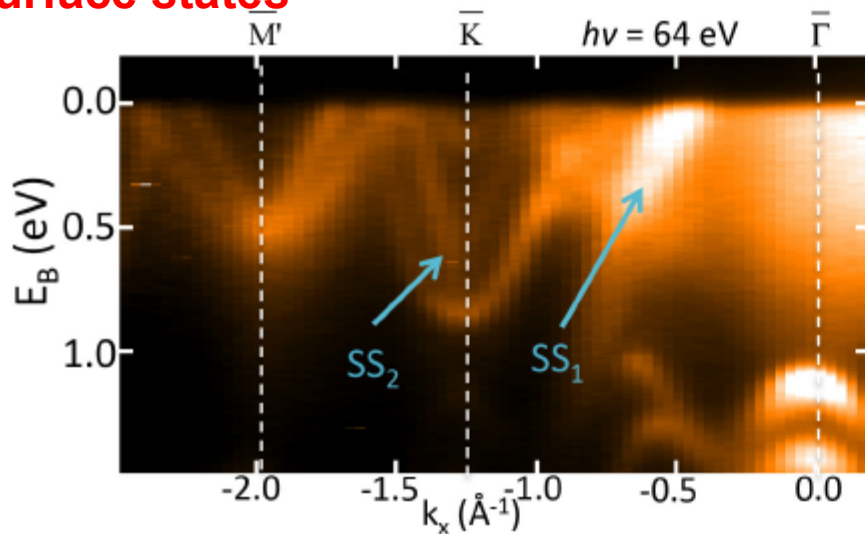
B Bulk Fermi ring



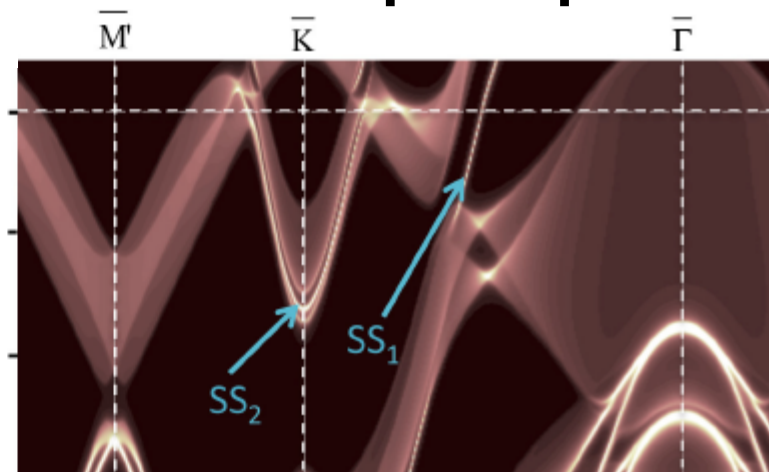
C

Surface states

ARPES



First-principles



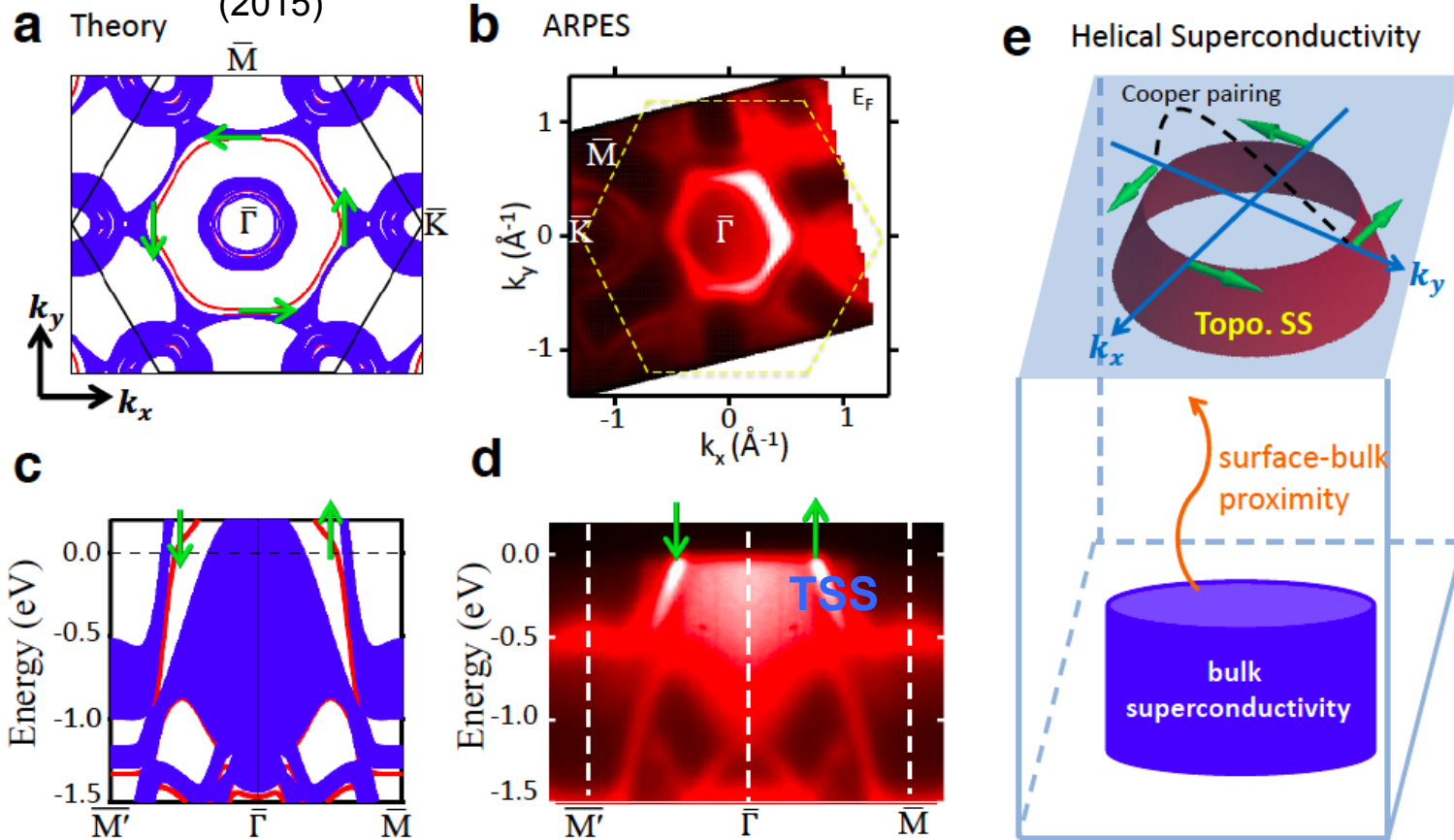
Topological Nodal-Line Semimetals: PbTaSe_2

PbTaSe_2 : Superconductivity $T_c = 3.8$ K proximity effect

Nontrivial Z_2 , topological surface states

Surface topological superconductivity

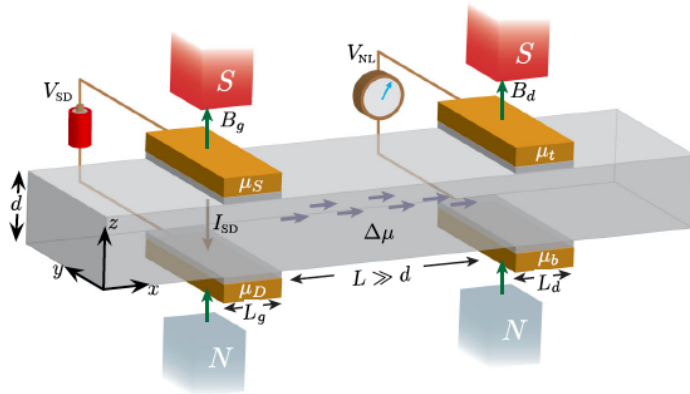
T.-R. Chang*, P.-J. Chen*, G. Bian* *et al.*, (MZH) arXiv:1511.06231



G. Bian, T.-R. Chang *et al.*, (MZH) arXiv:1508.07521 for nodal lines in TiTaSe_2

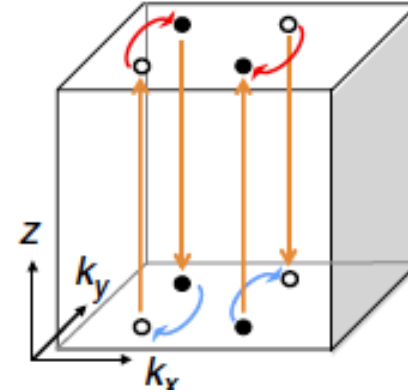
Future Weyl devices

Nonlocal transport



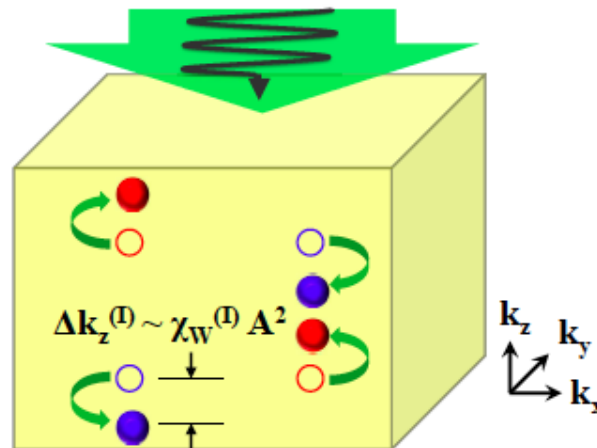
Parameswaran *et al.* *PRX* (2014)

Fermi arc transport

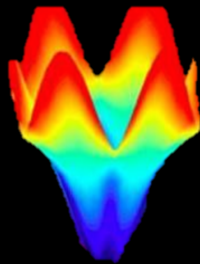


Potter *et al.* *Nature Commun.* (2014)
Huang, SYX *et al.* *Nature Commun.* (2015)

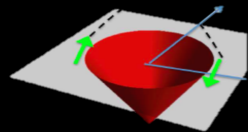
Chiral photon driven AHE



C.-K. Chan *et al.* arxiv:1509.05400 (2015).

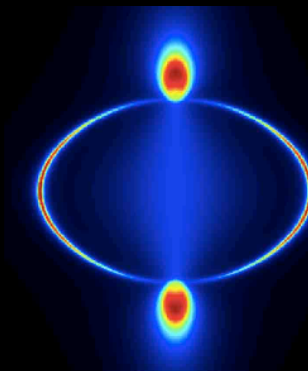


Topo. Insulator



Topo. Superconductors
Helical Pairing

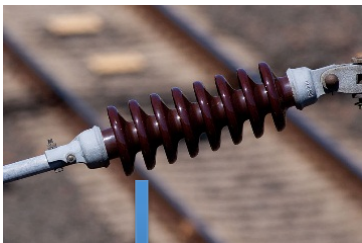
Majorana



Weyl Semimetals
Topological Fermi Arcs

Weyl Fermion & TNL Fermion
Weyl Superconductors (topological)
Weyl - Majorana

Insulators



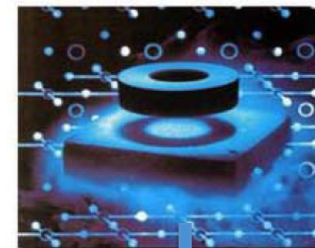
Magnets



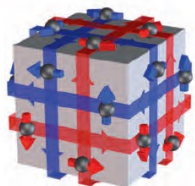
Semimetals



Superconductors

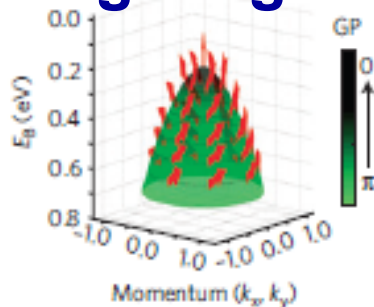


Topo Insulators



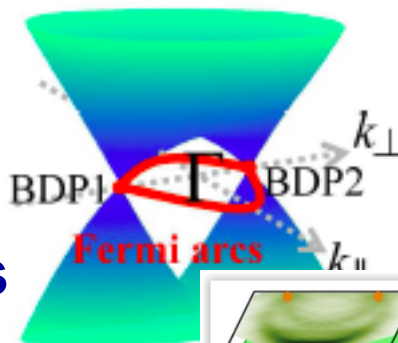
NATURE '08, SCIENCE '08
NATURE '09, SCIENCE '11

Hedgehog Magnet

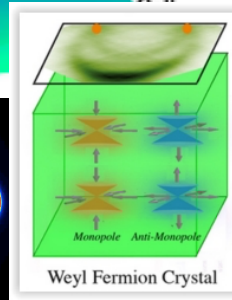


NATURE PHY '12, '11

Fermi-Arc Metal

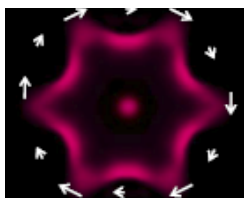
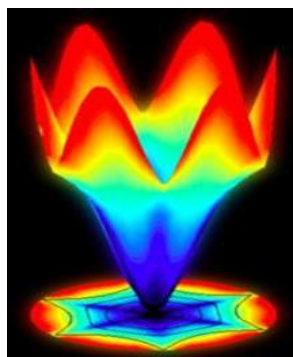
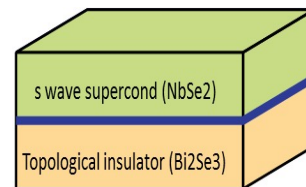


Fermi arcs

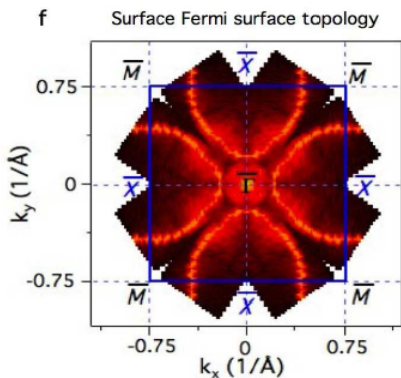


Weyl Fermion Crystal

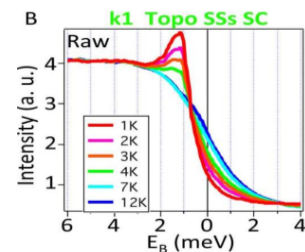
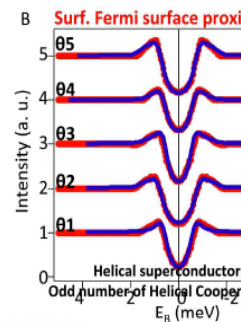
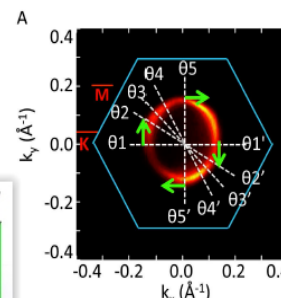
Topo. Supercond.



Kondo Insulators



SCIENCE 2014
SCIENCE 2015
Nature Phys '15



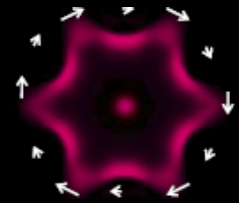
NATURE PHY '14

REVIEWS

M.Z.H. and C.L. Kane

Colloq.: “Topological Insulators” (& Superconductors)

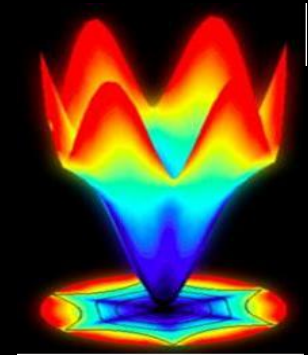
Rev. of Mod. Phys., (*RMP*) 82, 3045 (2010)



M.Z.H. and J.E. Moore

“Three Dimensional Topo. Insulators”

Ann. Rev. of Cond. Mat. Phys., 2, 78 (2011)



M.Z.H., D. Hsieh, Y. Xia, L. Wray

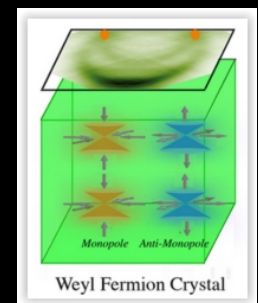
“Topological Surface States”

book Chapter in “Topological Insulators” (2013)

M.Z.H., S.-Y. Xu & I. Belopolski

“Weyl Fermions and Topological Semimetals” (2016)

Ann. Rev. of Cond. Mat. Phys., (in press)



Thanks !

MZH, Xu, Neupane *Topo Insulators, Topo Cryst. Insulators & Topo Kondo Insulators*, arXiv(2014)

MZH, Xia, Hsieh, Wray et.al., (Book ch.) *Topological Insulators*, Elsevier/Oxford (2013)

Nature '08 (sub. in **2007**)

Science '09

Nature Phys. '09

Nature '09

PhyRevLett '09

Nature '09

Nature Phys. '10

PhyRevLett. '10

Nature Mat. '10

RevModPhys. '10

AnnRevCMP. '11

Nature Phys. '11

PhyRevLett. '12

Nature Comm. '12

Science '11

Nature Phys. '12

Nature Comm. '13

Science '13

Nature Comm. '14a

Nature Comm. '14b

Nature Comm. '14c

Nature Phys '14

Nature Phys '14

Science 2014

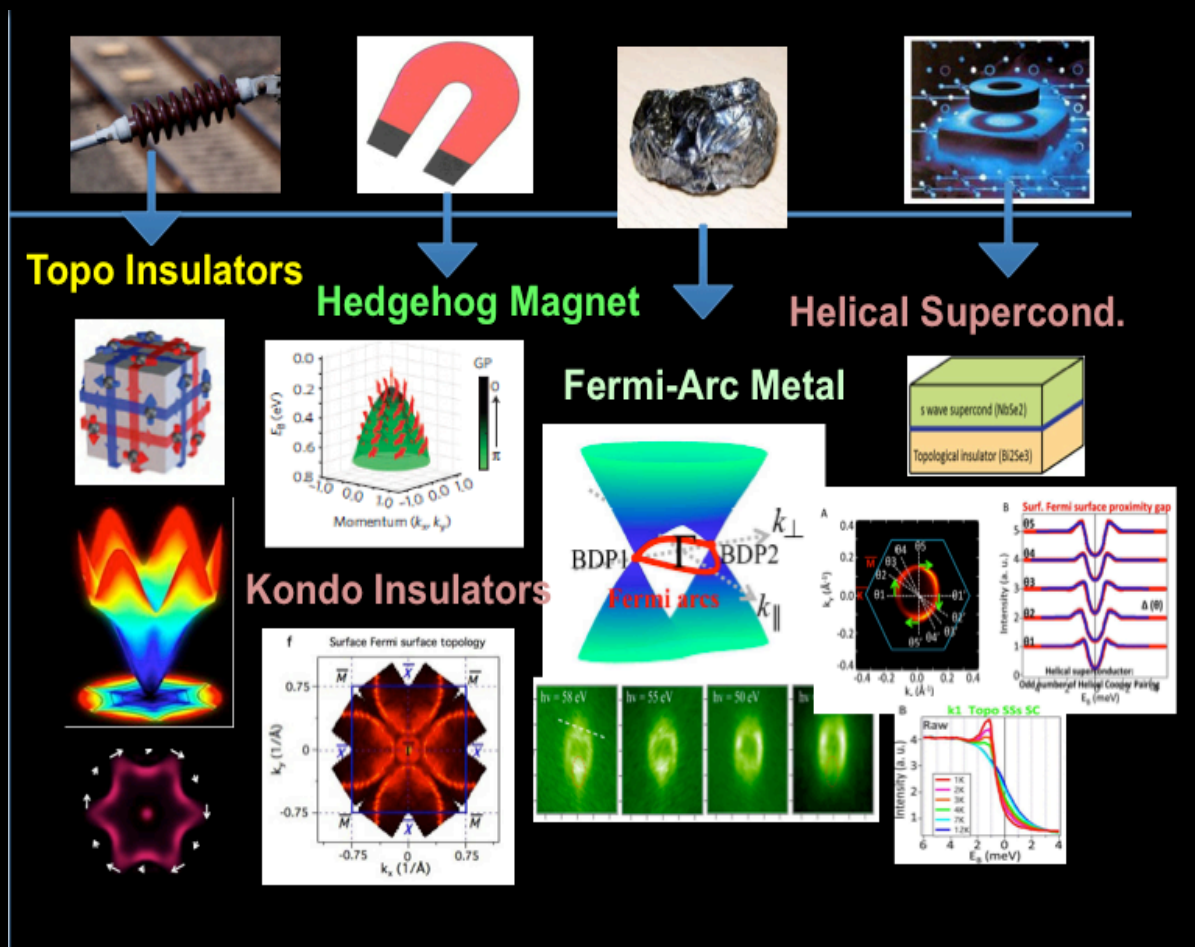
Science 2015

Science Adv '15

Nature Phys '15

MZH and C.L. Kane *Rev. of Mod. Phys., (RMP) 82*, 3045 (2010)

MZH and J.E. Moore *Ann. Rev. of Cond. Mat. Phy., 2*, 78 (2011)



Topological Condensed Matter Physics