

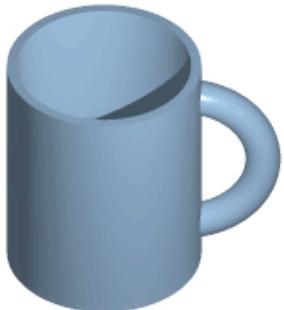


# Topological Semimetals

Zhong Fang  
Institute of Physics, CAS,  
Beijing

## Acknowledgement:

Theory: H. M. Weng, X. Dai, Z. J. Wang (IoP),  
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X. J. Zhou, Li Lu, Hong Ding, Y. Q. Li (IoP)  
Y. G. Shi, G. F. Chen (IoP)  
Ming Shi, N. Xu (PSI)



# 目 录

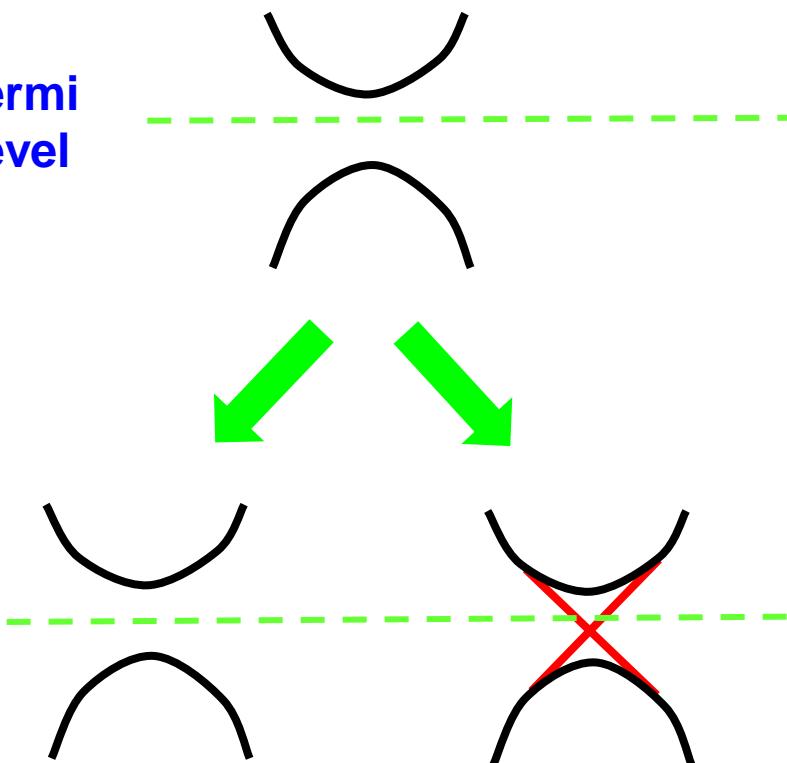
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1. Introduction: New state--Topological semi-metals.
2. Expected Novel Properties:
3. Prediction of Materials & Exp. Progresses.
  - (1) Dirac Semimetal:  $\text{Na}_3\text{Bi}$  &  $\text{Cd}_3\text{As}_2$
  - (2) Weyl semimetal:  $\text{HgCr}_2\text{Se}_4$ . &  $\text{TaAs}$   
 $(\text{TaP}, \text{NbAs}, \text{NbP})$

# 1. Introduction: Topological Metals?

## Insulators

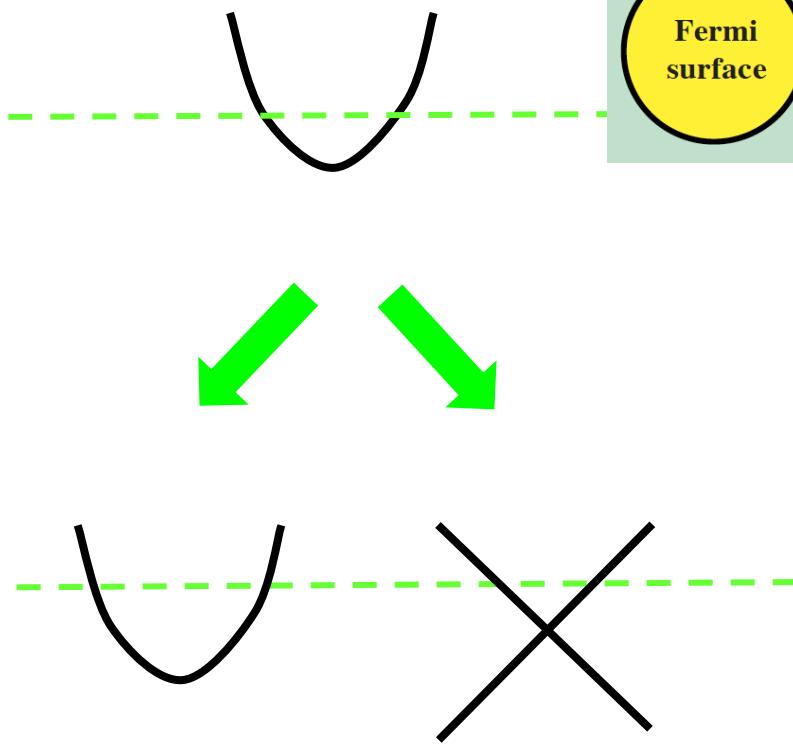
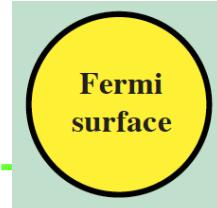
Fermi Level



Normal

## Metals

## Metals



Normal

Topological

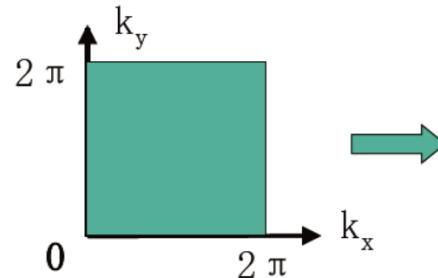
Gapless boundary states

Can metals be classified?  
How to define TM?

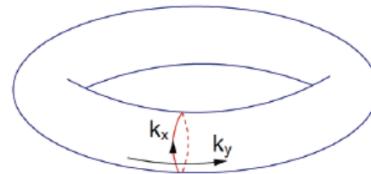
Topological  
Metal?

# 1. Introduction: Topological Invariants for Insulators

## Z-number for T-broken QH or QAH insulators (2D)



Winding Number  $N$



$$S_{xy} = -\frac{e^2}{2ph} \int_{BZ} W_z(k) d^2k = -n \frac{e^2}{h}$$

$n$ =Chern number

TKNN, PRL (1982):

$$n = \sum_{bands} \frac{i}{2\pi} \int d^2k \left( \left\langle \frac{\partial u}{\partial k_1} \middle| \frac{\partial u}{\partial k_2} \right\rangle - \left\langle \frac{\partial u}{\partial k_2} \middle| \frac{\partial u}{\partial k_1} \right\rangle \right)$$

Haldane, PRL (1988): Lattice Model (Honeycomb);

Onoda & Nagaosa: PRL (2003); S. C. Zhang: PRB (2006); PRL (2008)

Realization: Fang & Dai, Science 2010 (Theory); Xue, Science 2013 (Exp.)  
(Cr-doped (BiSb)Te<sub>3</sub> thin film)

## $Z_2$ number for Topological insulators with T-symmetry

2D: Kane & Mele (2005, 2006); Bernevig & Zhang (2006); HgTe, InAs/GaSb

3D: More & Balents (2007); Fu & Kane (2007);

H. J. Zhang, et. al. (2009); Y.Xia, et.al. (2009); Y.Chen (2010) Bi<sub>2</sub>Se<sub>3</sub>, Bi<sub>2</sub>Te<sub>3</sub>

Simple view: Two QAH-layers related by T-symmetry

# 1. Introduction: K-space as parameter space

**Bloch State:** 
$$\begin{cases} H(\vec{r})\psi_{nk}(\vec{r}) = \epsilon_{nk}\psi_{nk}(\vec{r}) \\ \psi_{nk}(\vec{r}) = e^{ik \cdot \vec{r}} u_{nk}(\vec{r}) \end{cases} \quad \rightarrow \quad \begin{cases} H_k(\vec{r})u_{nk}(\vec{r}) = \epsilon_{nk}u_{nk}(\vec{r}) \\ H_k = e^{-ik \cdot \vec{r}} H e^{ik \cdot \vec{r}} \end{cases}$$

**Gauge Freedom:**  $|u_{nk}^{\text{C}}\rangle = e^{i\tilde{f}(k)}|u_{nk}\rangle \quad \rightarrow \quad H_k|u_{nk}^{\text{C}}\rangle = \epsilon_{nk}|u_{nk}^{\text{C}}\rangle$

**Berry Connection:**  $\vec{A}_n(k) = i\langle u_{nk} | \vec{\nabla}_k | u_{nk} \rangle$

Gauge dependent

$$\vec{A}'_n(k) = i\langle u'_{nk} | \vec{\nabla}_k | u'_{nk} \rangle = \vec{A}_n(k) - \vec{\nabla}_k \phi(k)$$

**Berry Curvature:**  $\vec{\Omega}_n(k) = \vec{\nabla}_k \times \vec{A}_n(k) = i\langle \vec{\nabla}_k u_{nk} | \times | \vec{\nabla}_k u_{nk} \rangle$

Gauge invariant

$$\vec{\Omega}_n(k) = \vec{\nabla}_k \times \vec{A}'_n(k) = \vec{\nabla}_k \times \vec{A}_n(k)$$

**Symmetry:**  $\vec{\Omega}_n(k) = \vec{\Omega}_n(-k) \quad \text{for IS} \quad \vec{\Omega}_n(k) \equiv 0$

$$\vec{\Omega}_n(k) = -\vec{\Omega}_n(-k) \quad \text{for TRS} \quad \text{for IS and TRS}$$

# 1. Introduction: Magnetic Field in K-space

**Key quantity:**  $\vec{\Omega}(\mathbf{k}) = \nabla_{\mathbf{k}} \times \vec{A}(\mathbf{k}) = \nabla_{\mathbf{k}} \times i \langle u_{nk} | \nabla_{\mathbf{k}} | u_{nk} \rangle$

$A(\mathbf{k})$ : Berry connection,  $u_{nk}$ : periodic part of Bloch function

**can be viewed as magnetic field in k-space**

[ Sundaram & Niu, et.al, PRB (1999); Jungwirth & Niu, et.al, PRL (2002);  
Fang, et.al, Science (2003); Y. Yao & Niu, et.al. PRL (2004)]

## Analogies

Berry curvature  
 $\vec{\Omega}(\vec{k})$

Berry connection  
 $\vec{A}(\vec{k}) = \langle \psi | i \frac{\partial}{\partial \vec{k}} | \psi \rangle$

Geometric phase  
 $\oint d\vec{k} \cdot \vec{A}(\vec{k}) = \iint d^2k \Omega_z(\vec{k})$

$$\oint d\vec{k} \cdot \vec{A}(\vec{k}) = \iint d^2k \Omega_z(\vec{k})$$

Chern number  
 $\iint d^2k \Omega_z(\vec{k}) = \text{integer}$

Magnetic field  
 $\vec{B}(\vec{r})$

Vector potential  
 $\vec{A}(\vec{r})$

Aharonov-Bohm phase  
 $\oint d\vec{r} \cdot \vec{A}(\vec{r}) = \iint d^2r B_z(\vec{r})$

$$\iint d^2r B_z(\vec{r}) = \text{integer } h/e$$

Equation of motion:

$$\dot{\mathbf{r}} = \frac{1}{\hbar} \frac{\partial \epsilon(\mathbf{k})}{\mathbf{k}} - \vec{\mathbf{k}} \times \vec{\Omega}(\mathbf{k})$$

$$\hbar \dot{\mathbf{k}} = -e\mathbf{E}(\mathbf{r}) - e\dot{\mathbf{r}} \times \mathbf{B}(\mathbf{r})$$

Anomalous velocity

$$x_i = i \frac{\partial}{\partial k_i} - \tilde{A}_i(\vec{k}), \quad [x, y] = -i \Omega_z(\vec{k})$$

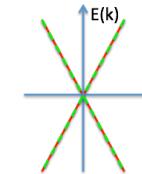


**Anomalous Hall Effect**

# 1. Introduction: Massless Dirac & Weyl Fermion

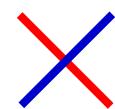
Massless Dirac (4x4):  
(Reducible !!)

$$H = \begin{bmatrix} 0 & -c\hat{S} \times \hat{p} & 0 & \bar{u} \\ 0 & 0 & c\hat{S} \times \hat{p} & \bar{d} \\ \bar{u} & \bar{d} & 0 & 0 \end{bmatrix}$$



Weyl representation (2x2):  
(Irreducible !!)

$$H(\vec{k}) = \pm \vec{k} \cdot \vec{\sigma} = \pm \begin{bmatrix} k_z & k_x - ik_y \\ k_x + ik_y & -k_z \end{bmatrix}$$



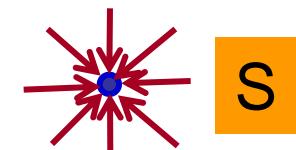
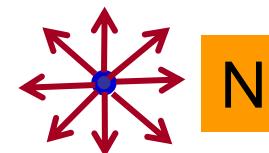
Left-hand + right-hand

## Weyl nodes:

- (1) Topological Objects
- (2) Gapless, no mass term
- (3) Chirality  $\pm$  (left or right-hand)
- (4) Protected by translation  
(k must be well defined)

## Magnetic Monopoles:

$$\vec{\Omega}(k) = \vec{\nabla}_k \times \vec{A}(k) = \pm \frac{\vec{k}}{2|k|^3} \quad \vec{\nabla} \cdot \vec{\Omega} \neq 0$$



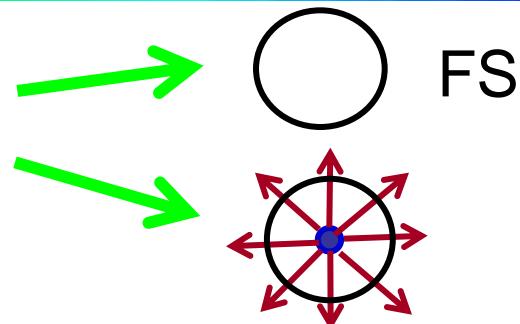
$$\frac{1}{2\pi} \oint_S \vec{\Omega}(k) \cdot d\vec{S}(k) = Q$$

magnetic Charge

Fang, Science (2003).

# 1. Introduction: Topological Invariant for Metals

**Definition:**  $\frac{1}{2\pi} \oint_{FS} \vec{\Omega}(k) \cdot d\vec{S}(k) = C_{FS}$



$C_{FS}=0$ , normal metal

$C_{FS}\neq 0$ , topological Weyl metal

if  $E_f$  at node ( $k=0$ )  $\rightarrow$  topological semimetal

Volovik, JETP (2002).

Z. J. Wang, et.al., PRB (2012)

## Notes:

- (1)  $|Q|$  can be more than 1
- (2)  $+Q$  &  $-Q$  monopoles have to appear in pair in lattice, but may separate in K. (No-go Theorem)
- (3)  $+Q$  &  $-Q$  monopoles can annihilate.
- (4) Defined only for 3D k-space

# 1. Introduction: Special Case: 3D Dirac Semimetal

If both T and I symmetry are present:

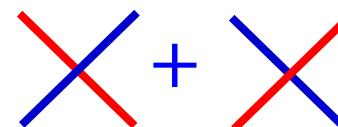
+Q & -Q Weyl nodes have to overlap in K-space

$$H(k) = \begin{pmatrix} \hat{e} & k \times S & M^* & \hat{u} \\ \hat{e} & M & -k \times S & \hat{u} \end{pmatrix}$$

Case I:  $M \neq 0$ , Insulator

$$H(k) = \begin{pmatrix} \hat{e} & k \times S & 0 & \hat{u} \\ \hat{e} & 0 & -k \times S & \hat{u} \end{pmatrix}$$

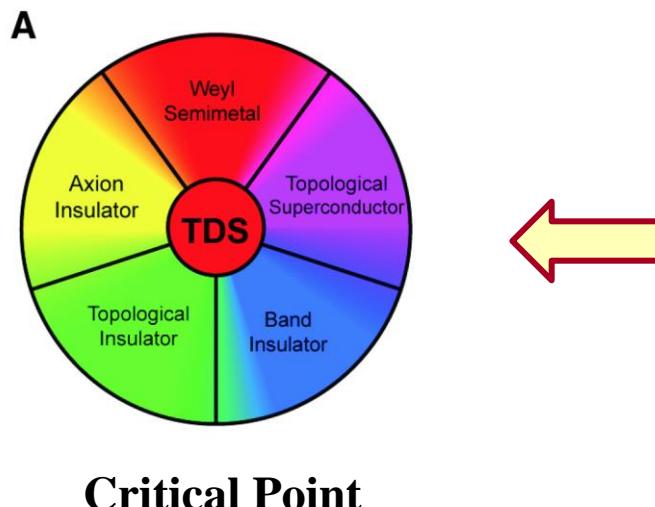
Case II:  $M=0$ , 3D Dirac Semimetal



Need crystal symmetry protection.

**3D Dirac semimetal:**

- (1) Pseudo fermi arcs on surface
- (2) Giant diamagnetism:  $\chi(\epsilon) \approx \log(1/\epsilon)$
- (3) Linear Quantum magneto-resistance.
- (4) QSHE in its quantum-well structure



Z. J. Wang, et.al., PRB (2012).  
S. M. Young, et.al., PRL (2012).

## 2. Novel Properties: Magnetic Monopoles in bulk

=> Anomalous/Spin Hall Effect,

[Fang, et.al, Science (2003)]

Quantum AHE/SHE for quantum well structure

(with higher plateaus & Tc, etc.)

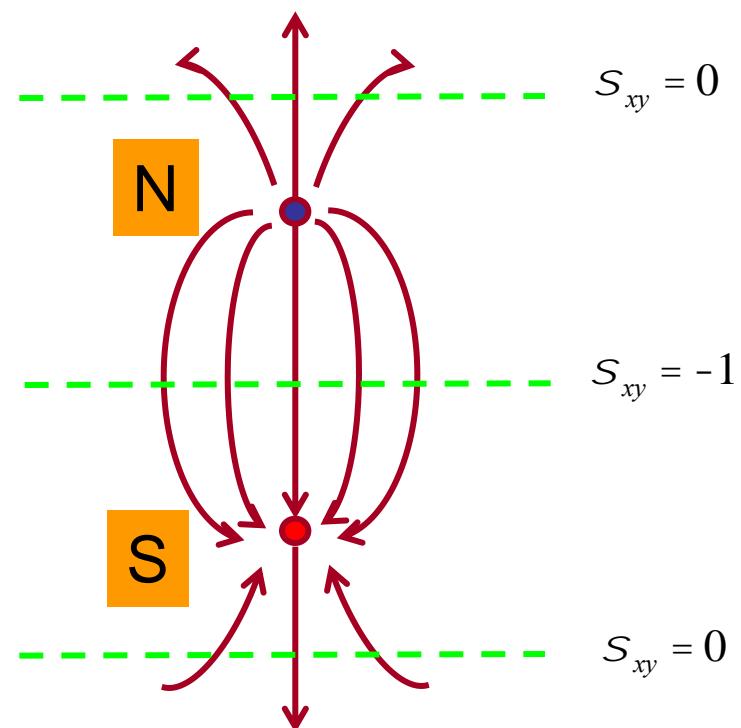
[X. Gu, et.al. PRL (2011), HgCr<sub>2</sub>Se<sub>4</sub> ]

A diagram showing a green rectangular plane representing a quantum well. On the plane, there is a central grey dot representing a magnetic monopole. From the monopole, several red arrows point outwards in various directions, representing the magnetic field lines. To the right of the diagram, two equations are shown:

$$S_{xy} = \frac{1}{2} \cdot \frac{e^2}{h}$$
$$S_{xy} = -\frac{1}{2}$$

A diagram showing a green rectangular plane representing a quantum well. On the plane, there is a central grey dot representing a magnetic monopole. From the monopole, several red arrows point outwards in various directions, representing the magnetic field lines. To the right of the diagram, two equations are shown:

$$S_{xy} = -\frac{1}{2}$$
$$S_{xy} = \frac{1}{2}$$

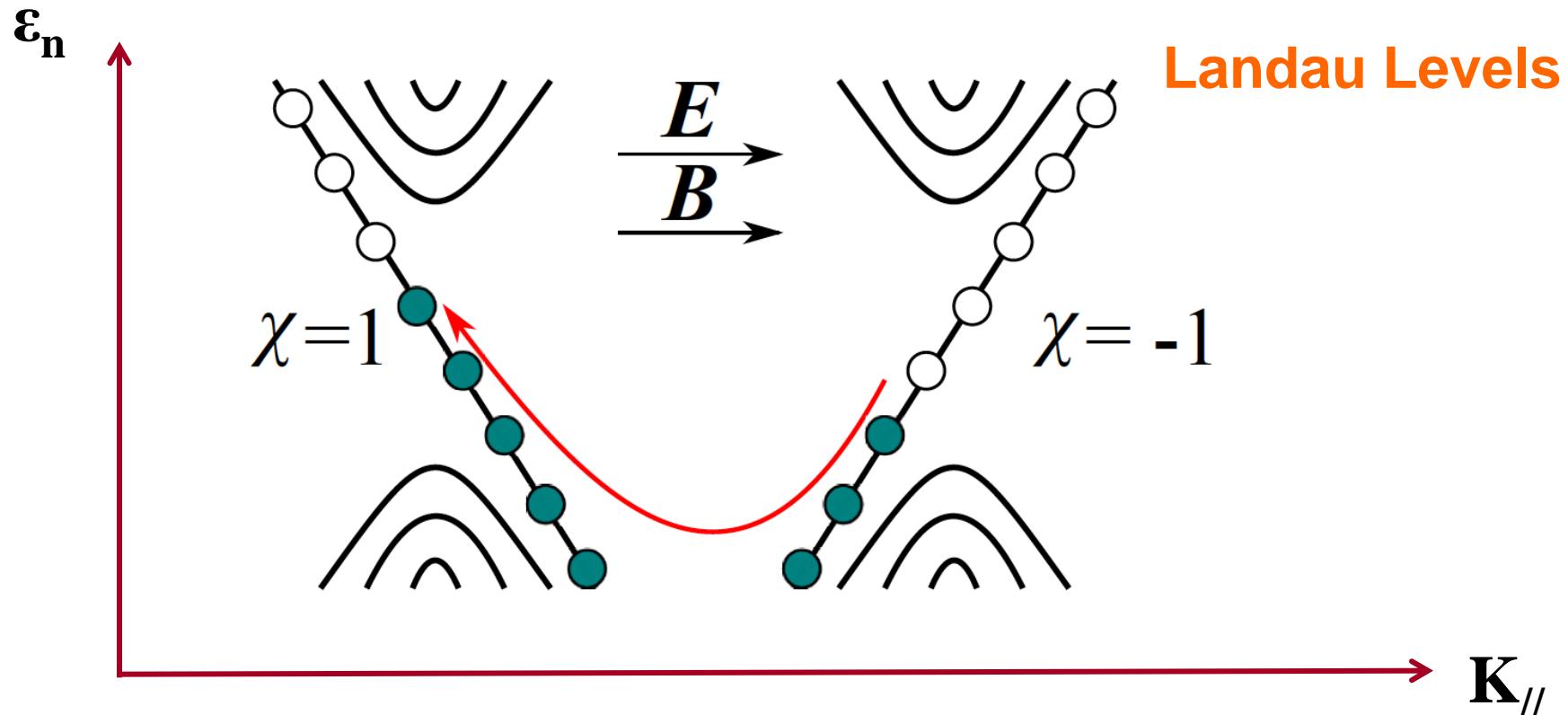


## 2. Novel Properties: Chiral Anomaly

=> Negative MR for E//B,  
Non-local Transport

[Nielsen & Ninomiya, Phys. Lett. (1983)]

[ S. A. Parameswaran, et.al. PRX (2013)]

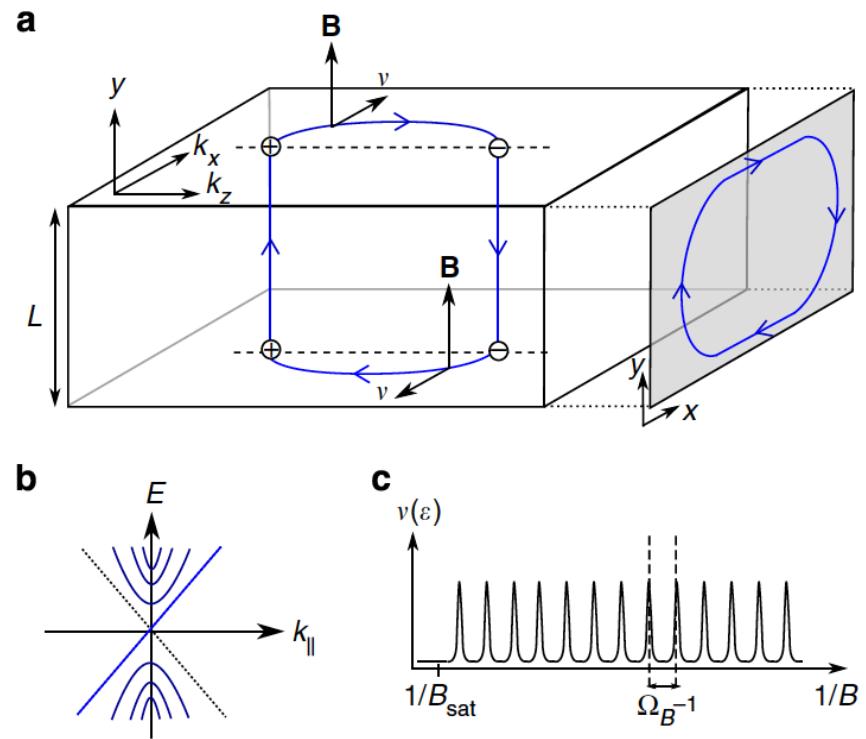
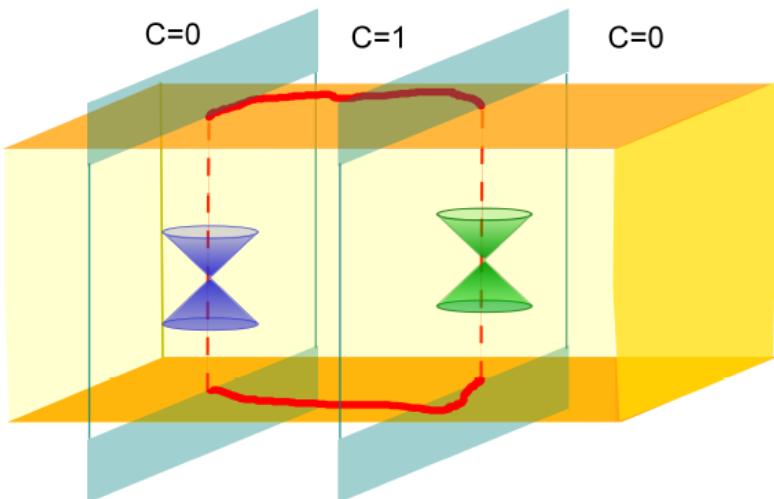


Intra-node: No back-scattering

## 2. Novel Properties: Fermi arcs on Surfaces

=> Surface Fermi arcs, [ X. Wan, et.al, PRL (2011) ]

Saturated Quantum Oscillation [A.C.Potter, et.al., Nature Comm. (2014)]



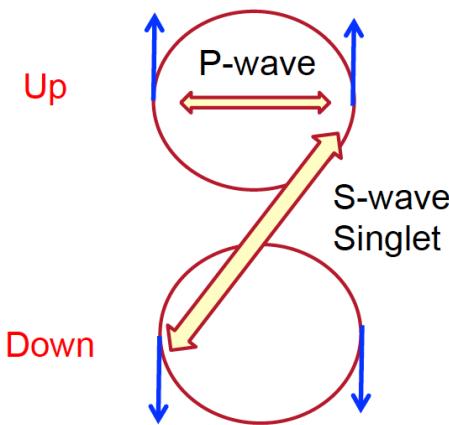
Thickness  $L$  dependent

## 2. Novel Properties: Spin-Momentum Lock in 3D

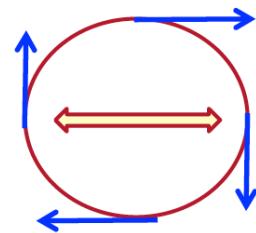
Doping  $\Rightarrow$  Topological Superconductor (TSC)

### Schematic

Conventional Metal



Weyl Metal



Singlet (BCS)  
Effective p+ip

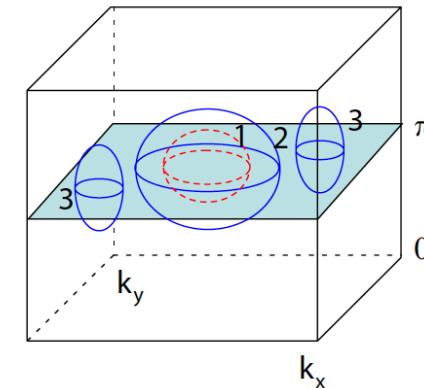
**Weak interaction limit:**

No T-invariant TSC  
in I-symmetric WSM or DSM

P. Hosur, et.al., PRB 90, 045130 (2014).

### Multiple FS in general

[ X. L. Qi, et.al, PRB (2010)]



**Topological Invariant:**

$$\nu = \frac{1}{2} \sum_{FS} C_{FS} \operatorname{sgn}(D_{FS})$$

**Criteria:**

- (1)  $C_{FS} \neq 0$
- (2)  $\Delta_{FS}$  have opposite signs.

### 3. Prediction & Exp.: Several Proposals

#### Break time-reversal symmetry

- $R_2\text{Ir}_2\text{O}_7$  with all-in/all-out magnetic order  
X. G. Wan *et al.*, Phys. Rev. B **83**, 205101 (2011)
- Ferromagnetic  $\text{HgCr}_2\text{Se}_4$   
G. Xu, Hongming Weng, *et al.* PRL **107**, 186806 (2011)
- $\text{Hg}_{1-x-y}\text{Cd}_x\text{Mn}_y\text{Te}$   
D. Bulmash, *et al.* PRB **89**, 081106 (2014)
  - artificial superlattice of (magnetically doped) TI and NI  
Burkov & Balents, PRL **107**, 127205(2011), Halasz & Balents PRB **85**, 035103 (2012).

#### Break inversion symmetry

- Solid solution:  $\text{TI}_n\text{Bi}(\text{S}_{1-x}\text{R}_x)_2$   
B. Singh *et al.*, Phys. Rev. B **86**, 115208 (2012)
- Solid solution:  $L_n\text{Bi}_{1-x}\text{Sb}_x\text{Te}_3$   
J. P. Liu *et al.*, Phys. Rev. B **90**, 155316 (2014)
- High pressure Se/Te  
M. Hirayama *et al.*, arXiv:1409.7517

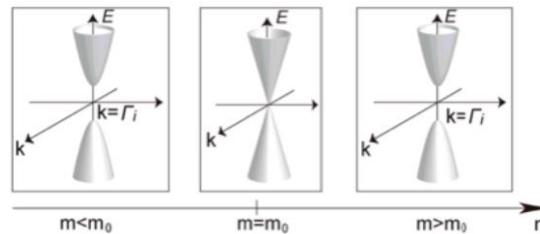
#### Problems/Disadvantages:

- complex magnetic domain structure
- ARPES requires full screening of magnetic field
- Magnetoresistance measurement: external magnetic field vs. magnetization
- Sophisticated fine tuning in both sample fabrications and measurements.

This list is not complete.

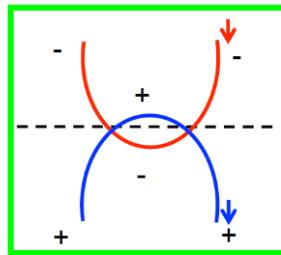
### 3. Prediction & Exp.: Band Inversion Mechanism

Transition State between TI and NI:  
( Murakami, arXiv:1006.1183)

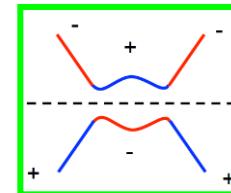


Fragile

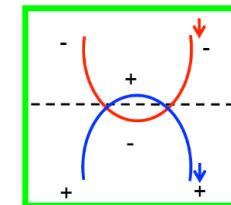
#### Weyl Semimetal:



SOC  
→

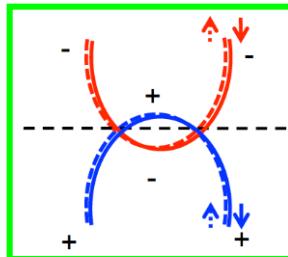


Gapped in 2D

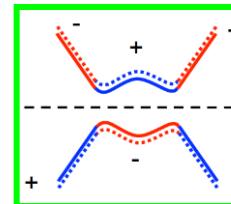


Gapless in 3D

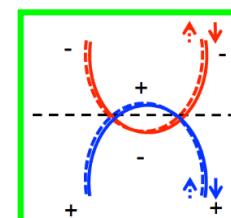
#### Dirac Semimetal:



SOC  
→



Gapped in  
both 2D & 3D

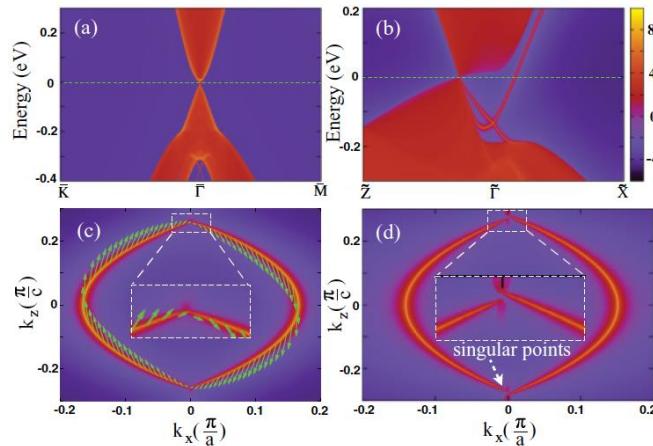


Gapless if  
+ Crystal symmetry

### 3. Prediction & Exp.: Dirac Semimetals

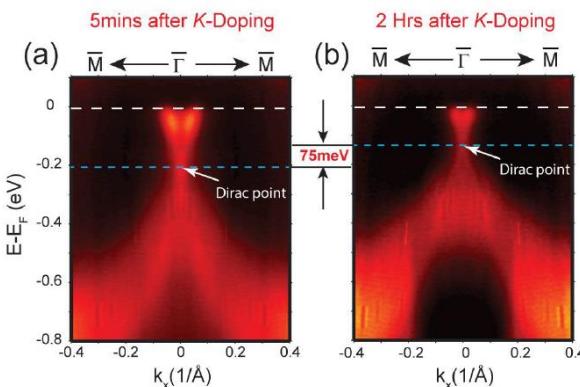
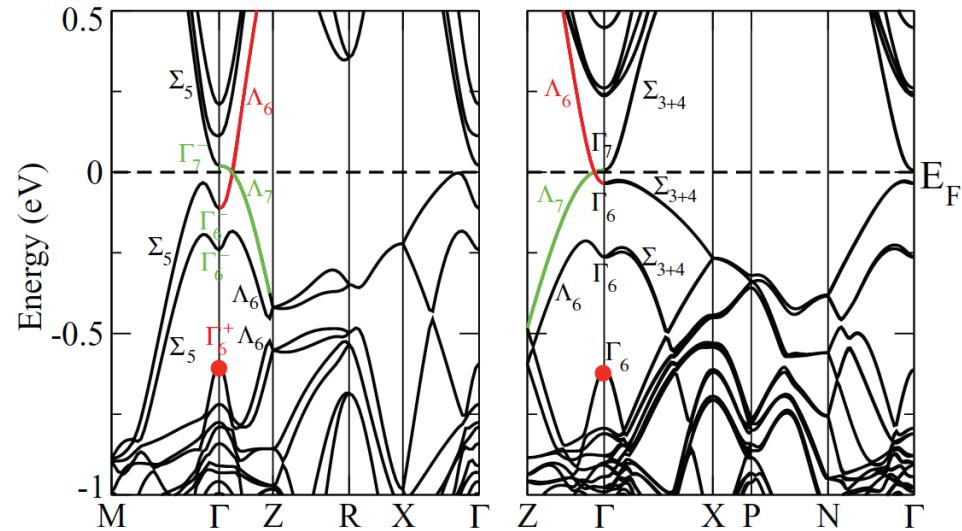
**Na<sub>3</sub>Bi**

Z. J. Wang, PRB 85, 195320 (2012)



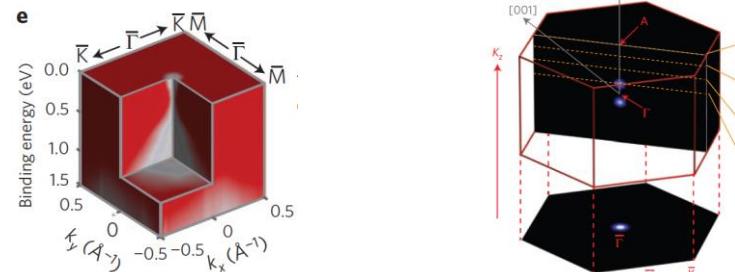
**Cd<sub>3</sub>As<sub>2</sub>**

Z. J. Wang, PRB 88, 125423 (2013)



**ARPES:**

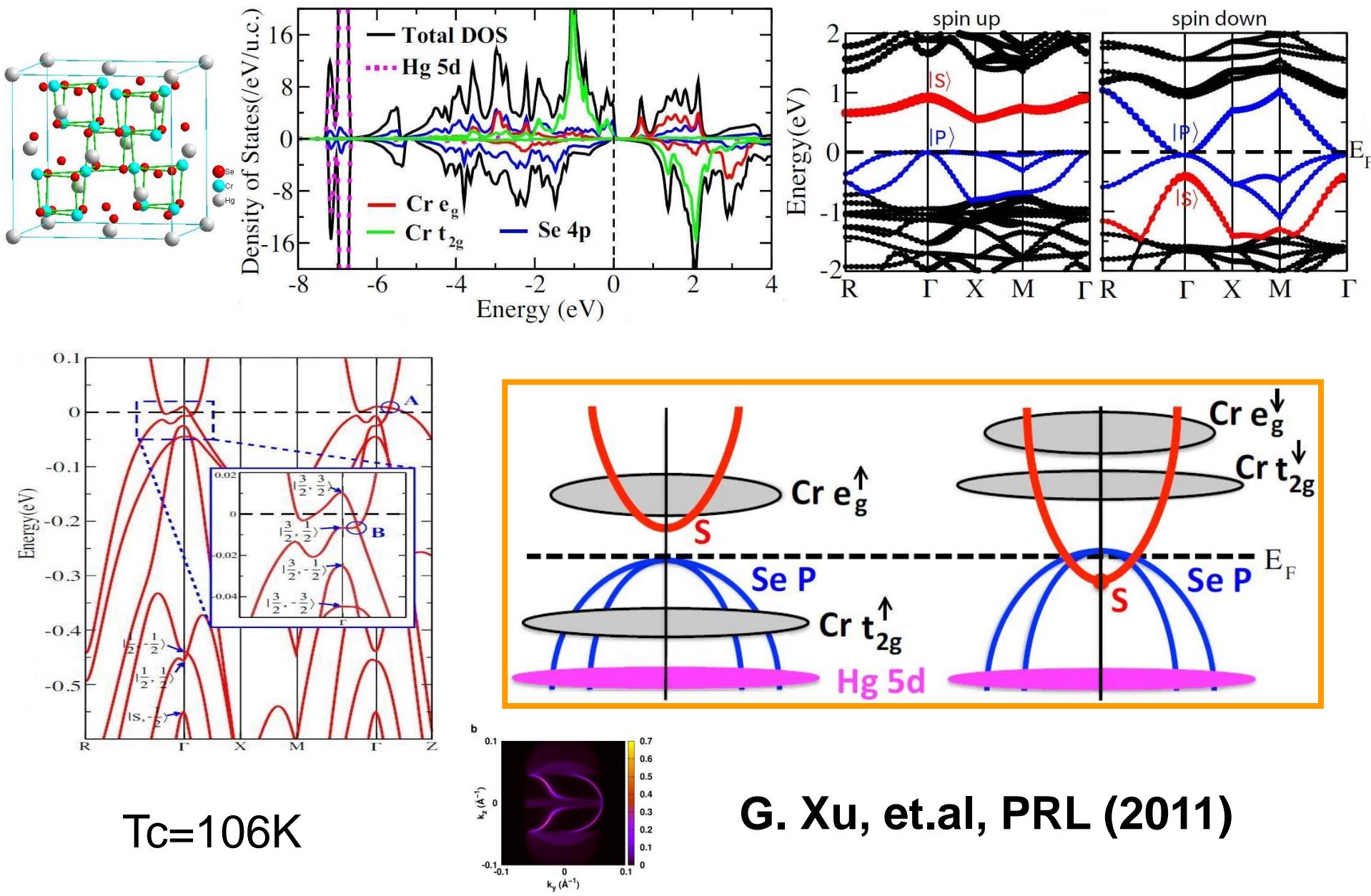
Z. K. Liu, Science (2014).  
S. Y. Xu, Science (2014).



**ARPES:**

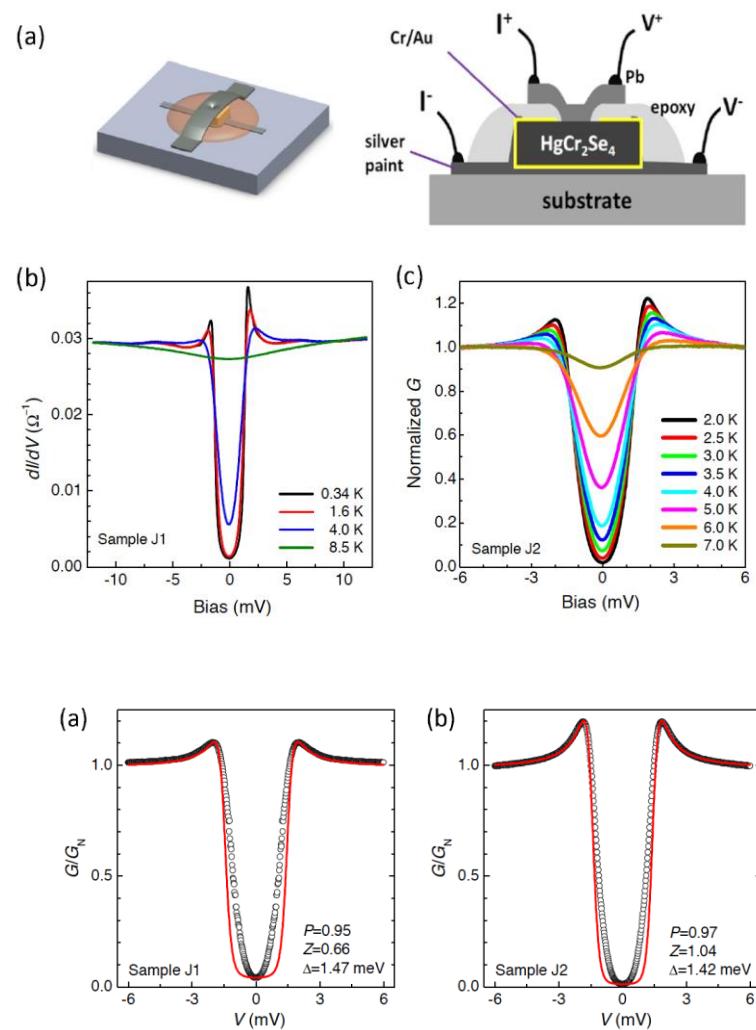
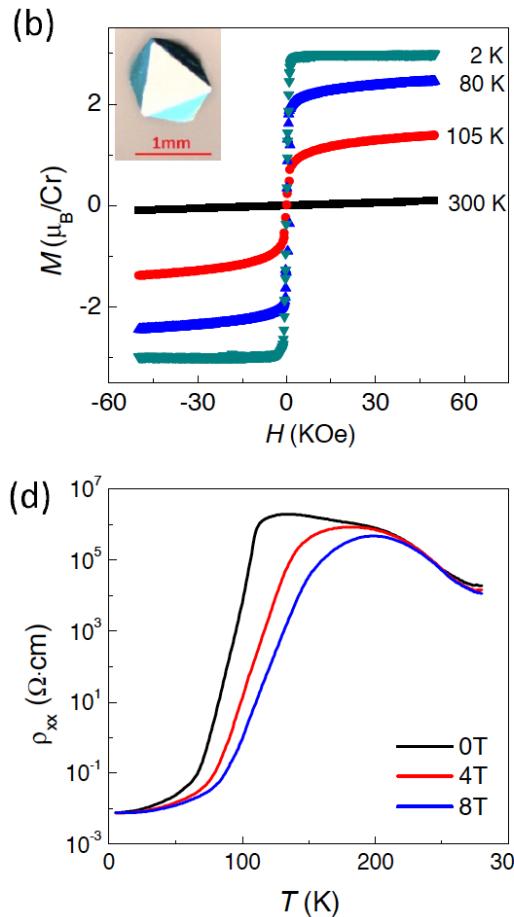
Z. K. Liu, Nature Mater. (2014).  
M. Neupane, Nature Comm. (2014).  
S. Borisenko, PRL (2014).

### 3. Predictions & Exp: T-broken Weyl Semimetal: $\text{HgCr}_2\text{Se}_4$



### 3. Predictions & Exp: T-broken Weyl Semimetal: $\text{HgCr}_2\text{Se}_4$

Single s-band Half Metallicity:

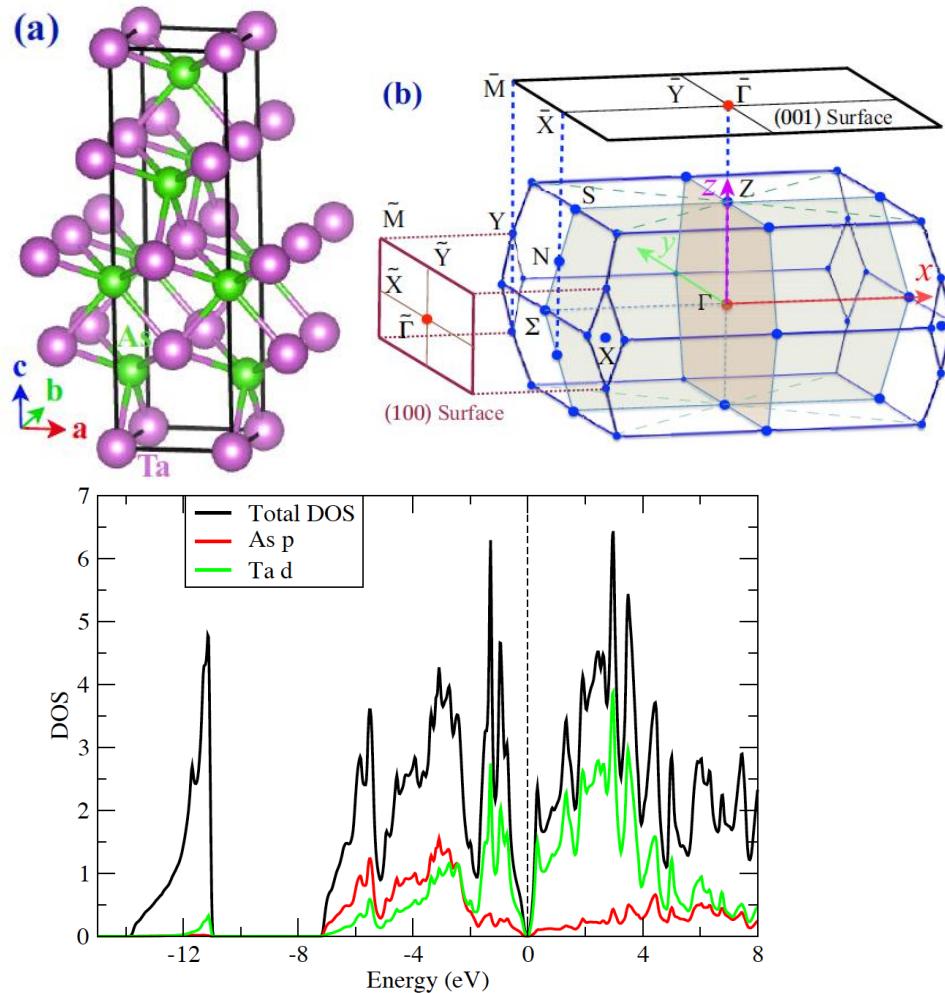


Y. Q. Li, et.al, (2014).

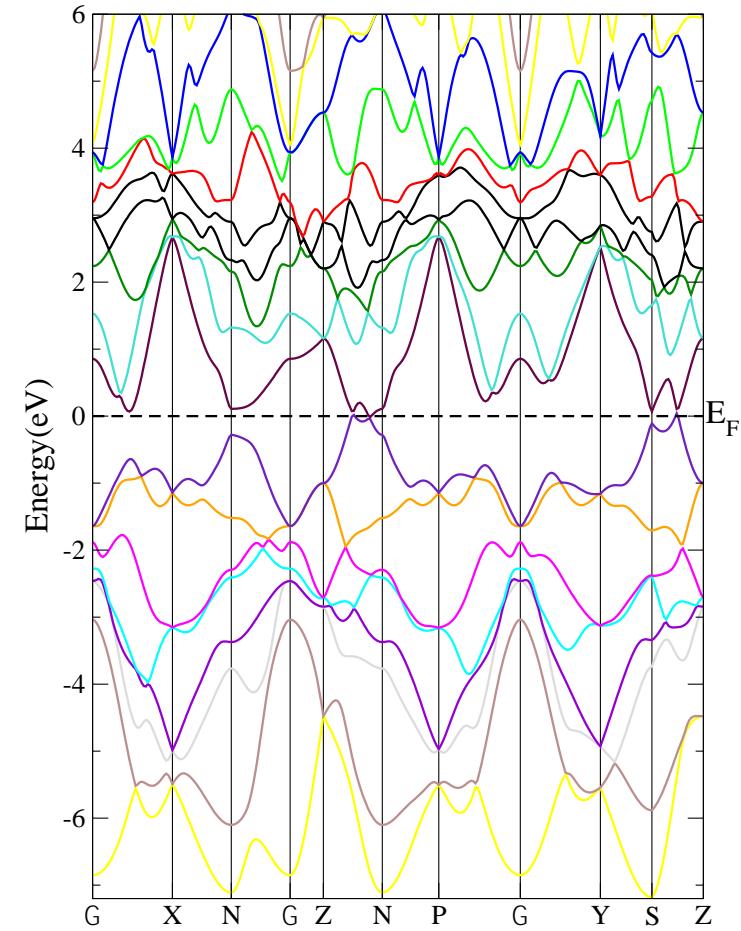
$P = 95\%, 97\%$

### 3. Prediction & Exp: T-invariant WSM: TaAs family

**Family: TaAs, TaP, NbAs, NbP ( $I4_1md$ , 109,  $C4v$ )**



Nominal valence:  $Ta^{+3}As^{-3}$ ,  $Ta-5d^2$   
 Ta-5d, yz/zx occupied



**Important Symm.:  $M_x, M_y$   
 $M_{xy}, M_{-xy}$  + glide**

### 3. Prediction & Exp: T-invariant WSM: TaAs family

## Known properties of TaAs family

NbAs

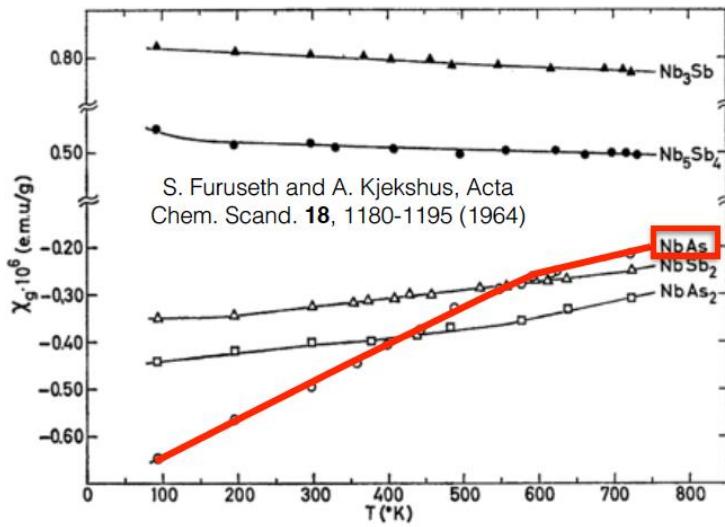


Fig. 5. The magnetic susceptibilities of  $\text{NbAs}$ ,  $\text{NbAs}_2$ ,  $\text{Nb}_3\text{Sb}$ ,  $\text{Nb}_5\text{Sb}_4$ , and  $\text{NbSb}_2$  as a function of temperature.

TaAs

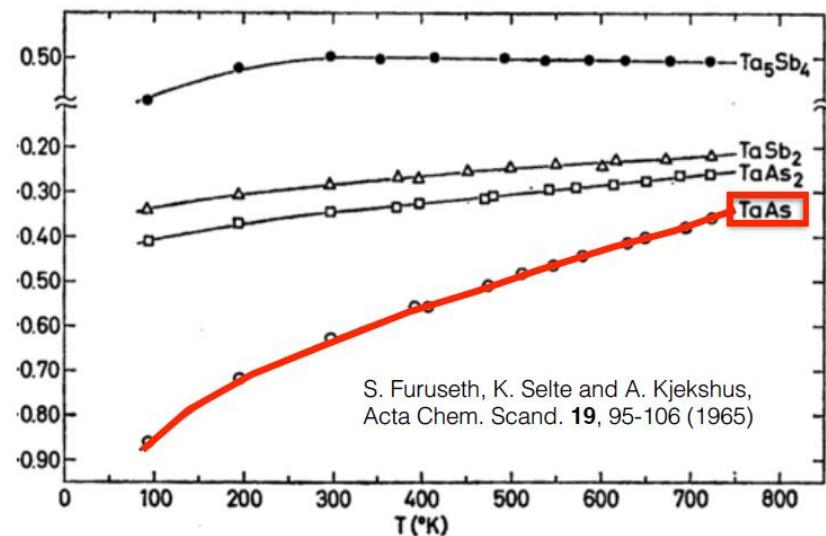
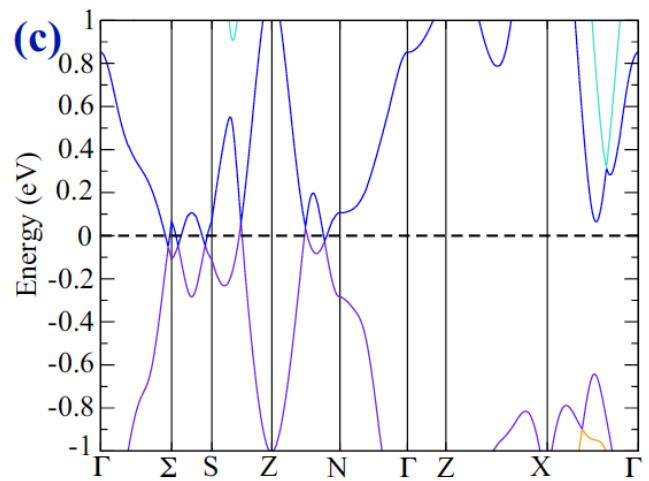


TABLE V. Magnetic susceptibilities of  $\text{NbP}$  and  $\text{TaP}$ .

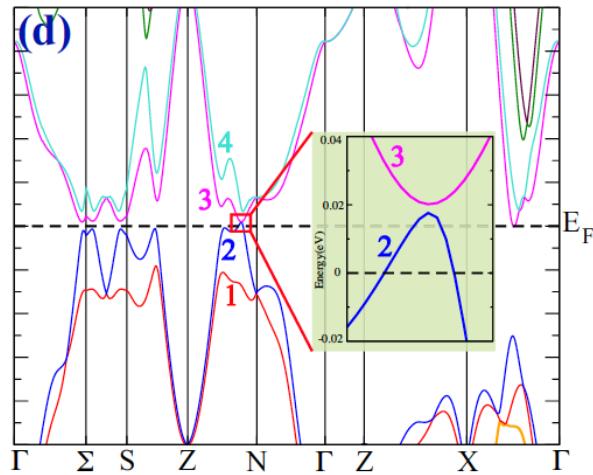
Compound	$T$ (°K)	$X_g (10^{-6} \text{ cgs/g})$
<b>NbP</b>	78	$-0.45 \pm 0.03$
	201	$-0.57 \pm 0.03$
	297	$-0.52 \pm 0.02$
	373	$-0.55 \pm 0.03$
<b>TaP</b>	78	$-0.70 \pm 0.03$
	201	$-0.65 \pm 0.03$
	297	$-0.62 \pm 0.02$
	373	$-0.59 \pm 0.02$

B. A. Scott, G. R. Eulenberger, and R. A. Bernheim, J. Chem. Phys. **48**, 263 (1968)

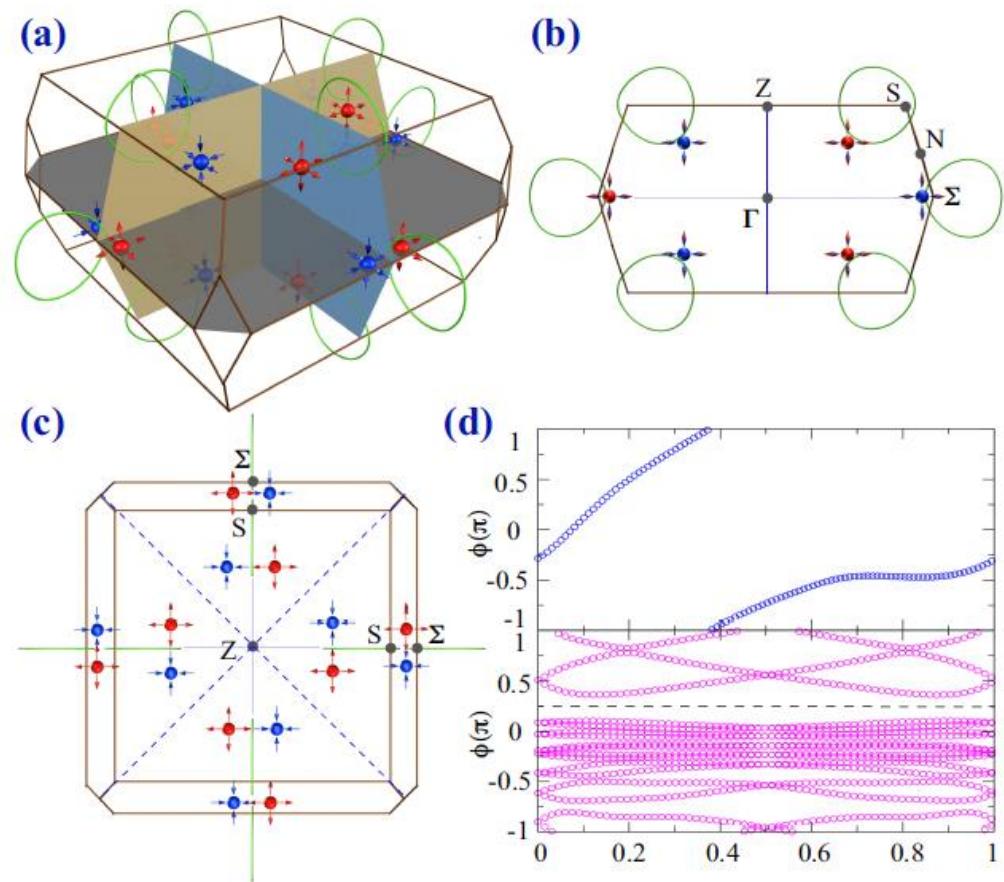
### 3. Prediction & Exp: T-invariant WSM: TaAs family



GGA



GGA+SOC

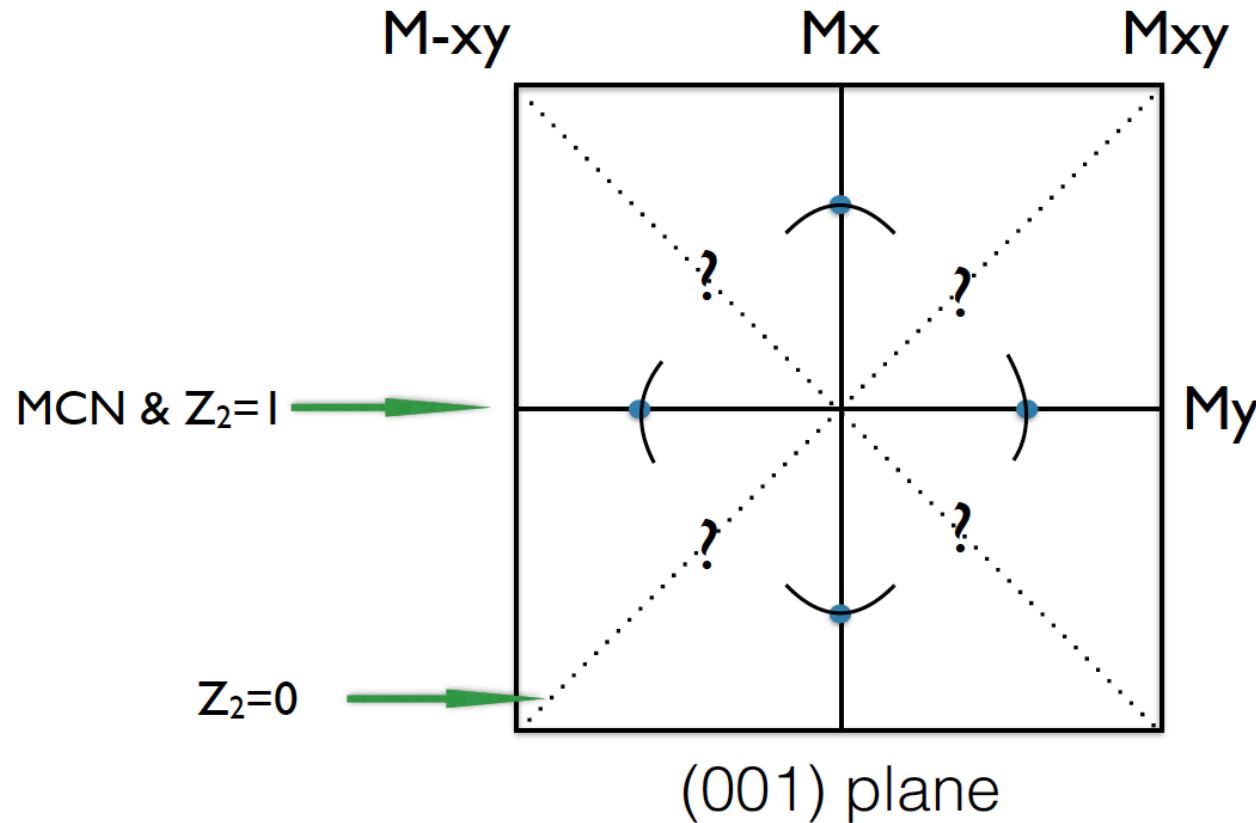


	Weyl Node 1	Weyl Node 2
TaAs	(0.949, 0.014, 0.0)	(0.520, 0.037, 0.592)
TaP	(0.955, 0.025, 0.0)	(0.499, 0.045, 0.578)
NbAs	(0.894, 0.007, 0.0)	(0.510, 0.011, 0.593)
NbP	(0.914, 0.006, 0.0)	(0.494, 0.010, 0.579)

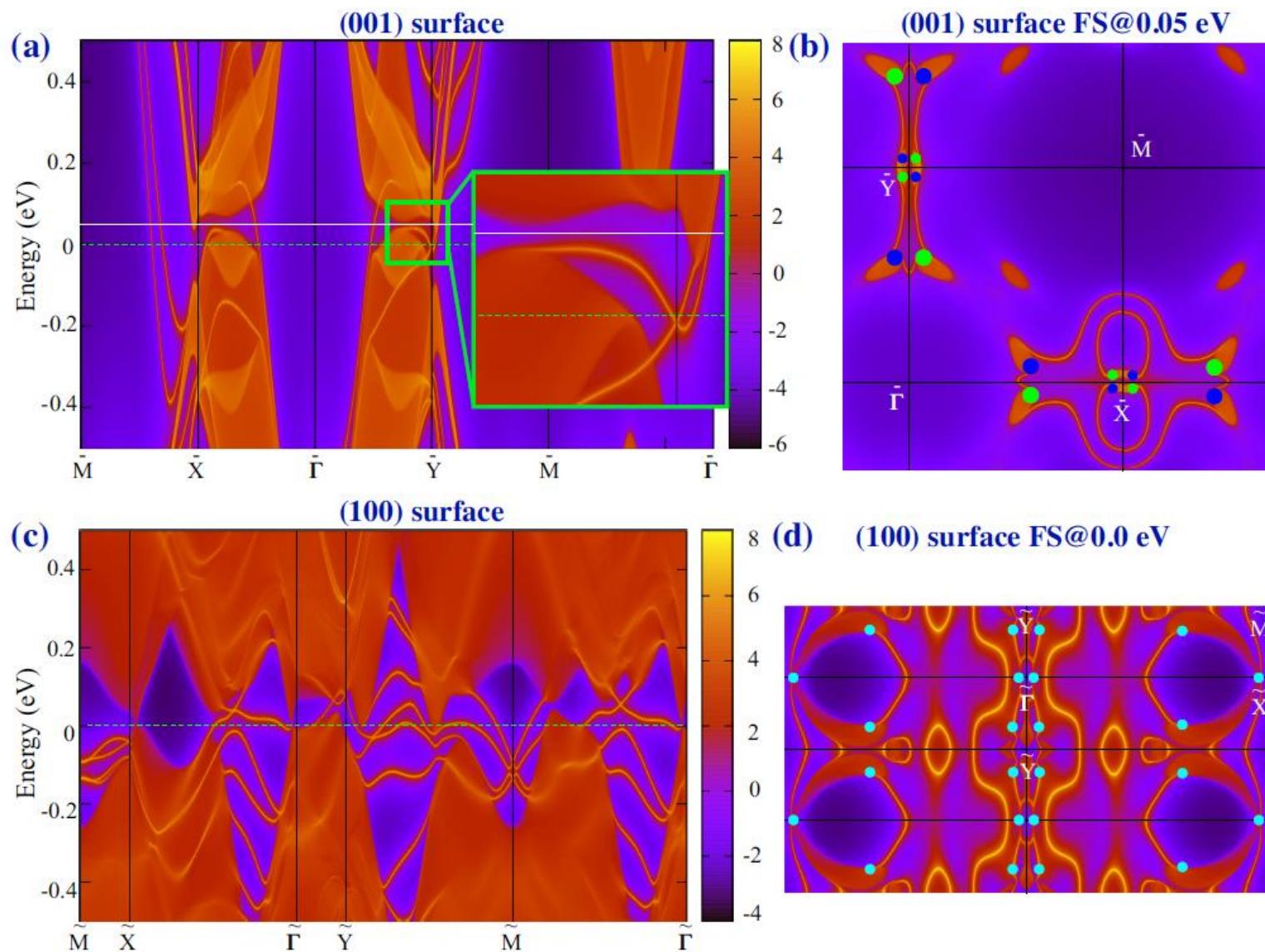
- ◆ 12 pairs of Weyl nodes.
- ◆ MCN=1 ( $M_x, M_y$ )
- ◆  $Z_2=0$  for  $M_{xy}$

### 3. Prediction & Exp: T-invariant WSM: TaAs family

Fermi circle or arcs?



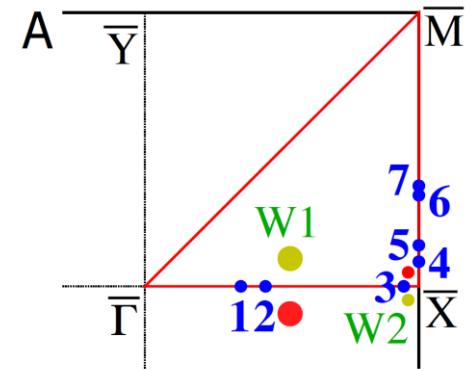
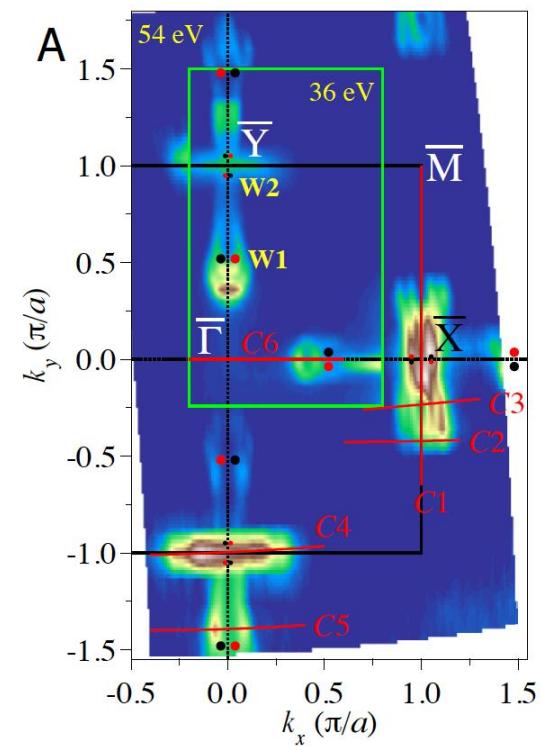
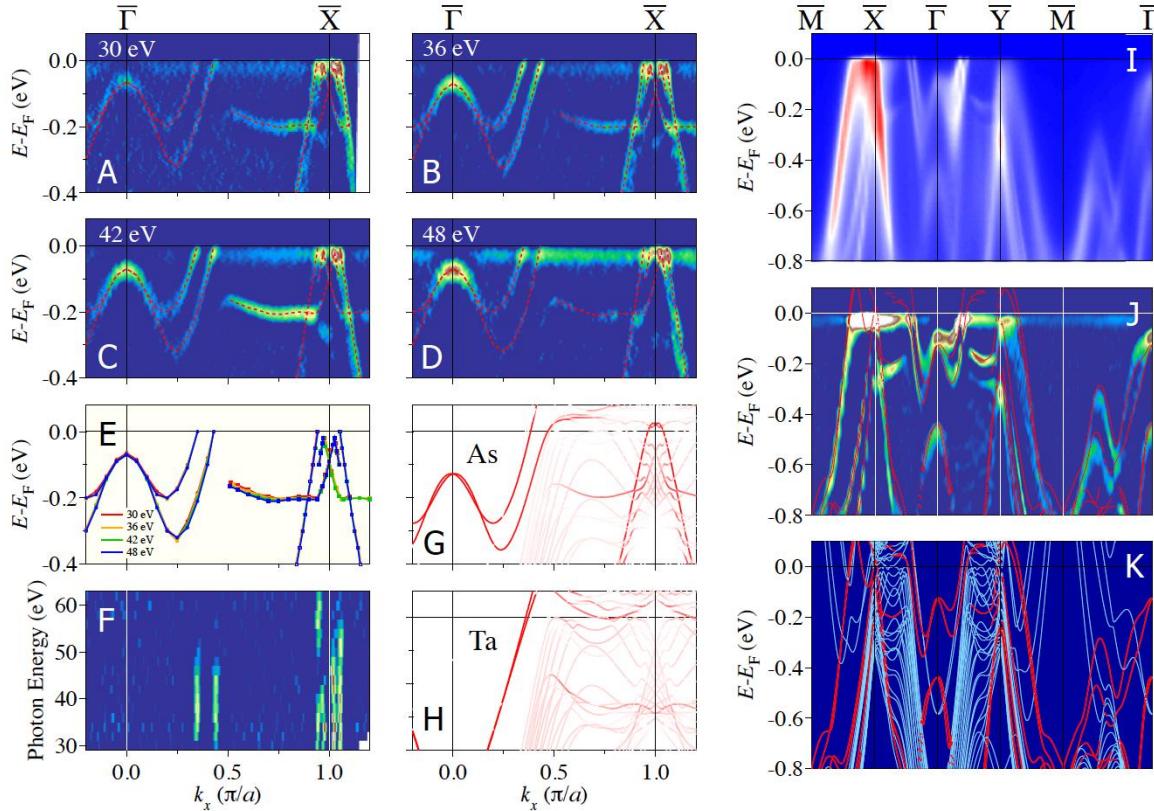
### 3. Prediction & Exp: T-invariant WSM: TaAs family



Calculated Surface States

### 3. Prediction & Exp: T-invariant WSM: TaAs family

**ARPES:** B. Q. Lu, et.al., arXiv:1502.04684 (2015).  
See also, 1502.03807 (2015).

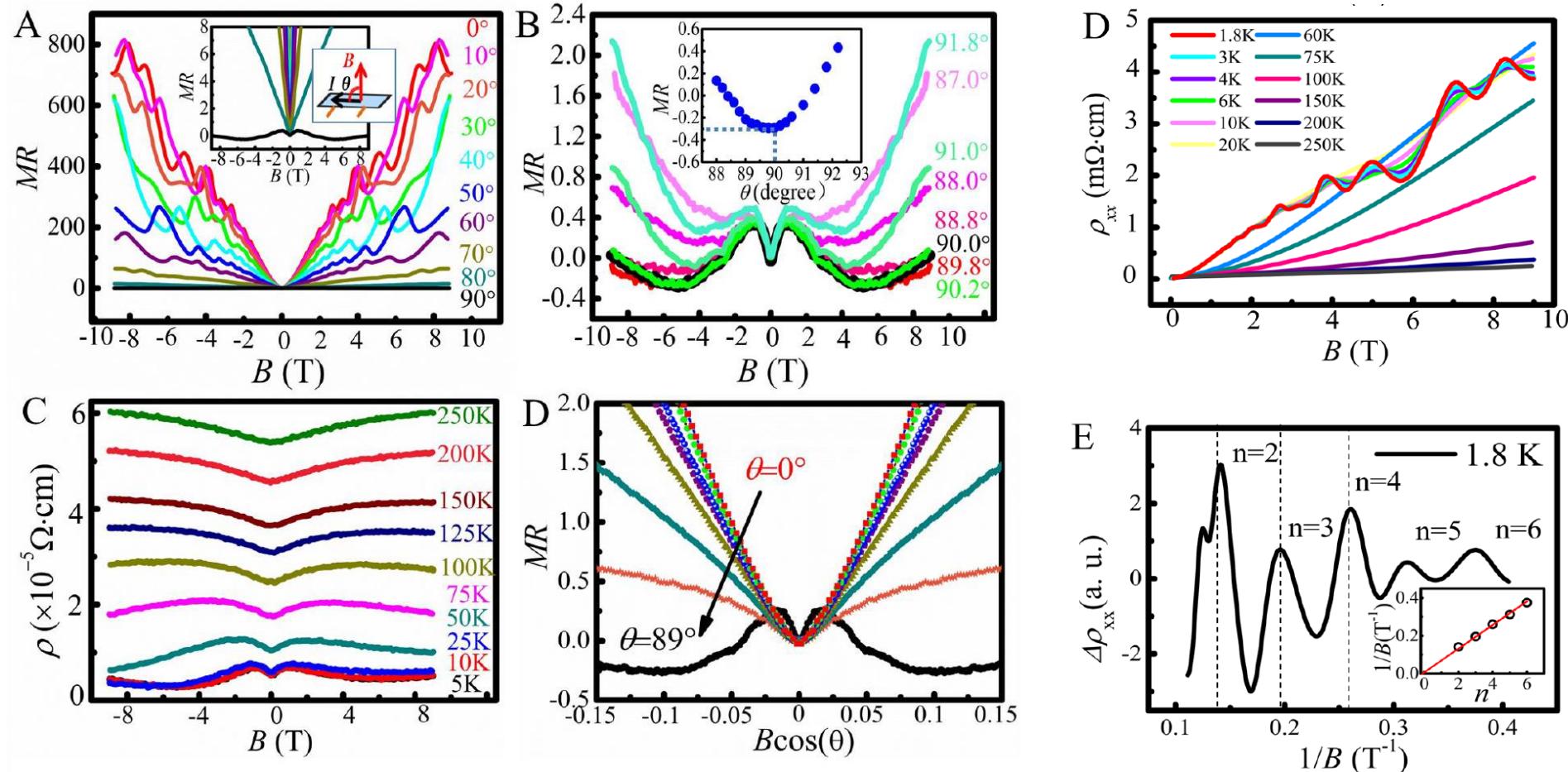


**Fermi Arcs: odd Number of Fermi cuts**

### 3. Prediction & Exp: T-invariant WSM: TaAs family

**Transport:** X. C. Huang, et.al., arXiv:1503.01304 (2015).

See also, 1502.00251 (2015).



Negative MR is observed for  $E \parallel B$ .

# Summary:

1. Definition of Topological Metals
2. Novel Properties of TSM.
3. Dirac SM:  $\text{Na}_3\text{Bi}$ ,  $\text{Cd}_3\text{As}_2$
4. Weyl SM:  $\text{HgCr}_2\text{Se}_4$ ,  $\text{TaAs}$ ,  $\text{NbAs}$ ,  $\text{TaP}$ ,  $\text{NbP}$

