Topological Electronic States

---- From Insulators to Semimetals

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Theory: H. M. Weng, X. Dai, Z. J. Wang (IoP),
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   (3) Dirac Semimetal: Na_3Bi & Cd_3As_2

   (4) Weyl semimetal: $HgCr_2Se_4$ & TaAs (TaP, NbAs, NbP)

1. Introduction: Topological Electronic States

Local Order Phase:
(Landau's Symm-Breaking Theory)

(1) Local Order Parameter
Such as: M(r) for magnetic states

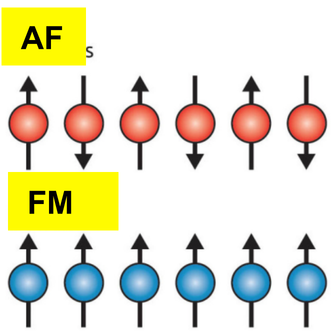
(2) Symm-Breaking for Phase-transition
M(r) breaks the spin rotation.

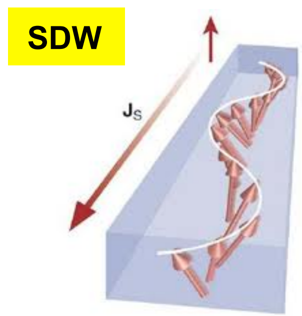
Global Order Phase:
(Topological phase)

(1) Topological Invariant

(2) No symm-change for phase transition

(3) Insensitive to perturbation





Edges = "2" "1"

g=0 g=1

Gauss–Bonnet Theorem:

$$\frac{1}{2\pi}\int_S K\,dA = 2(1-g)$$

$\rho = \langle \Psi | \Psi \rangle$ vs. $|\Psi\rangle = e^{i\phi(k)} |\psi\rangle$ Phase is important

Observable & Measurable in condensed matters!

1. Introduction: K-space as parameter space

Bloch State:

$$\begin{cases} H(\vec{r})\psi_{nk}(\vec{r}) = \varepsilon_{nk}\psi_{nk}(\vec{r}) \\ \psi_{nk}(\vec{r}) = e^{ik\cdot r}u_{nk}(\vec{r}) \end{cases} \Rightarrow \begin{cases} H_k(\vec{r})u_{nk}(\vec{r}) = \varepsilon_{nk}u_{nk}(\vec{r}) \\ H_k = e^{-ik\cdot r}He^{ik\cdot r} \end{cases}$$

Gauge Freedom:

$$\left|u'_{nk}\right\rangle = e^{i\phi(k)}\left|u_{nk}\right\rangle \Rightarrow H_k\left|u'_{nk}\right\rangle = \varepsilon_{nk}\left|u'_{nk}\right\rangle$$

Berry Connection:

$$\vec{A}_n(k) = i\left\langle u_{nk}\middle|\vec{\nabla}_k\middle|u_{nk}\right\rangle$$

Gauge dependent

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

Berry Curvature:

$$\vec{\Omega}_n(k) = \vec{\nabla}_k \times \vec{A}_n(k) = i\left\langle \vec{\nabla}_k u_{nk}\middle|\times\middle|\vec{\nabla}_k u_{nk}\right\rangle$$

Gauge invariant

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

Symmetry:

$\vec{\Omega}_n(k) = \vec{\Omega}_n(-k)$ for IS

$\vec{\Omega}_n(k) = -\vec{\Omega}_n(-k)$ for TRS

$\vec{\Omega}_n(k) \equiv 0$ for IS and TRS

1. Introduction: Magnetic Field in K-space

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

$A(\mathbf{k})$: Berry connection, $u_{n\mathbf{k}}$: 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 $\vec{\Omega}(\vec{k})$	Magnetic field $\vec{B}(\vec{r})$
Berry connection $\vec{A}(\vec{k}) = \langle \psi | i\frac{\partial}{\partial \vec{k}} | \psi \rangle$	Vector potential $\vec{A}(\vec{r})$
Geometric phase $\oint d\vec{k} \bullet \vec{A}(\vec{k}) = \iint d^2k \; \Omega_z(\vec{k})$	Aharonov-Bohm phase $\oint d\vec{r} \bullet \vec{A}(\vec{r}) = \iint d^2r \; B_z(\vec{r})$
Chern number $\oiint d^2k \;\; \Omega_z(\vec{k}) = \text{integer}$	Dirac monopole $\oiint d^2r \;\; B_z(\vec{r}) = \text{integer } h/e$

Equation of motion:

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

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

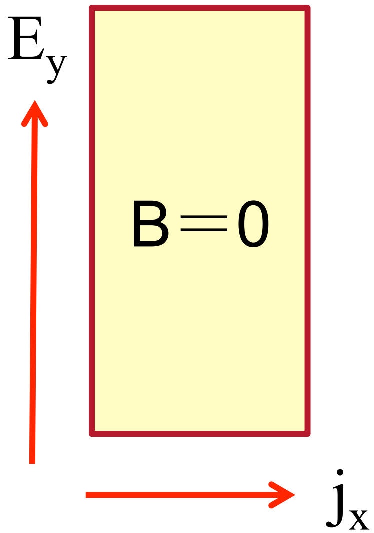
Anomalous velocity

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

⇓

Observable:
Anomalous Hall Effect

1. Introduction: Hall conductivity as observable!



$$j_x = -ev_x = -e\sum_n \int_{BZ} \frac{d^3\mathbf{k}}{(2\pi)^3} f_n(\mathbf{k})(-\dot{\mathbf{k}} \times \boldsymbol{\Omega}_n(\mathbf{k}))_x$$

$$= -\frac{e^2}{\hbar}\sum_n \int_{BZ} \frac{d^3\mathbf{k}}{(2\pi)^3} f_n(\mathbf{k})(\mathbf{E} \times \boldsymbol{\Omega}_n(\mathbf{k}))_x$$

$$= -\frac{e^2}{\hbar}\sum_n \int_{BZ} \frac{d^3\mathbf{k}}{(2\pi)^3} f_n(\mathbf{k}) E_y \Omega_{n,z}(\mathbf{k})$$

Hall conductivity: $$\sigma_{xy} = \frac{j_x}{E_y} = -\frac{e^2}{\hbar}\sum_n \int_{BZ} \frac{d^3\mathbf{k}}{(2\pi)^3} f_n(\mathbf{k}) \Omega_{n,z}(\mathbf{k})$$

For 2D insulators: f_n(k)=1 or 0

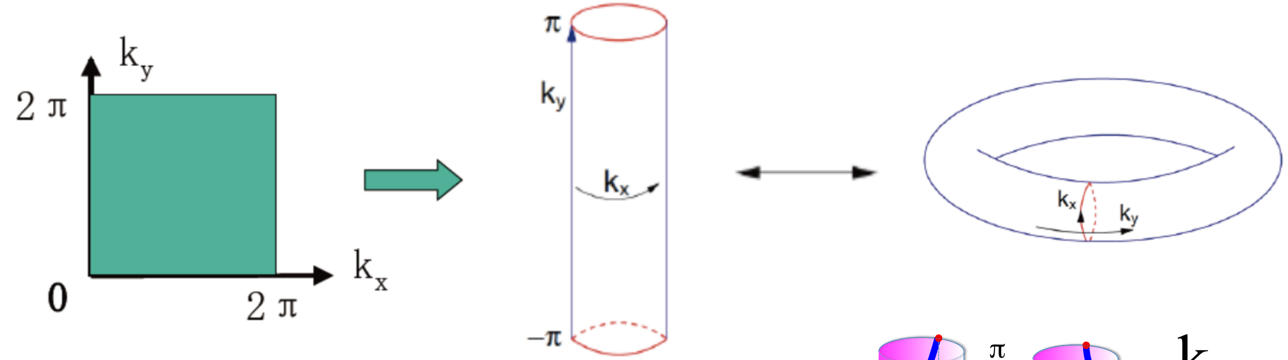
$$\sigma_{xy} = -\frac{e^2}{\hbar}\sum_n \int_{BZ} \frac{d^2\mathbf{k}}{(2\pi)^2} f_n(\mathbf{k}) \Omega_{n,z}(\mathbf{k})$$

$$= -\frac{e^2}{2\pi h}\int_{BZ} d^2\mathbf{k} \sum_{n(occ)} \Omega_{n,z}(\mathbf{k})$$

1. Introduction: Topological Insulators

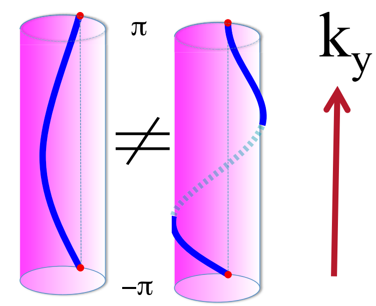
2D Chern Insulators:

2D Brillouin Zone:



Topological Invariant: Chern Number Z

$$\int_{\mathcal{S}} \mathbf{\Omega}(\mathbf{k}) \cdot d\mathcal{S} = 2\pi Z \qquad Z\text{=interger}$$

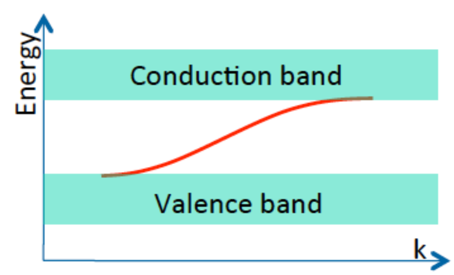


Winding Numer of Wannier Center

QAHE:

$$\int_{BZ} d^2\mathbf{k}\Omega_z(\mathbf{k}) = \int_{\mathcal{S}} \mathbf{\Omega}(\mathbf{k}) \cdot d\mathcal{S}$$

$$\sigma_{xy} = \frac{e^2}{2\pi h} \times 2\pi Z = Z\frac{e^2}{h}$$

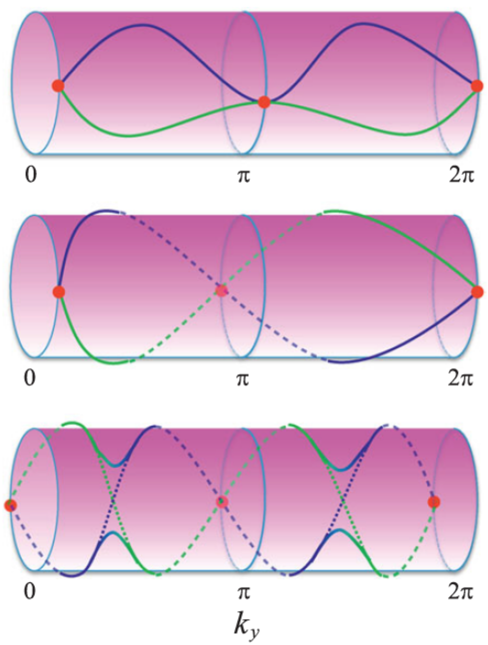


Ref: TKNN, PRL (1982); Haldane, PRL (1988); etc.

Realized recently!

1. Introduction: Topological Insulators

2D Z_2 Insulators with TRS: SPT



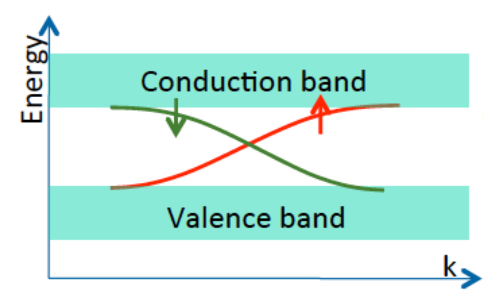
ψ_{nk}

ψ^{I} $\longleftrightarrow$ ψ^{II}

TRS

Z **-Z**

Invariant: Z_2=Z mod 2



QSHE: Spin-Hall

$$\sigma_{xy}^{s} = \frac{\hbar}{2e} \times 2 \frac{e^2}{h} = \frac{e}{2\pi}$$

Ref: (1) Hasan & Kane, RMP (2010).
(2) Qi & Zhang, RMP (2011).

1. Introduction: Topological Insulators

Z_2 Insulator can be extended to 3D

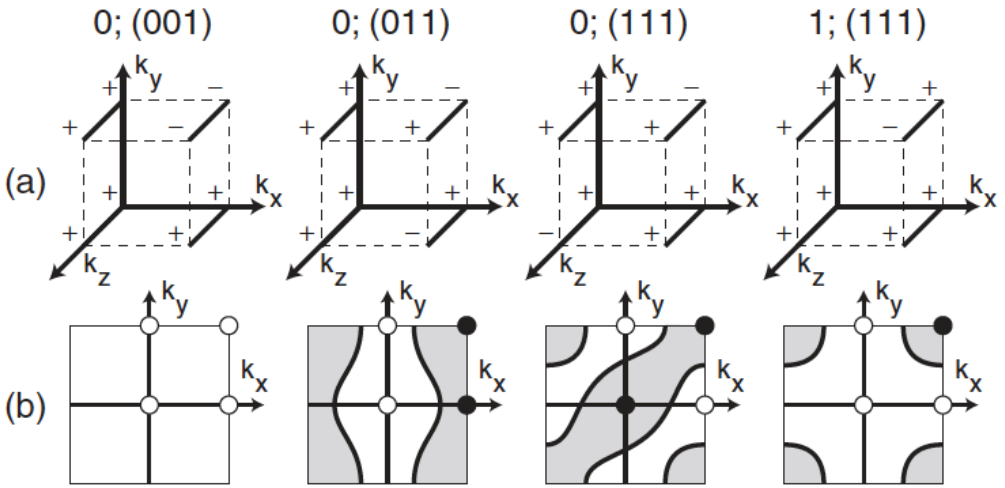
Topological Indices:

$$\nu_0; (\nu_1 \nu_2 \nu_3)$$

$$\delta_i = \sqrt{\det[w(\Gamma_i)]}/\mathrm{Pf}[w(\Gamma_i)] = \pm 1$$

$$(-1)^{\nu_0} = \prod_{n_j=0,1} \delta_{n_1 n_2 n_3},$$

$$(-1)^{\nu_{i=1,2,3}} = \prod_{n_{j\neq i}=0,1; n_i=1} \delta_{n_1 n_2 n_3}$$

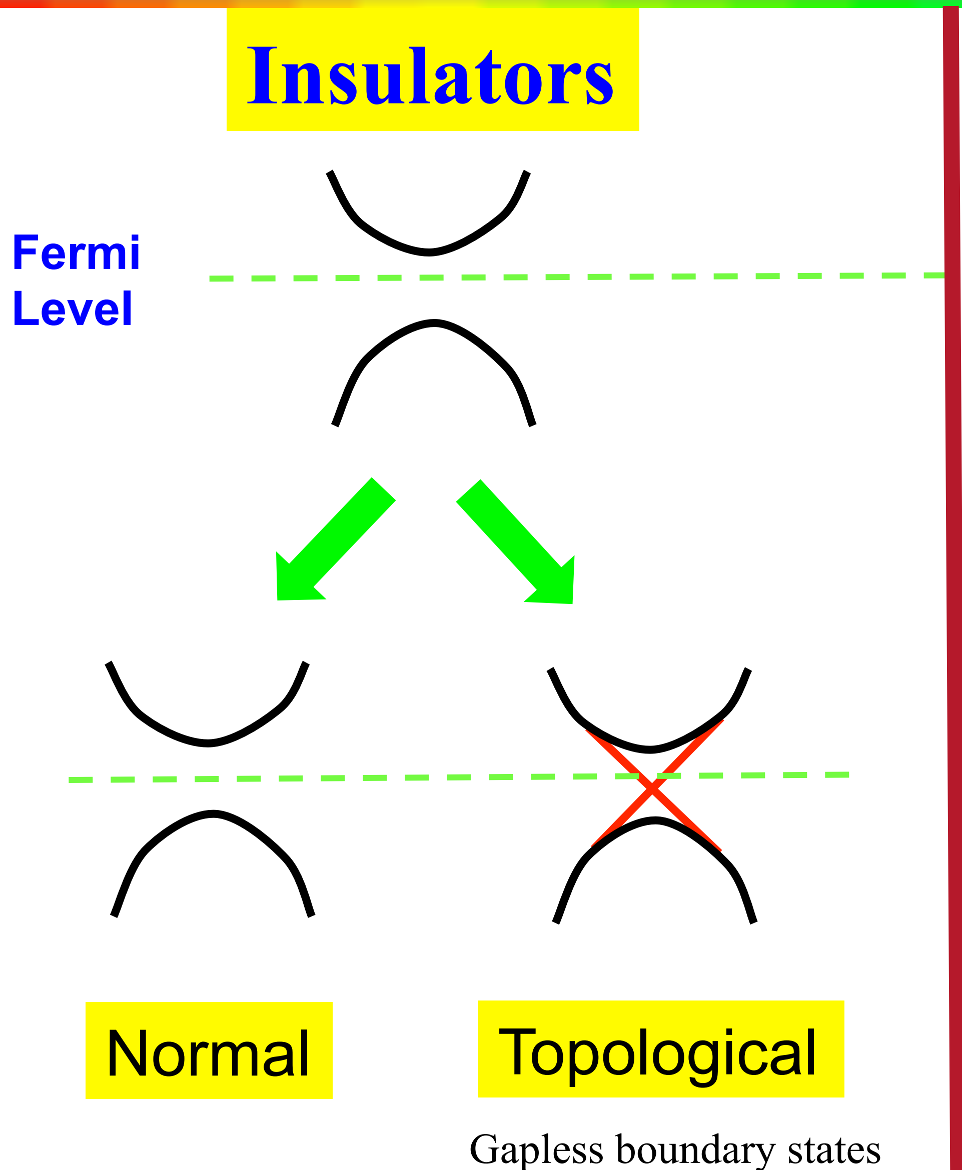


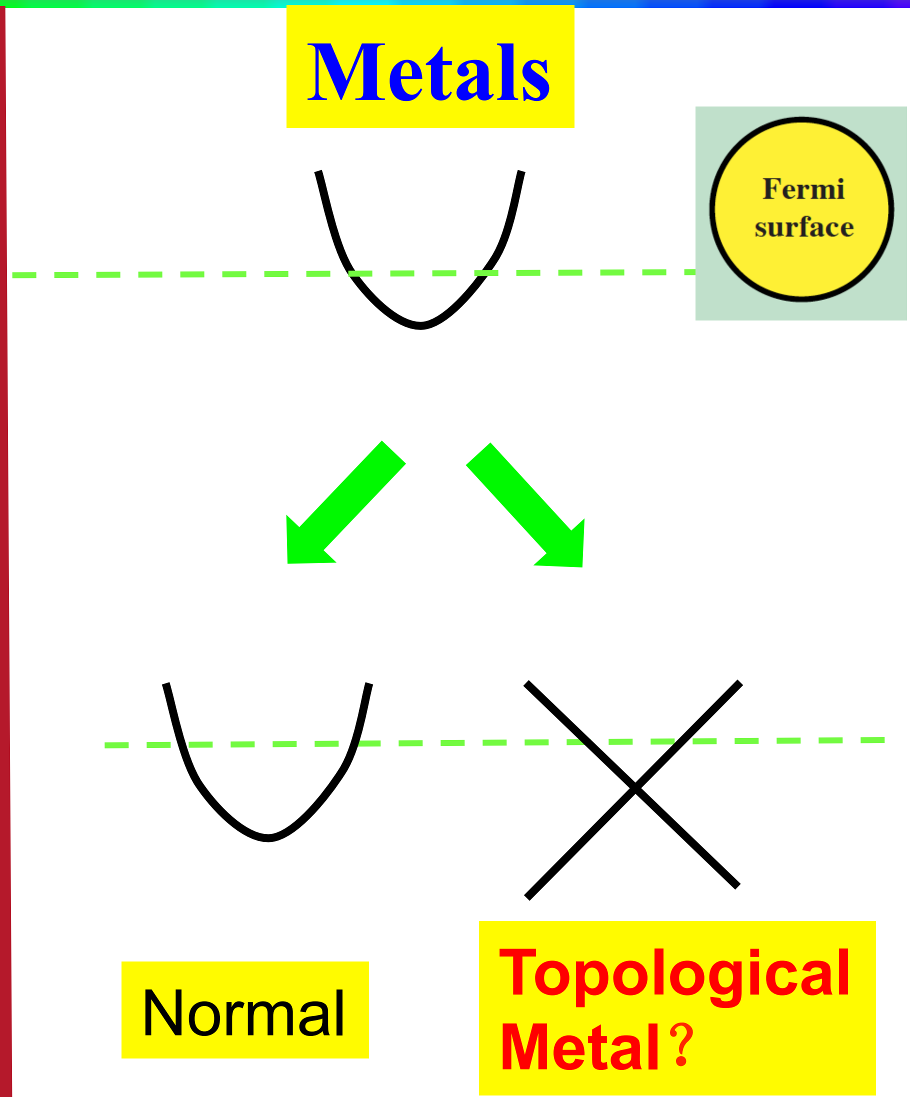
Ref: Fu, Kane & Mele, PRL (2007)

Dirac-cone type Surface states:

Further extension to TCI.
See, Fu, PRL (2011)

2. Topological Metals?



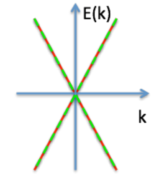


Can metals be classified?
How to define TM?

2. Topological Metals: Massless Dirac & Weyl Fermion

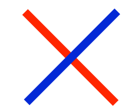
Massless Dirac (4x4):
(Reducible !!)

$$H = \begin{bmatrix} -c\hat{\sigma}\cdot\hat{p} & 0 \\ 0 & c\hat{\sigma}\cdot\hat{p} \end{bmatrix}$$



Weyl representation (2x2):
(Irreducible !!)
Left-hand + right-hand

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



Weyl nodes:

(1) Topological Objects

(2) Gapless, no mass term

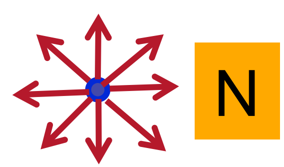
(3) Chirality ± (left or right-hand)

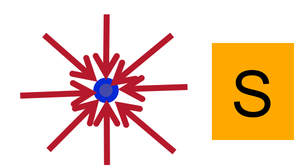
(4) Protected by translation

(k must be well defined)

Magnetic Monopoles:

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



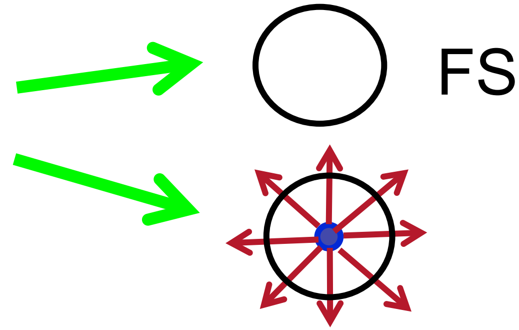


$$\frac{1}{2\pi}\oint_S \vec{\Omega}(k)\cdot dS(k) = Q$$ magnetic Charge

Fang, Science (2003).

2. Topological Metals: Topological Invariant

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



$C_{FS}=0$, normal metal

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

if E_f at node (k=0) ➔ 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

2. Topological Metals: Special Case: 3D Dirac metal

If both T and I symmetry are present:

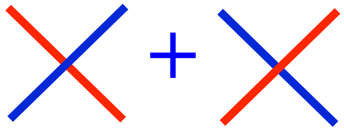
+Q & -Q Weyl nodes have to overlap in K-space

$$H(k)=\begin{bmatrix} k\cdot\sigma & M^* \\ M & -k\cdot\sigma \end{bmatrix}$$

Case I: M≠0, Insulator

$$H(k)=\begin{bmatrix} k\cdot\sigma & 0 \\ 0 & -k\cdot\sigma \end{bmatrix}$$

Case II: M=0, 3D Dirac Semimetal



Need crystal symmetry protection.

3D Dirac semimetal:

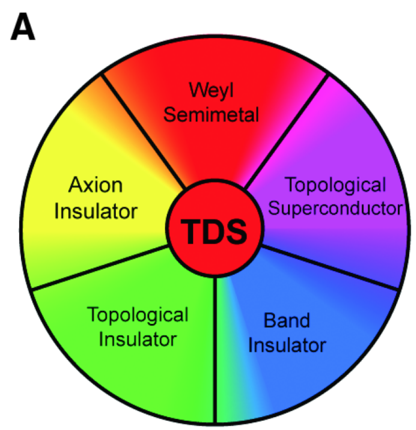
(1) Pseudo fermi arcs on surface

(2) Giant diamagnetism: $\chi(\varepsilon)\approx\log(1/\varepsilon)$

(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).



Critical Point

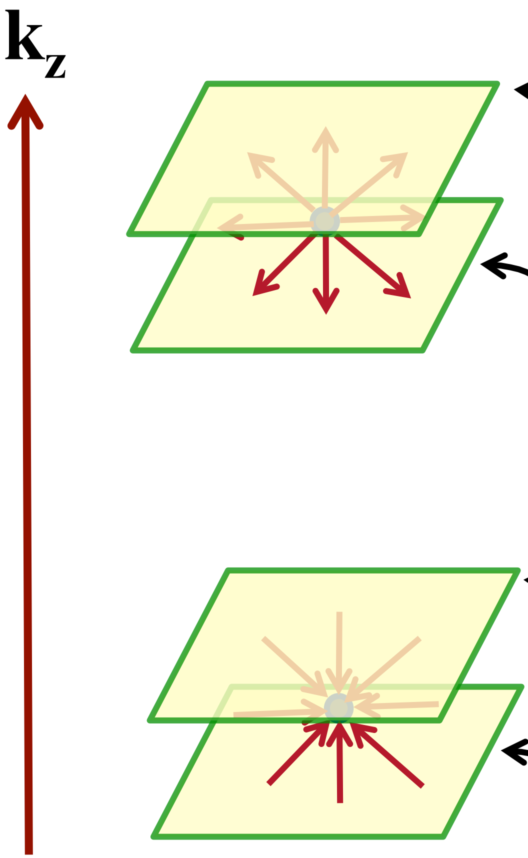
2. Topological Metals: Novel Properties

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), $HgCr_2Se_4$]

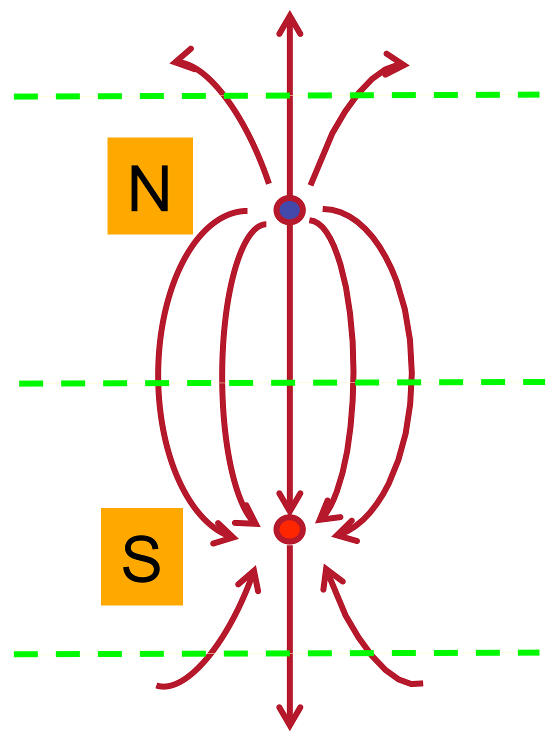


$$\sigma_{xy} = \frac{1}{2} \times \frac{e^2}{h}$$

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

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

$$\sigma_{xy} = \frac{1}{2}$$



$$\sigma_{xy} = 0$$

$$\sigma_{xy} = -1$$

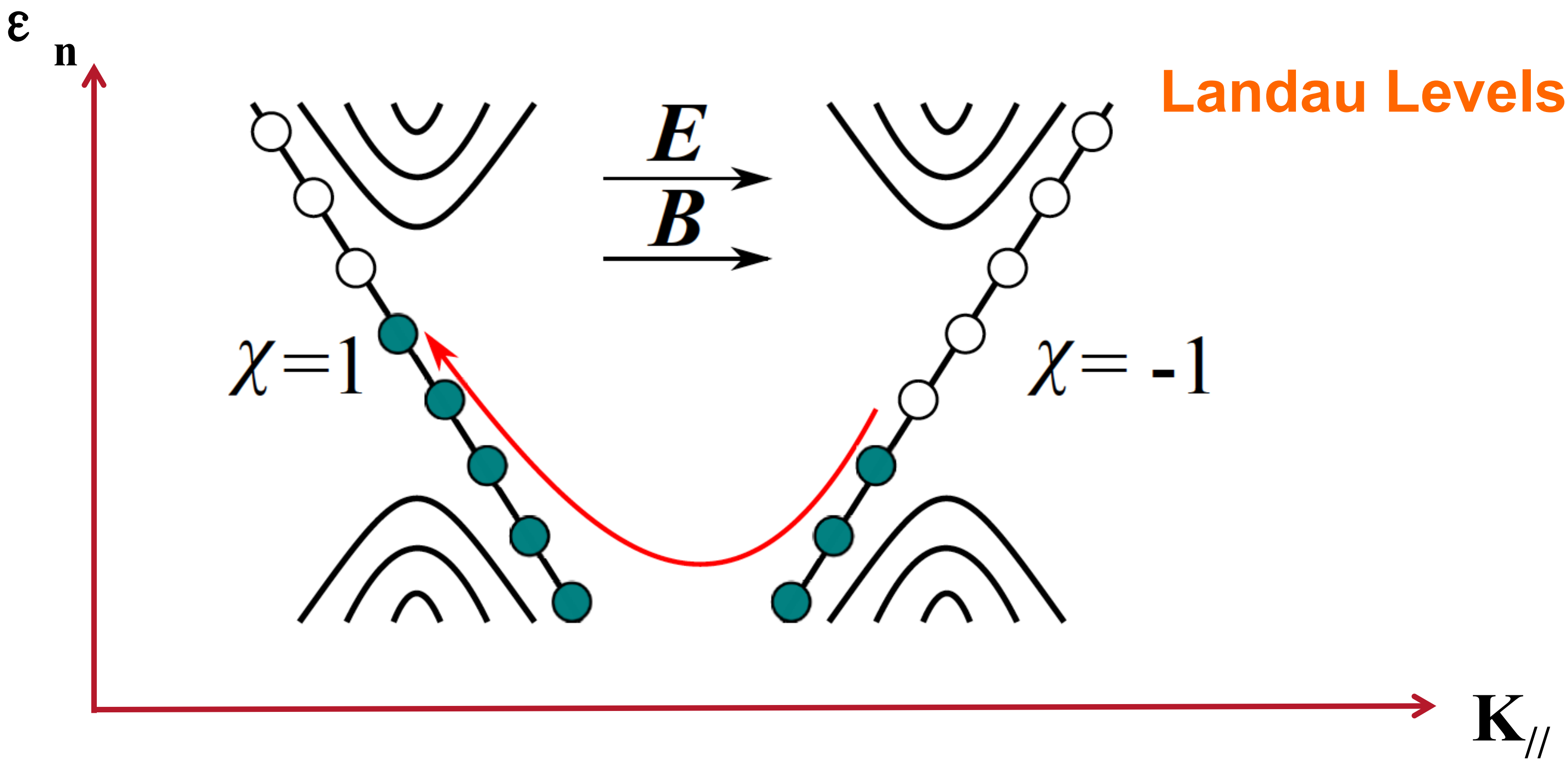
$$\sigma_{xy} = 0$$

2. Topological Metals: Novel Properties

Chiral Anomaly

=> Negative MR for E//B, [Nielsen & Ninomiya, Phys. Lett. (1983)]

Non-local Transport [S. A. Parameswaran, et.al. PRX (2013)]



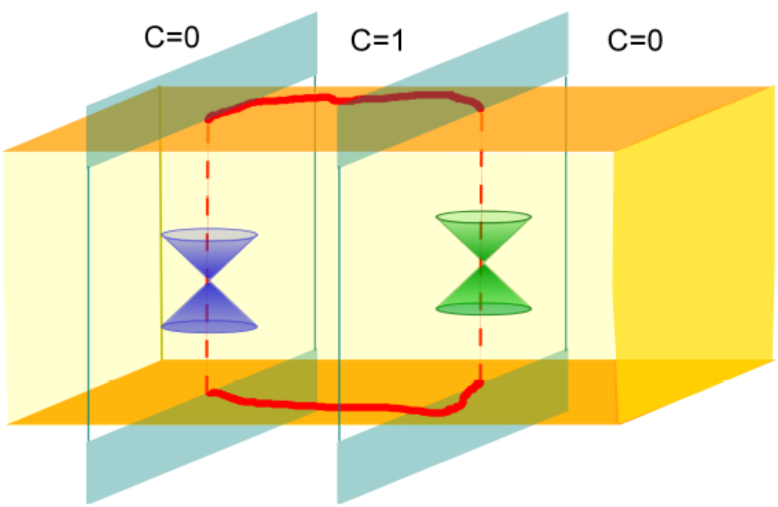
Intra-node: No back-scattering

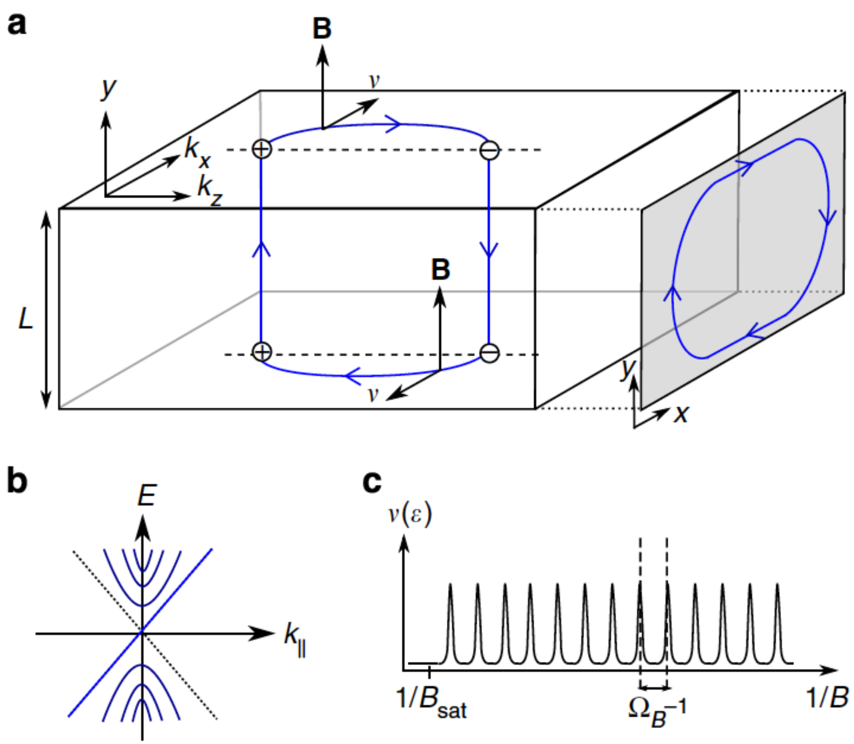
2. Topological Metals: Novel Properties

Fermi arcs on surfaces

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

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



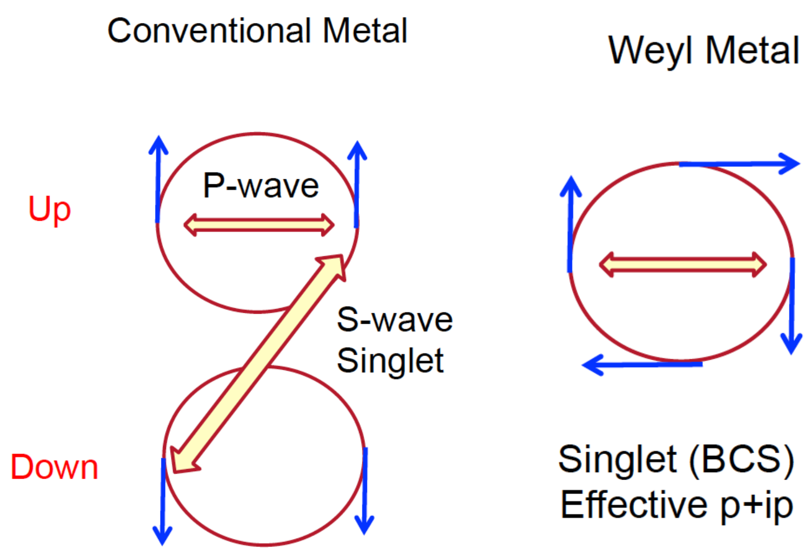


Thickness L dependent

2. Topological Metals: Novel Properties

Spin-Momentum Lock in 3D.
Doping => Topological Superconductor (TSC)

Schematic



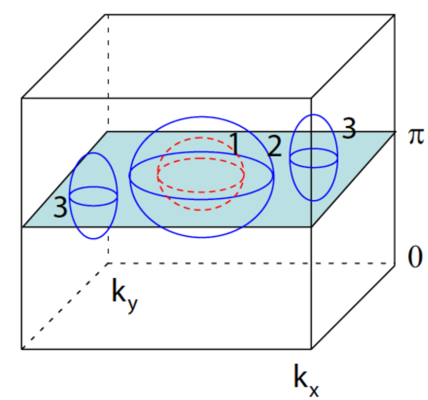
Weak interaction limit:

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:

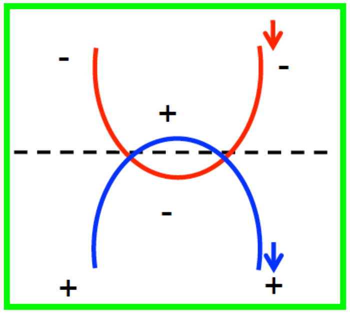
$$\nu = \frac{1}{2}\sum_{FS} C_{FS}\,\mathrm{sgn}(\Delta_{FS})$$

Criteria:

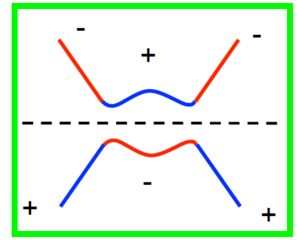
(1) $C_{FS} \neq 0$
(2) Δ_{FS} have opposite signs.

3. Prediction & Exp.: Band Inversion Mechanism

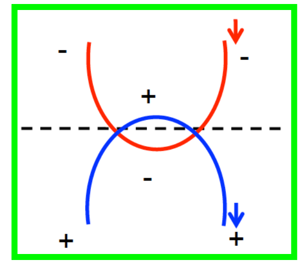
Without TRS:



SOC

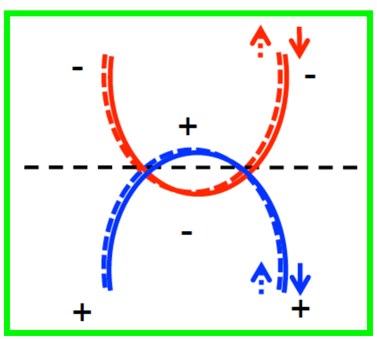


Gapped in 2D
Chern Insulator

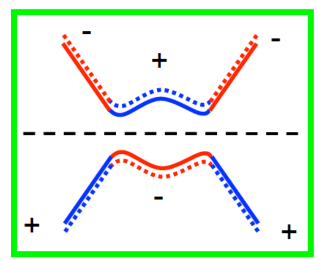


Gapless in 3D
Weyl semimetal

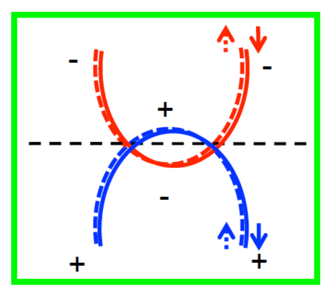
With TRS:



SOC



Gapped in both 2D & 3D
Z2 TIs



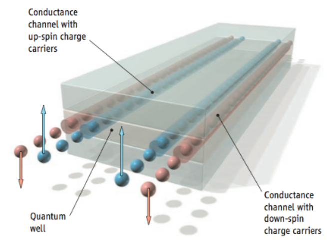
Gapless if
+ Crystal symmetry
3D Dirac semimetal

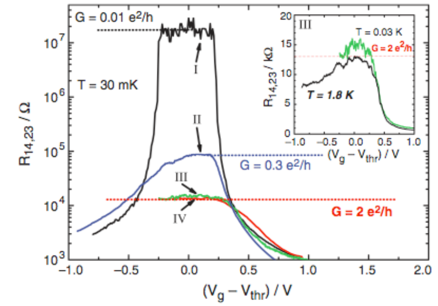
3. Prediction & Exp.: Calculations Play predictive roles.

2D TI (QSH Insulator): HgTe Quantum Well

Theory: Bernevig, Science (2006),

Exp: Konig, Science (2007).



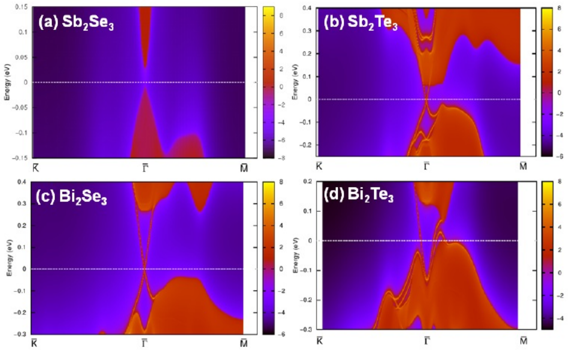


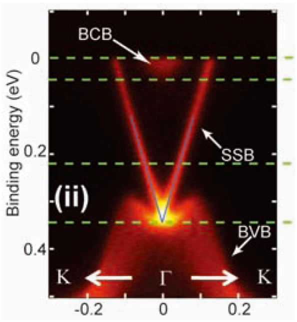
3D TI: Bi_2Se_3, Bi_2Te_3, Sb_2Te_3

Theory: H. J. Zhang, Nat. Phys. (2009),

Exp: Y. Xia, Nat. Phys. (2009)

Y. L. Chen, Science (2009).

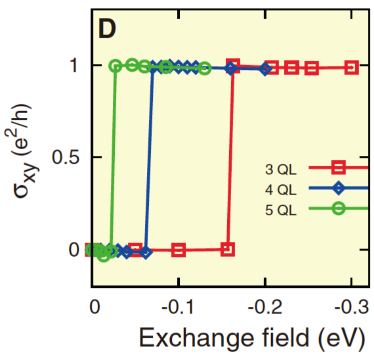


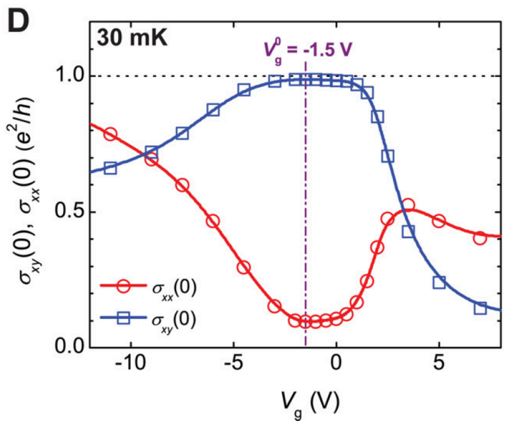


QAHE Insulator: Cr-doped Bi_2Te_3

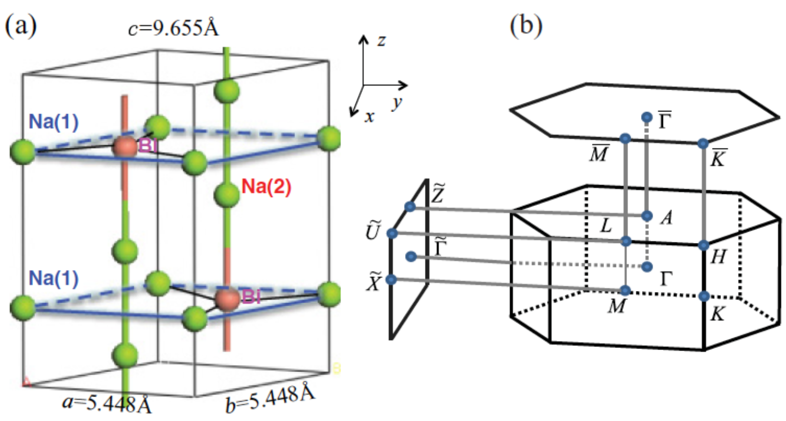
Theory: R. Yu, Science. (2010),

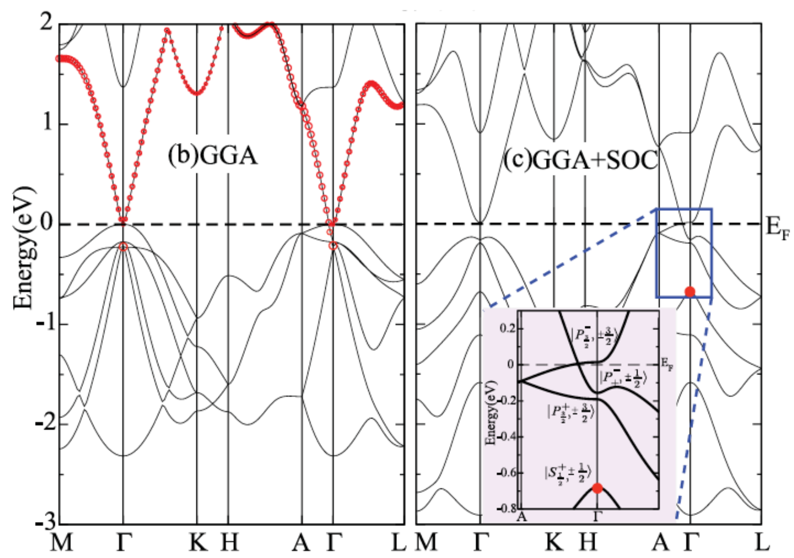
Exp: C. Z. Chang, Science (2013).

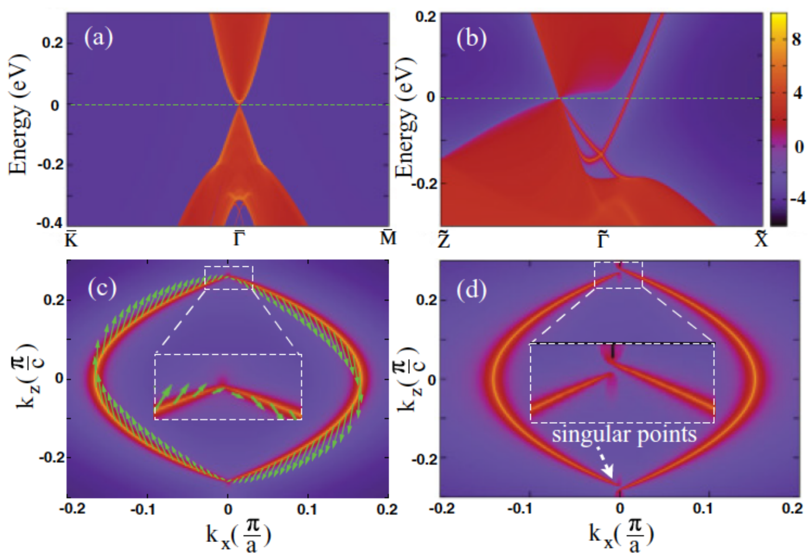




3. Prediction & Exp.: Dirac Semimetal: Na_3Bi (K or Rb).







Surface States

(1) S state is lower than P at Γ

(2) Band-crossing along Γ-Z

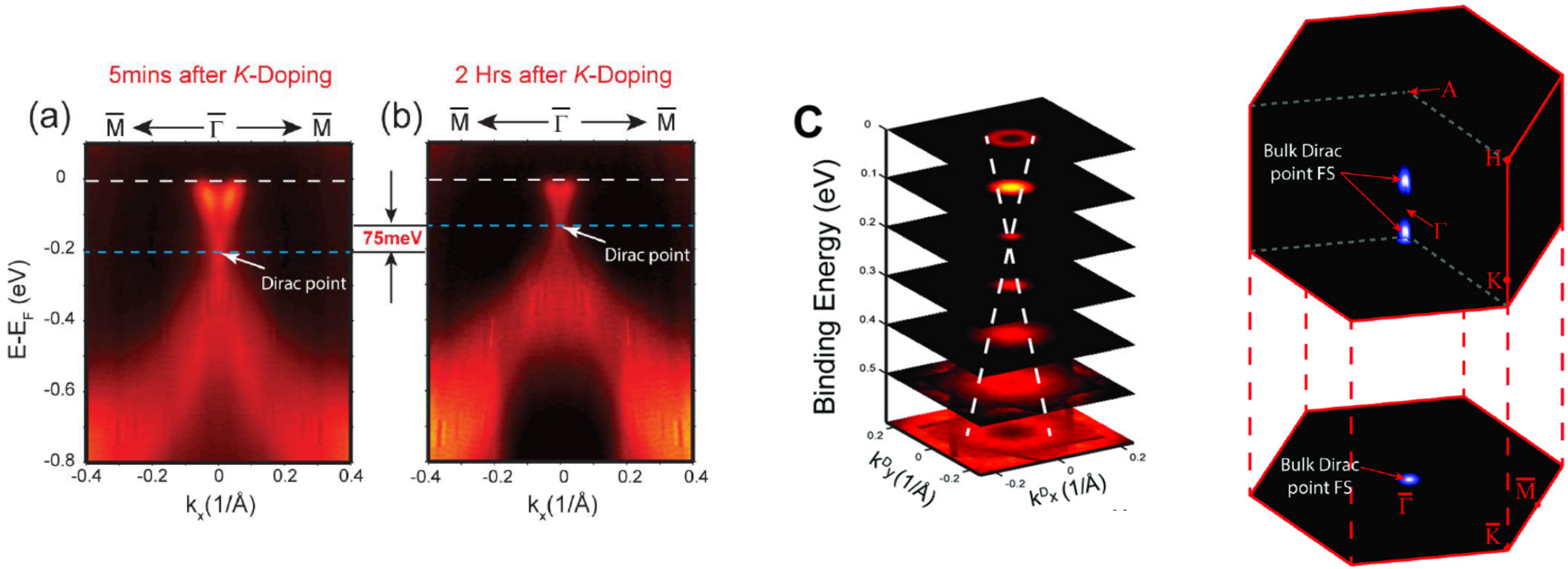
(3) Protected by C_3

(4) 3D Dirac Cone at $(0,0,\pm k_z^c)$

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

3. Prediction & Exp.: Dirac Semimetal: Na_3Bi.

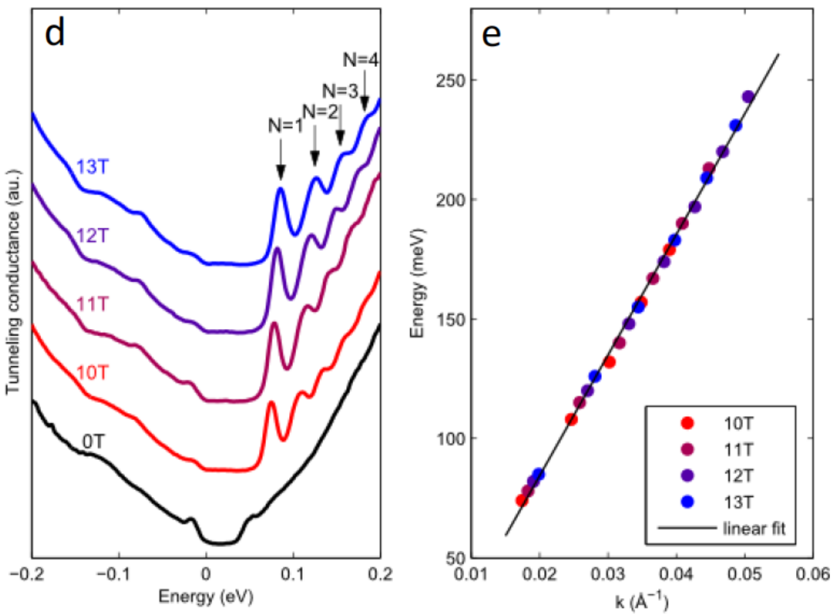
ARPES: Z. K. Liu, et.al. Science 343, 864 (2014).



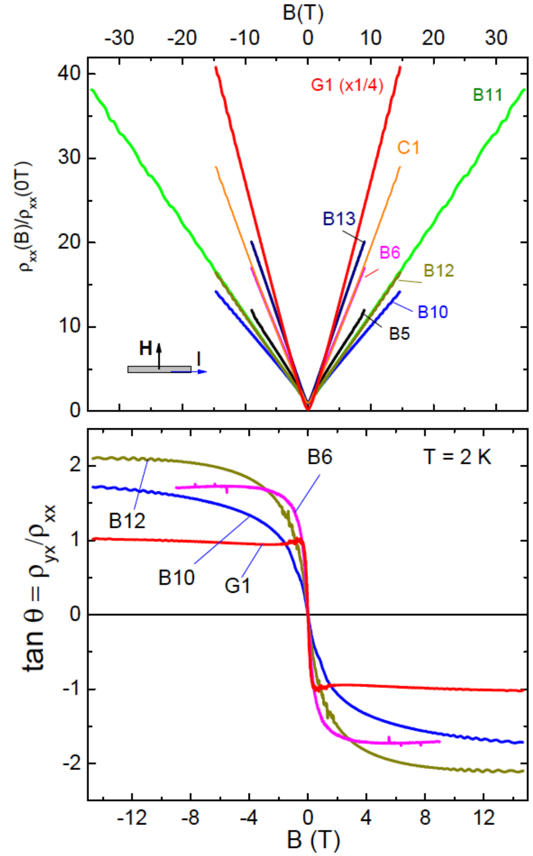
Other ARPES: S. Y. Xu, et.al. Science 10.1126 (2014).

3. Prediction & Exp.: Dirac Semimetal: Na_3Bi.

Transport:



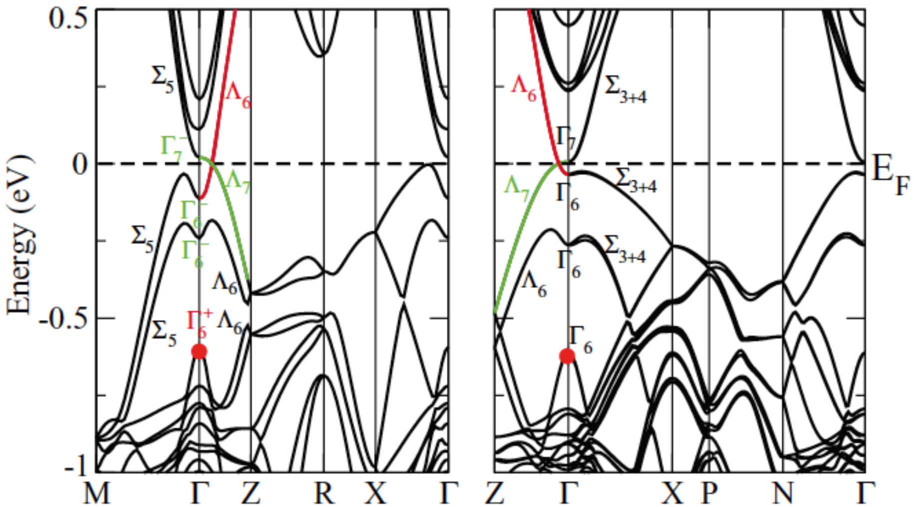
Quantum Oscillation
Arxiv: 1502.03547 (2015)

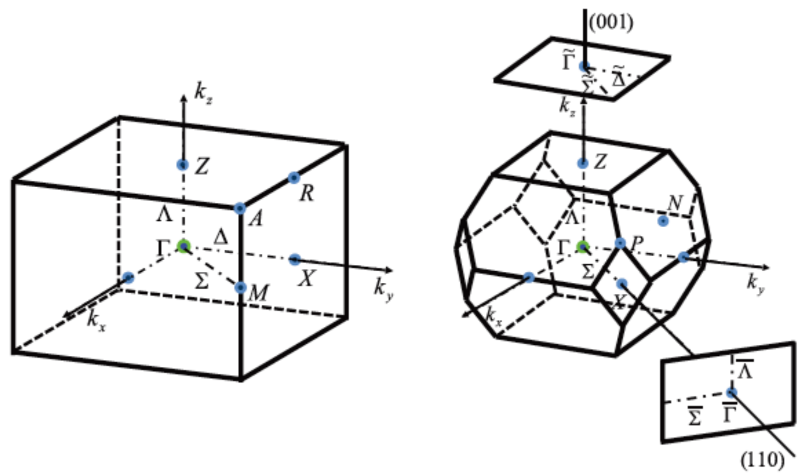


Linear MR & Large Hall angle
Arxiv: 1502.06266 (2015)

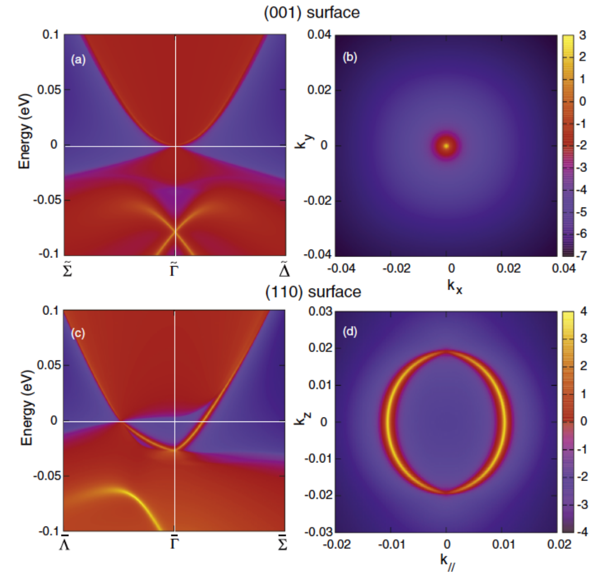
Negative MR is observed recently:
N. P. Ong, APS March Meeting (2015)

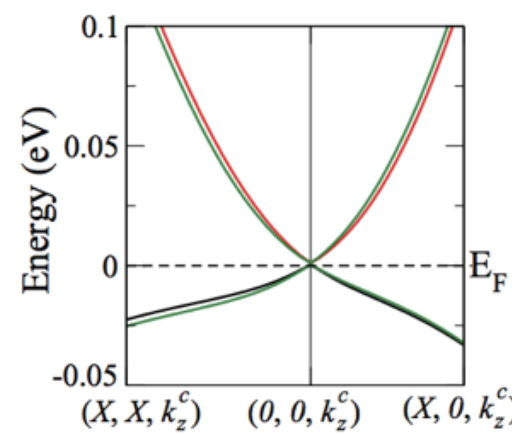
3. Prediction & Exp.: Dirac Semimetal: Cd_3As_2.





(a) structure I (b) structure II





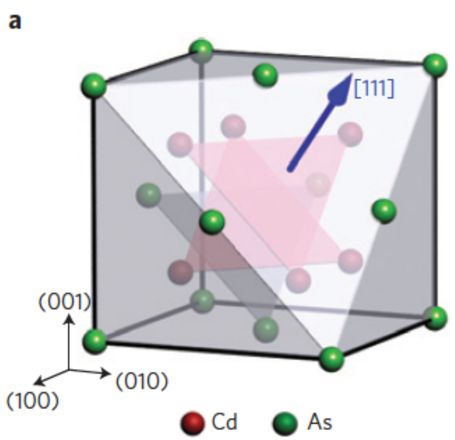
Z. J. Wang, et.al, PRB 88, 125427 (2013).
Stable compound with high mobility.

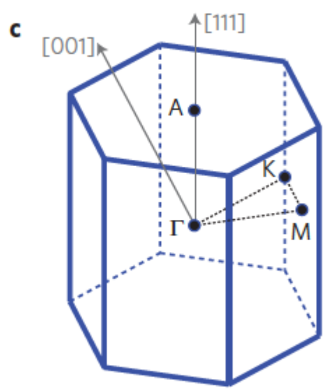
(1) Protected by C4

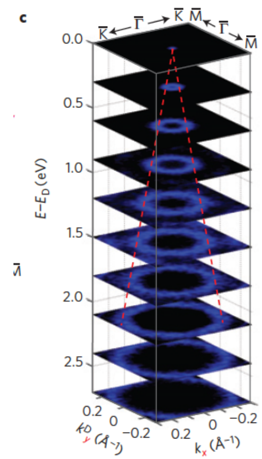
(2) Band-Splitting

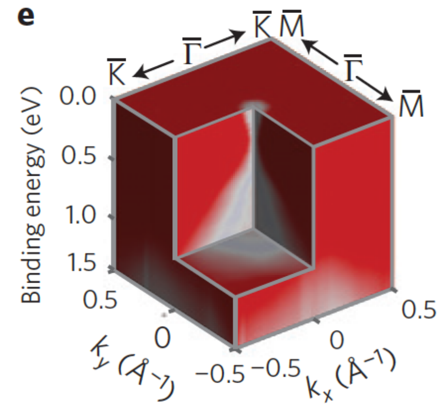
3. Prediction & Exp.: Dirac Semimetal: Cd_3As_2.

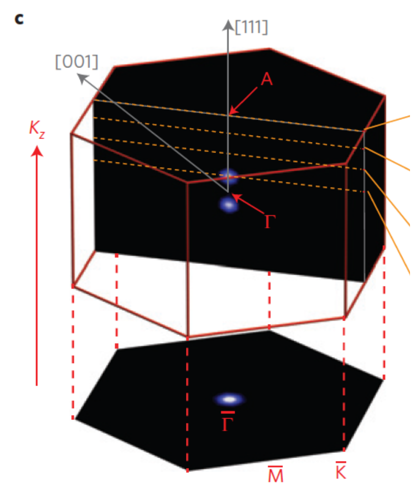
ARPES: Z. K. Liu, et.al. Nature Materials, 13, 677 (2014).









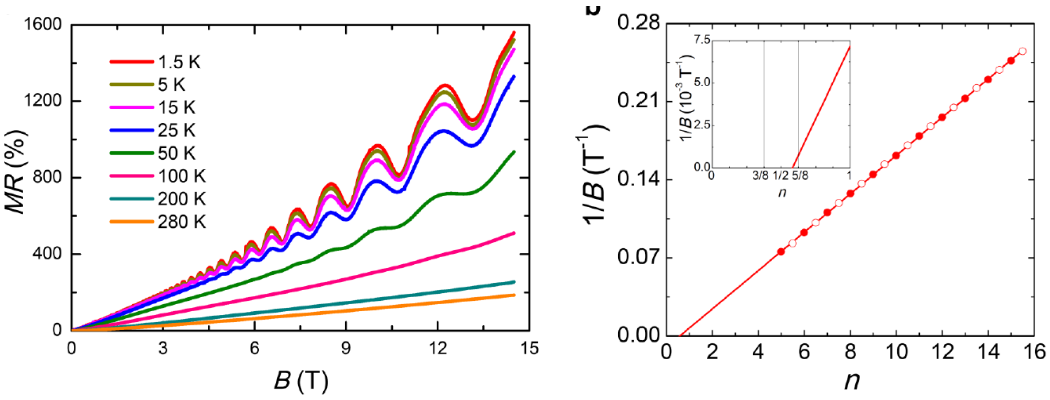


Other ARPES:

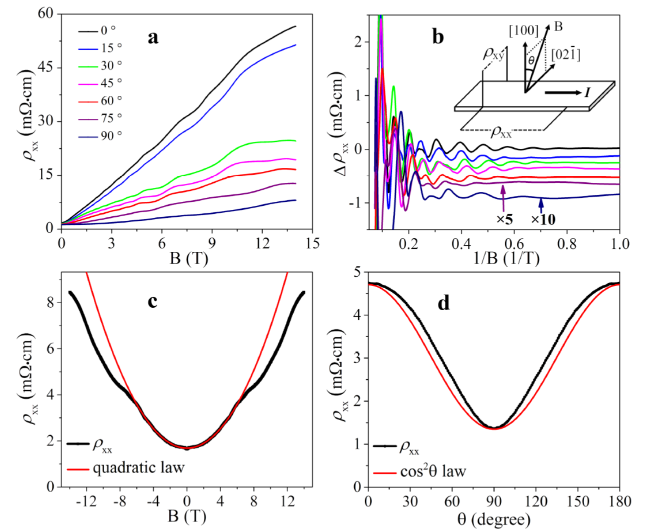
M. Neupane, et.al. Nature Comm. 5, 3786 (2014).
S. Borisenko, et.al, PRL 113, 027603 (2014).
H. Yi, et.al., Scientific Reports, 4, 6106 (2014).

3. Prediction & Exp.: Dirac Semimetal: Cd_3As_2.

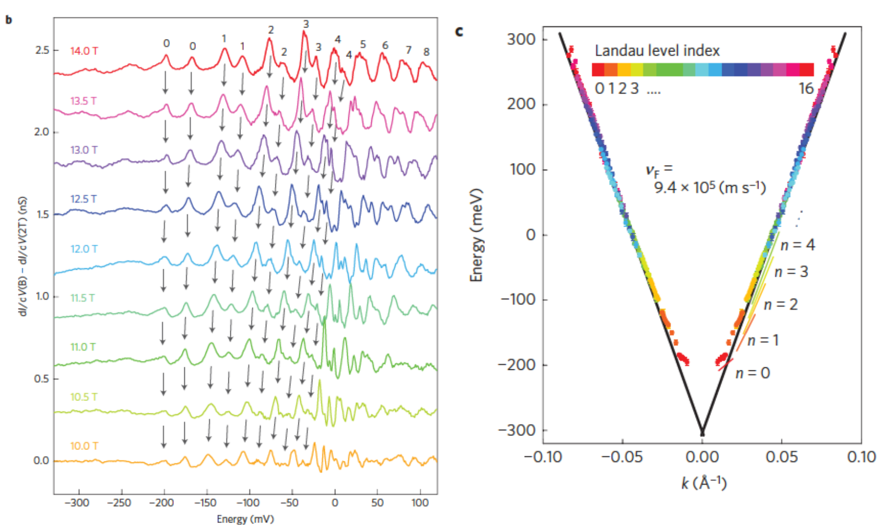
Transport: Linear MR & Qscillations



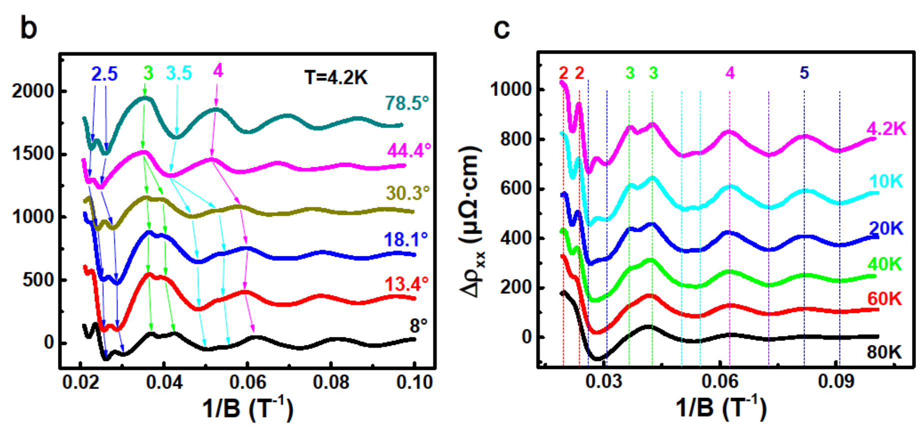
L. P. He, et.al. PRL 113, 246402 (2014)



J. Y. Feng, et.al. arXiv: 1405.6611



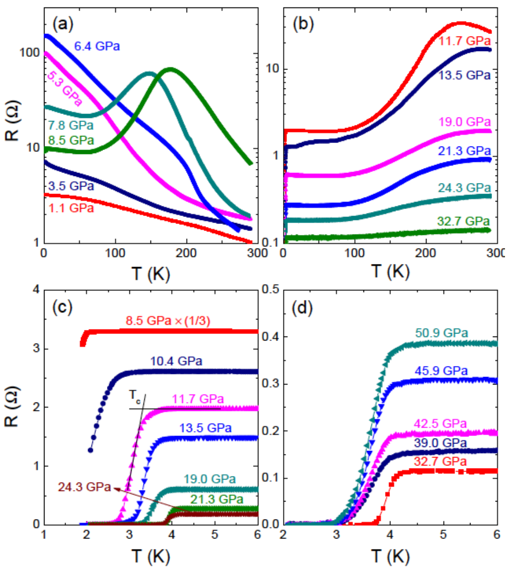
S. Jeon, et.al., Nature Matterials, 13, 851 (2014).

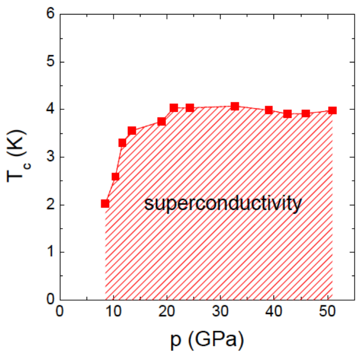


J. Z. Cao, et.al., arXiv: 1412.0824.

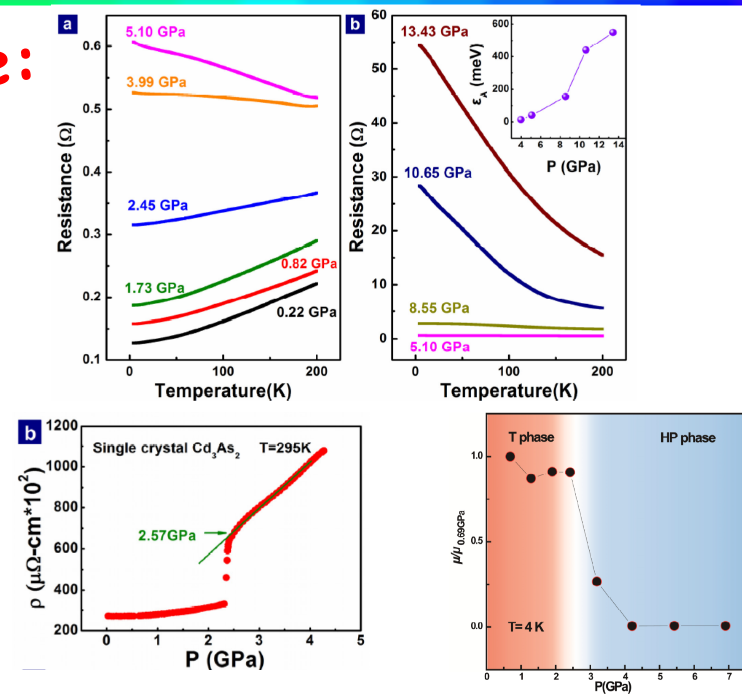
3. Prediction & Exp.: Dirac Semimetal: Cd_3As_2.

Superconductivity under pressure:



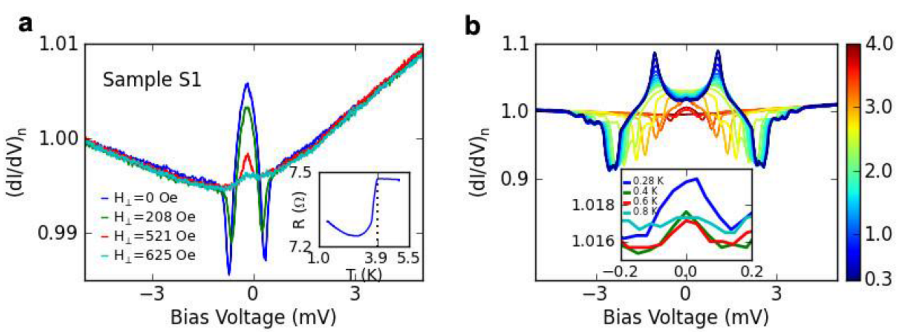


L. P. He, et.al.
arXiv: 1502.2509

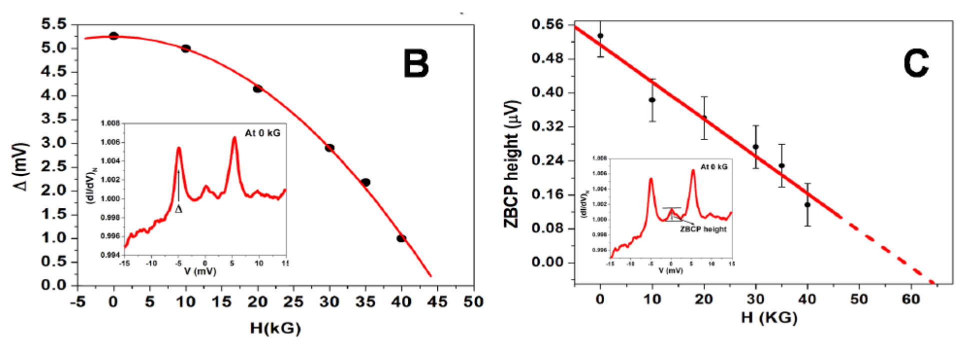


S. Zhan, et.al. arXiv: 1410.3213

SC & ZBCP in point contact:

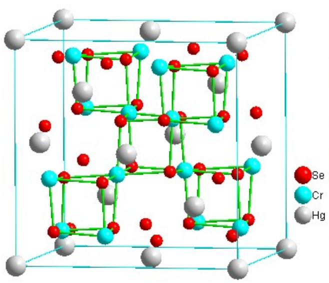


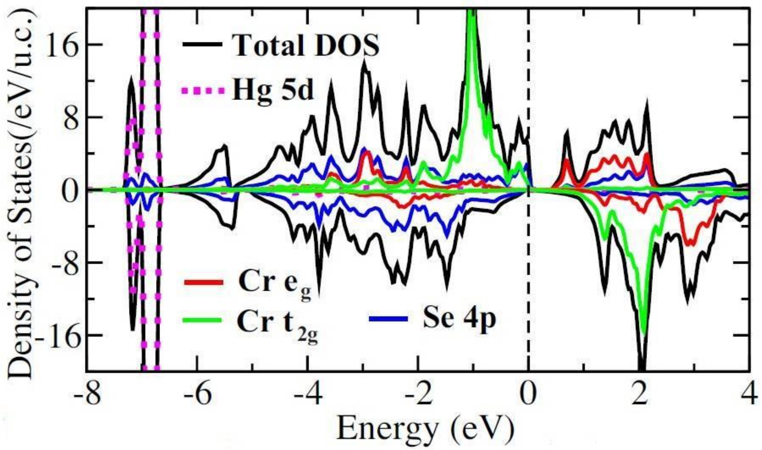
H. Wang, et.al. arXiv: 1501.0418

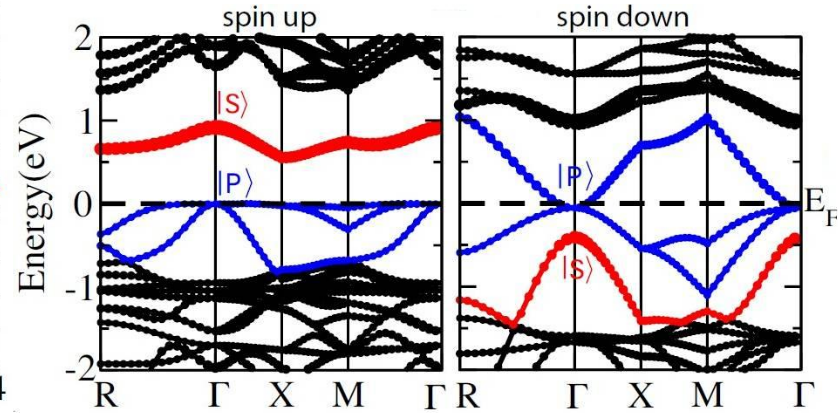


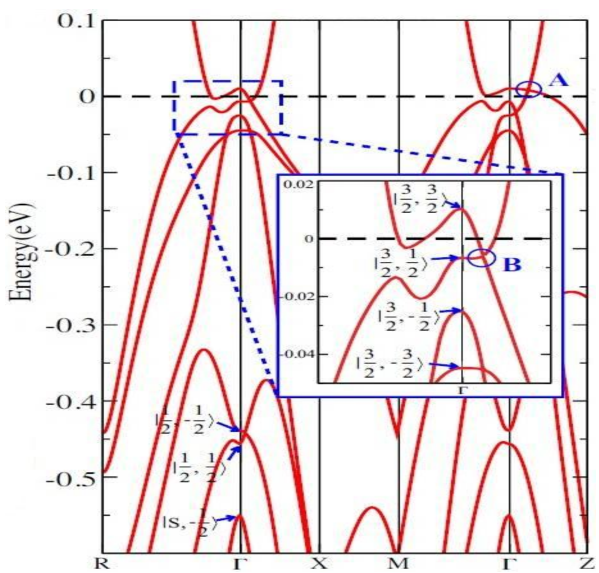
L. Aggarwal, et.al. arXiv: 1410.2072

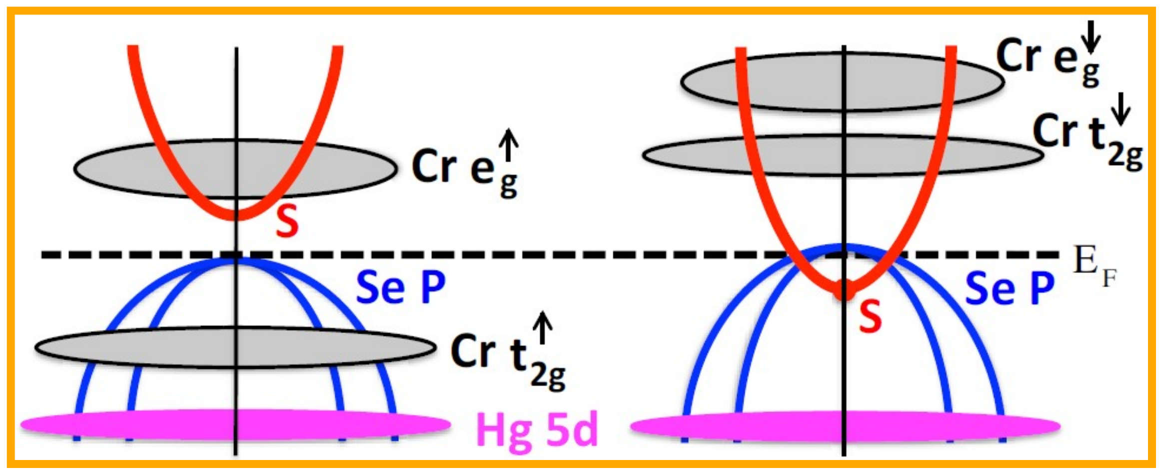
3. Predictions & Exp: T-broken Weyl Semimetal: $HgCr_2Se_4$

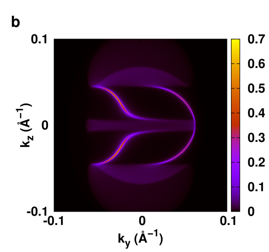










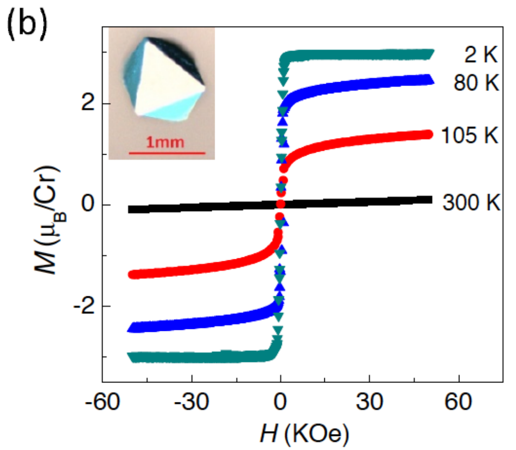


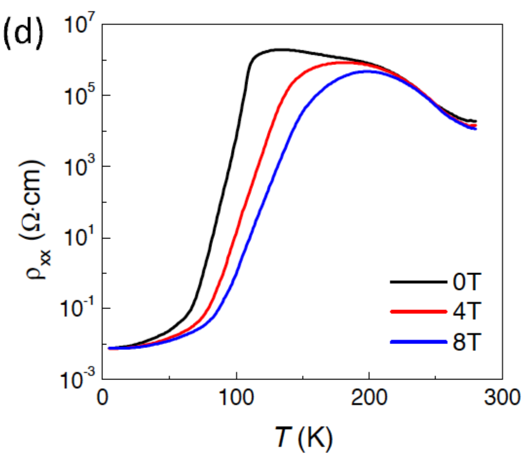
Tc=106K

G. Xu, et.al, PRL (2011)

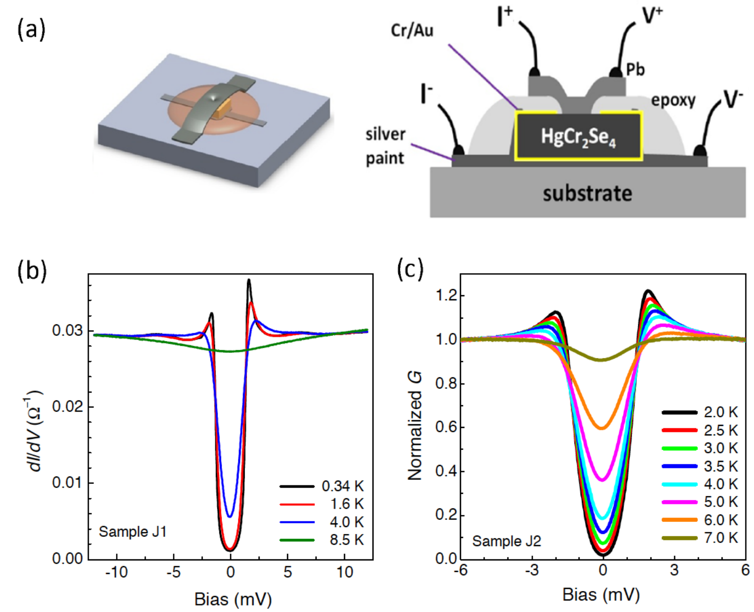
3. Predictions & Exp: T-broken Weyl Semimetal: $HgCr_2Se_4$

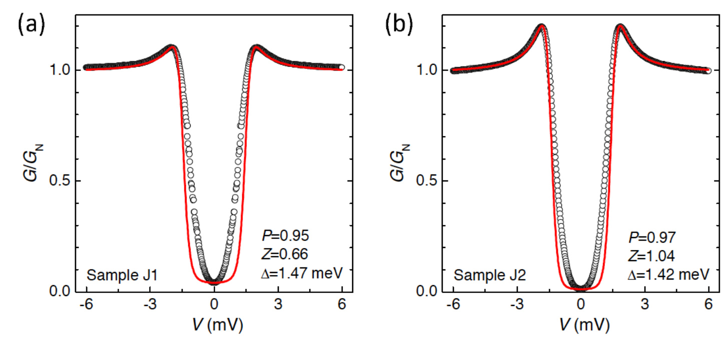
Single s-band Half Metallicity:





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

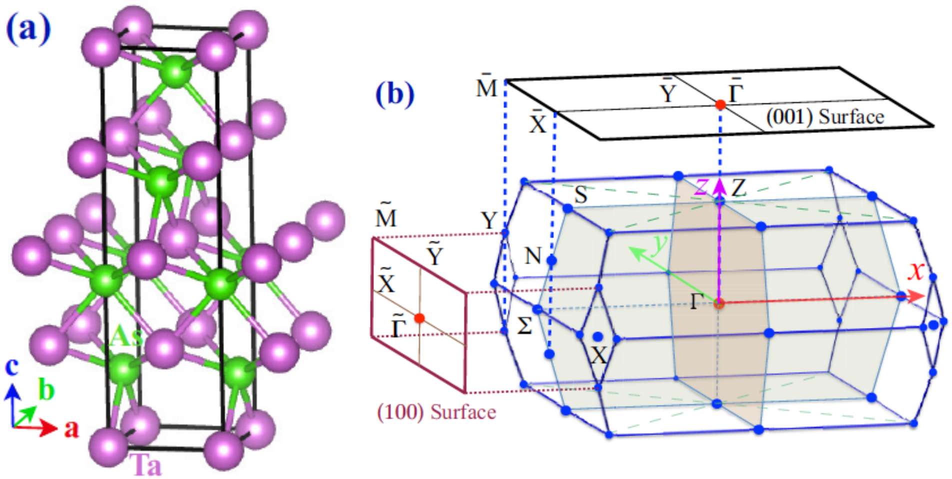


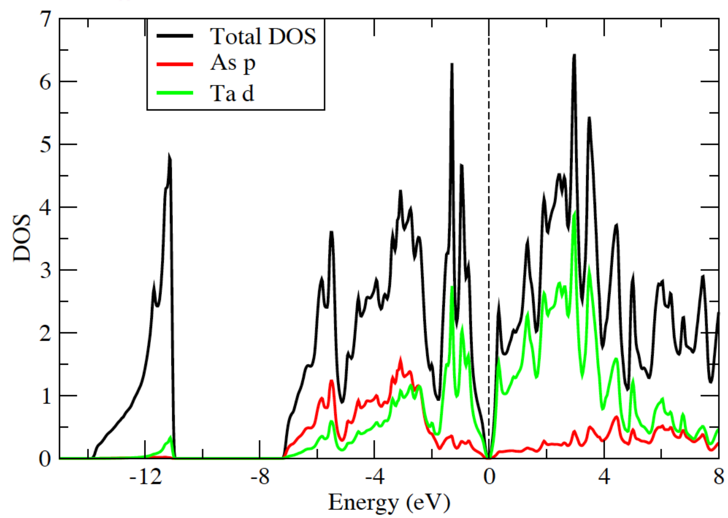


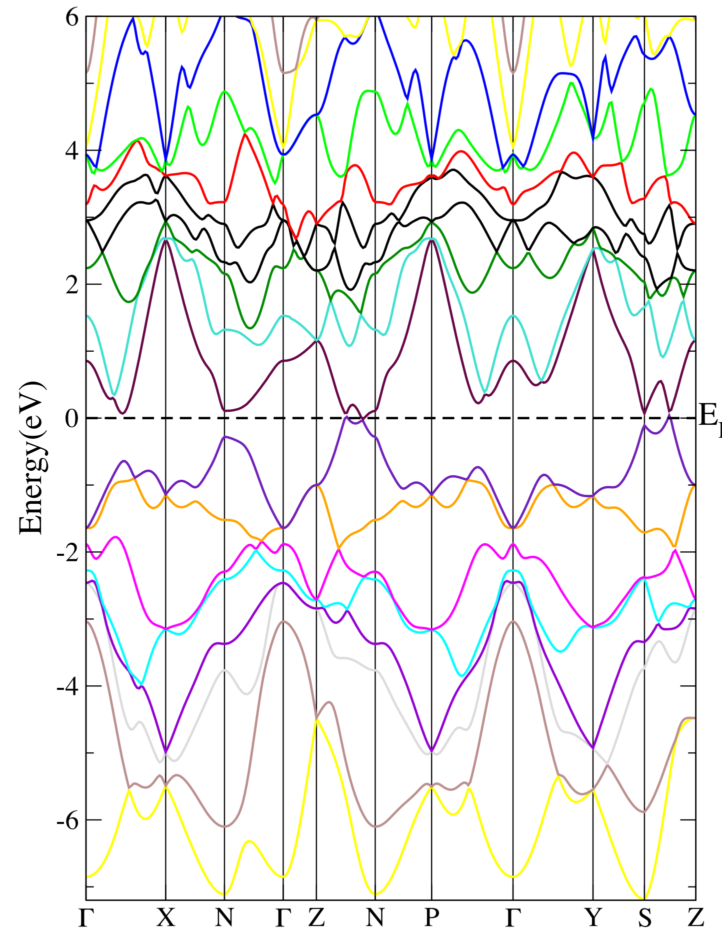
P = 95%, 97%

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

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







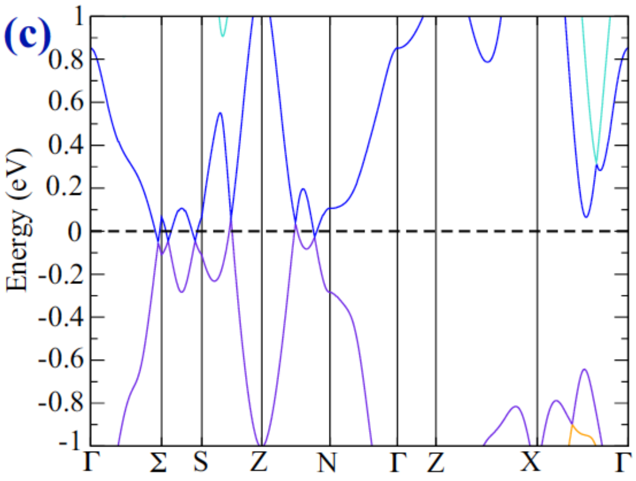
Nominal valence: $Ta^{+3}As^{-3}$, Ta-5d^2

Ta-5d, yz/zx occupied

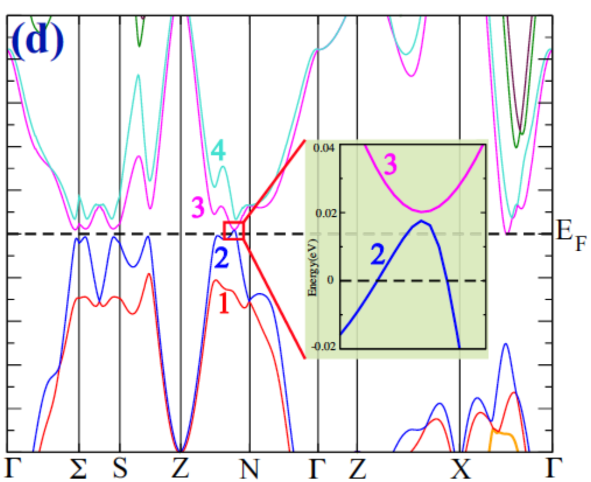
Important Symm.: Mx, My

M_{xy}, M_{-xy} + glide

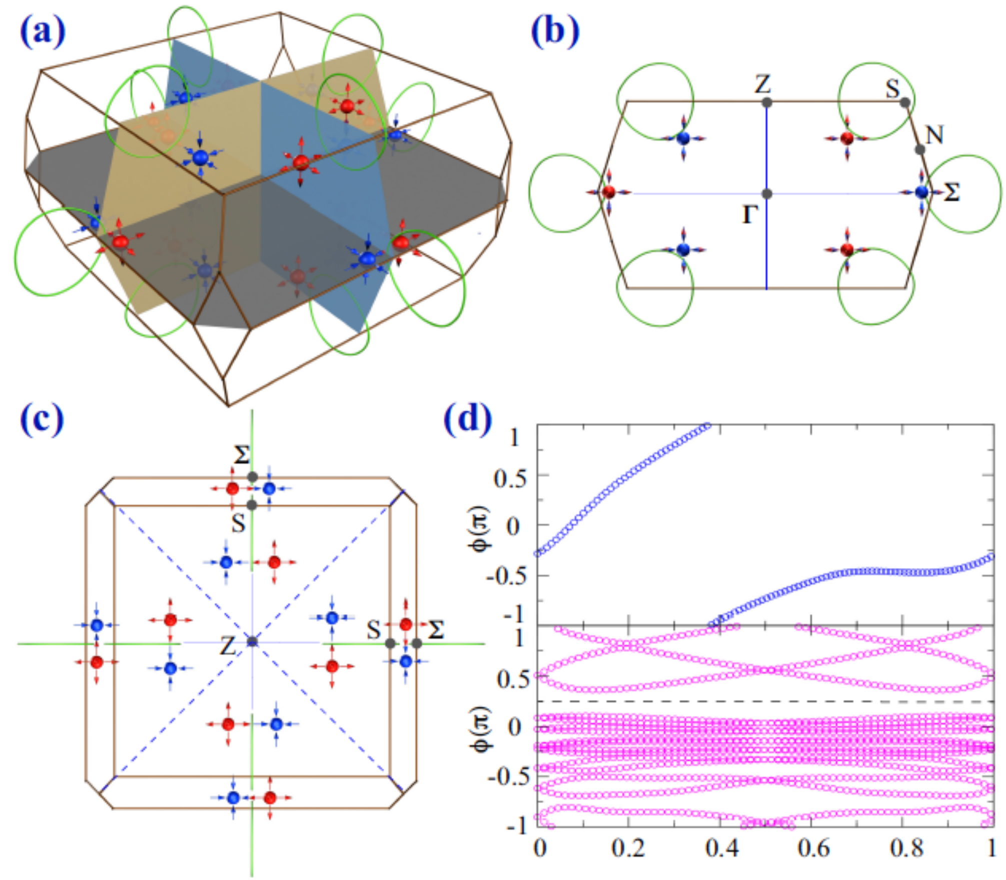
3. Prediction & Exp: T-invariant WSM: TaAs family



GGA



GGA+SOC

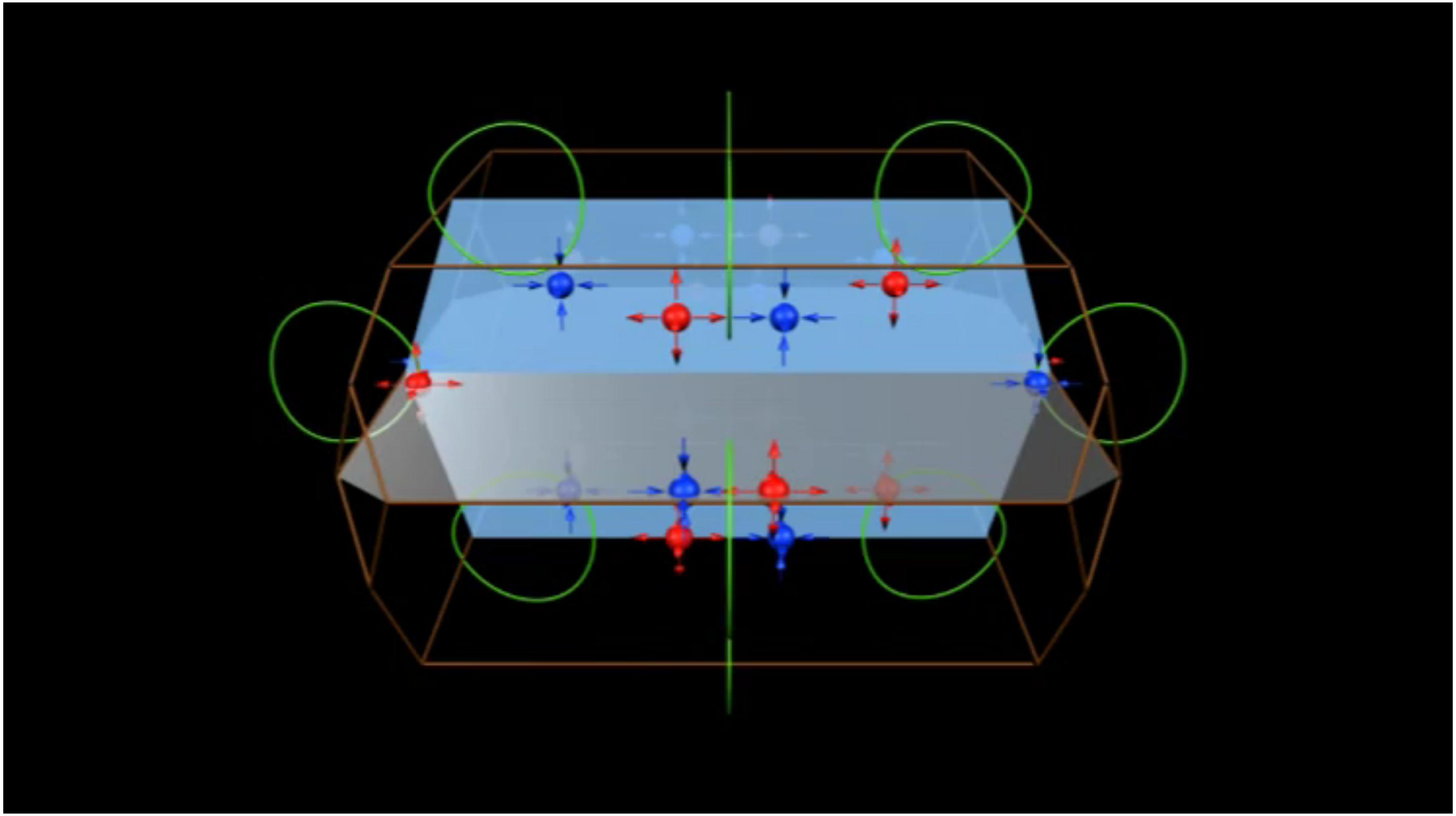


	Weyl Node 1	Weyl Node 2
TaAs	(0.949, 0.014, 0.0)	(0.520, 0.037, 0.592)
TaP	(0.955, 0.025, 0.0)	(0.499, 0.045, 0.578)
NbAs	(0.894, 0.007, 0.0)	(0.510, 0.011, 0.593)
NbP	(0.914, 0.006, 0.0)	(0.494, 0.010, 0.579)

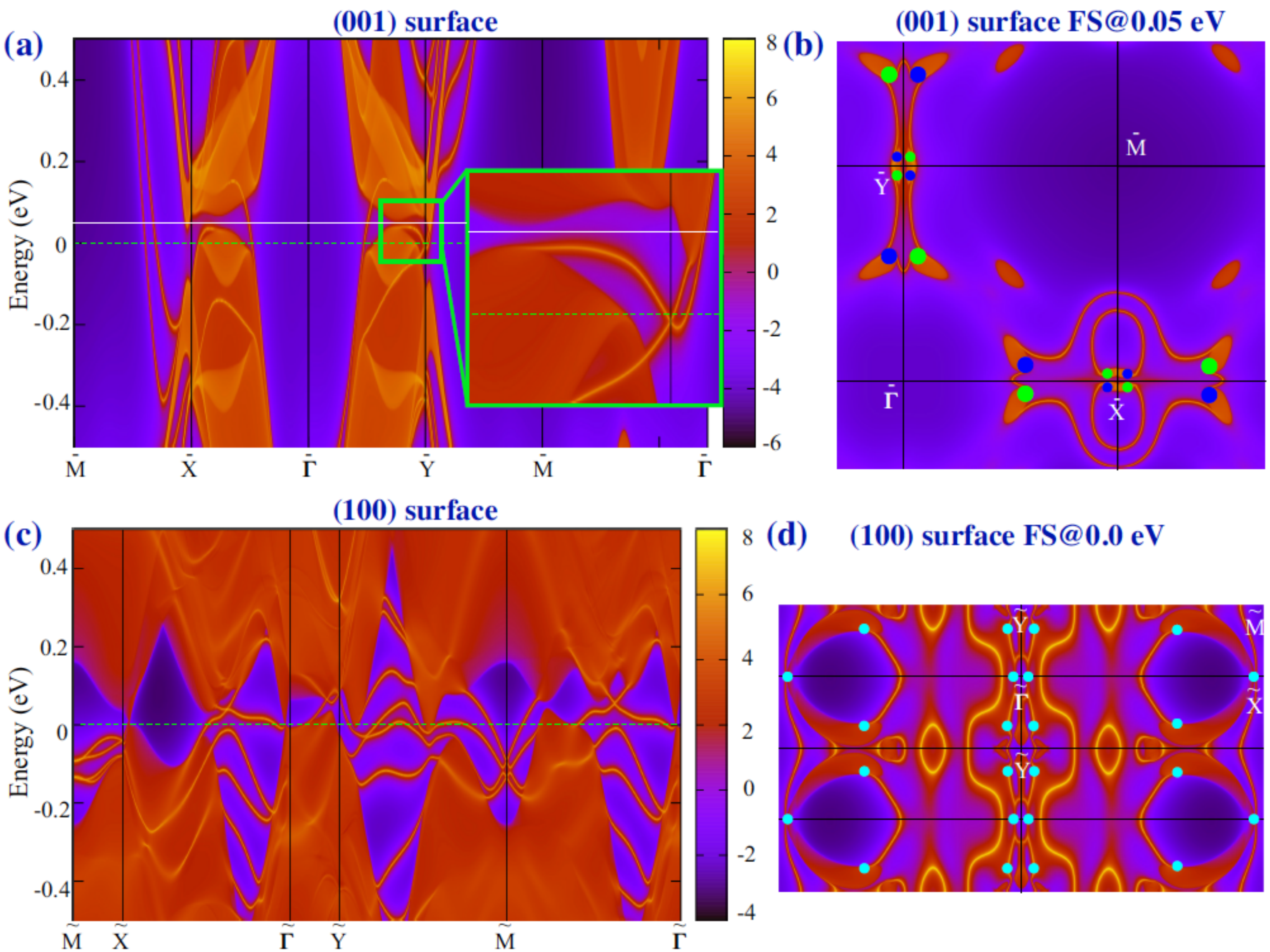
- **12 pairs of Weyl nodes.**
- **MCN=1 (M_x, M_y)**
- **Z_2=0 for M_{xy}**

H.M.Weng, et.al, PRX (2015).

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

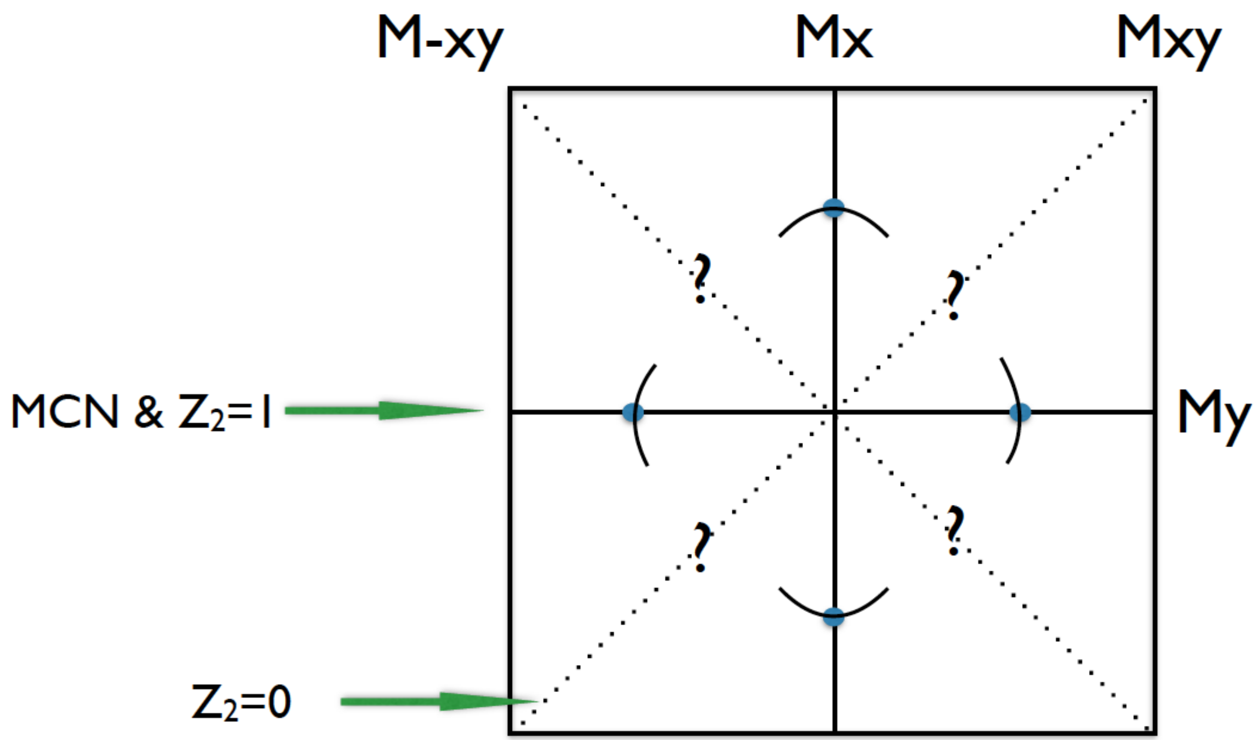


3. Prediction & Exp: T-invariant WSM: TaAs family



Calculated Surface States

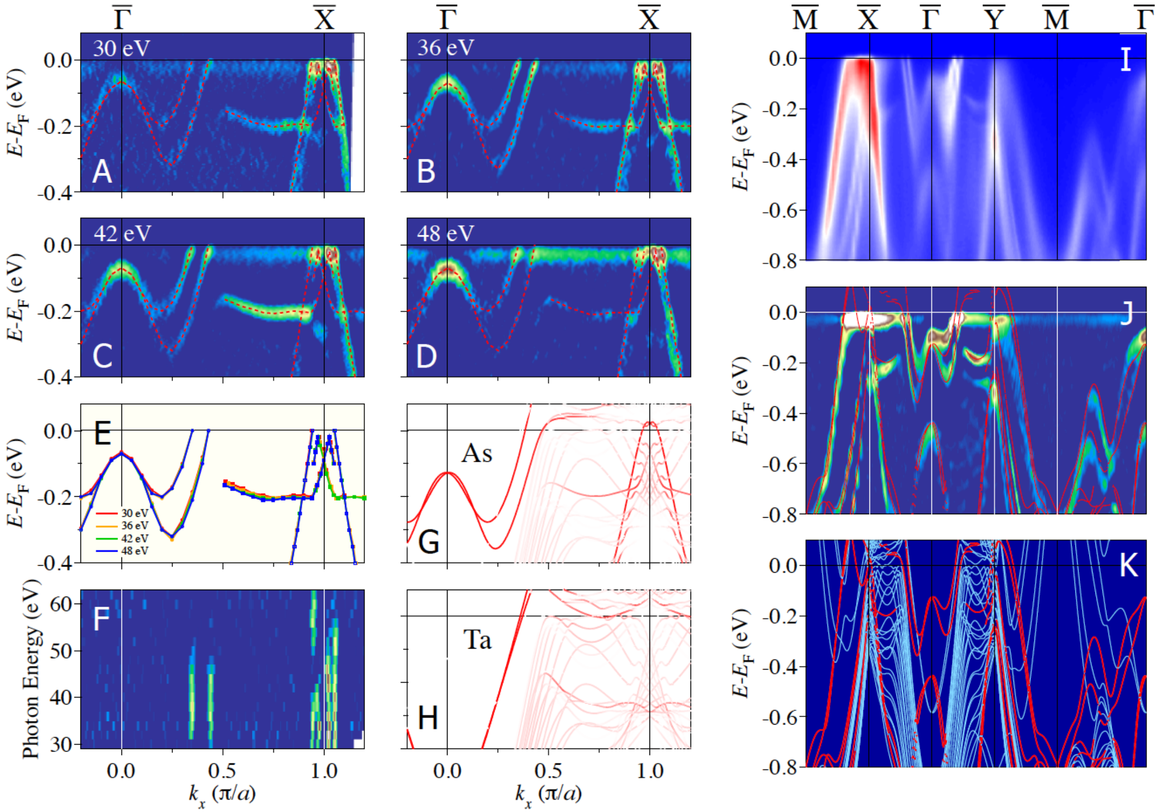
Fermi circle or arcs?

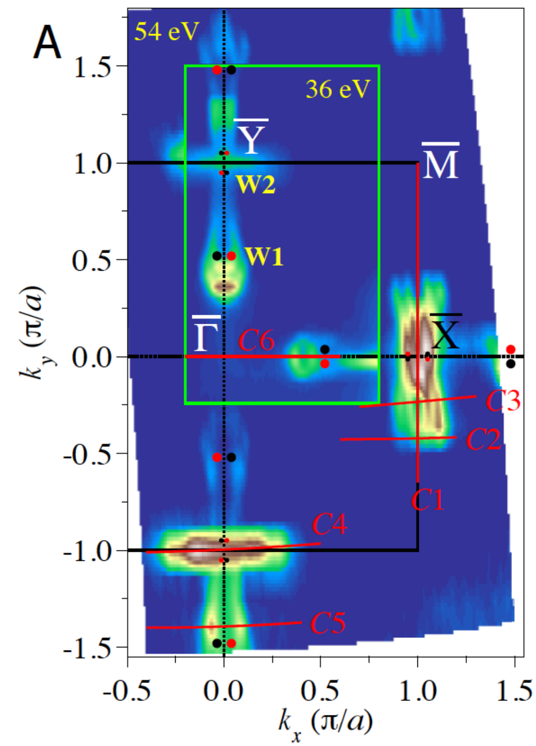


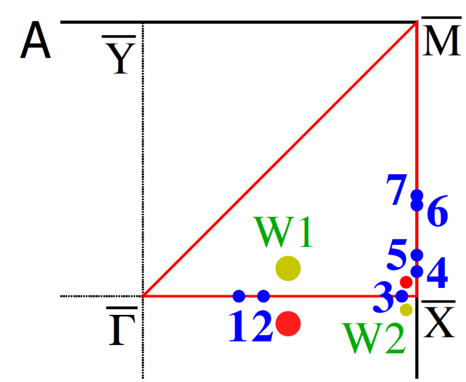
(001) plane

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

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



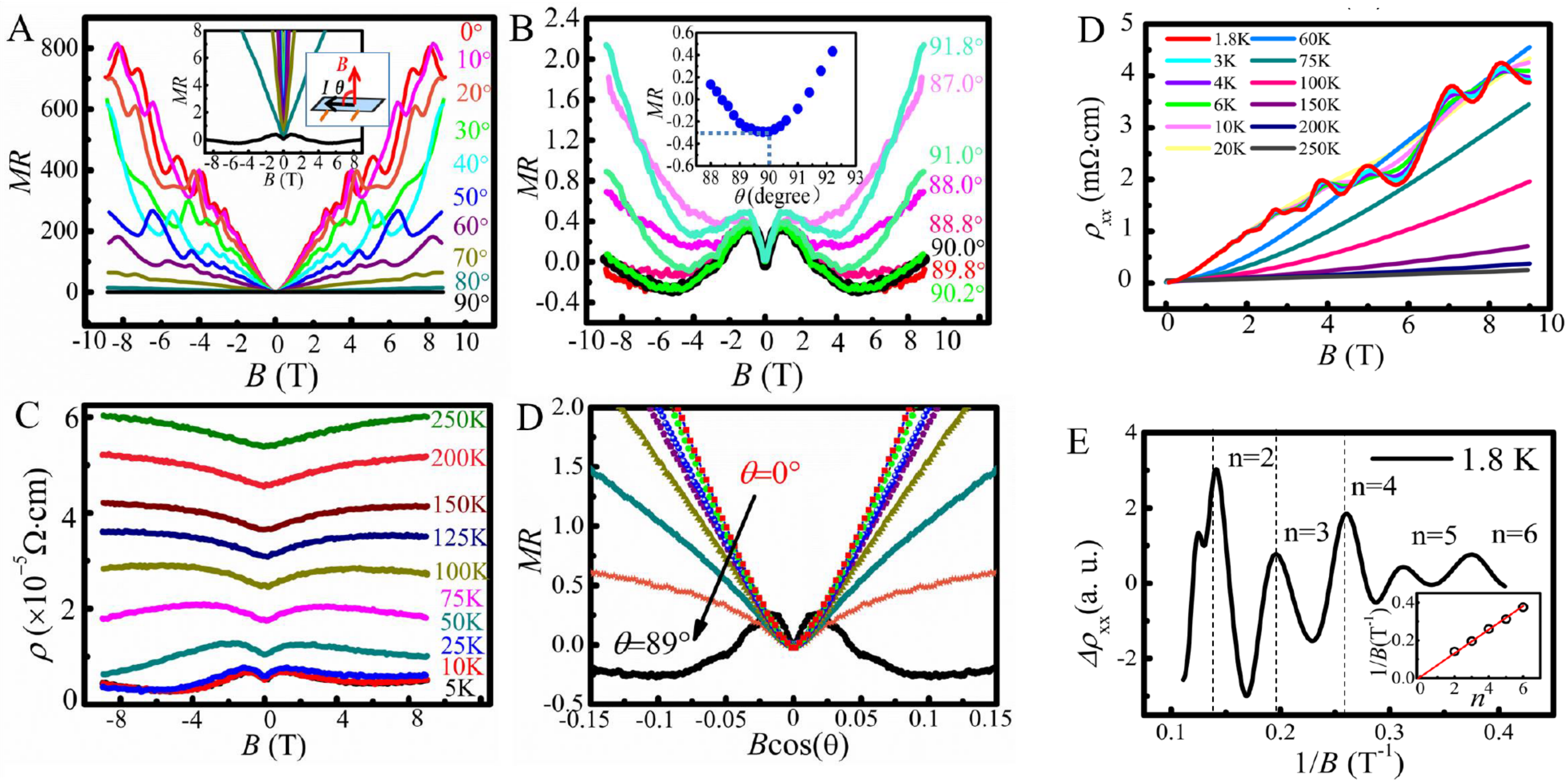




Fermi Arcs: odd Number of Fermi cuts

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

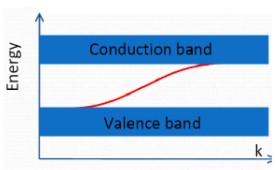
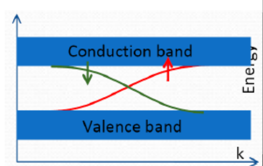
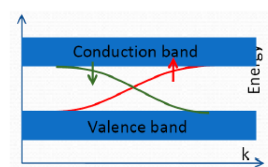
Transport: X. C. Huang, et.al., arXiv:1503.01304 (2015).
See also, 1502.00251 (2015).



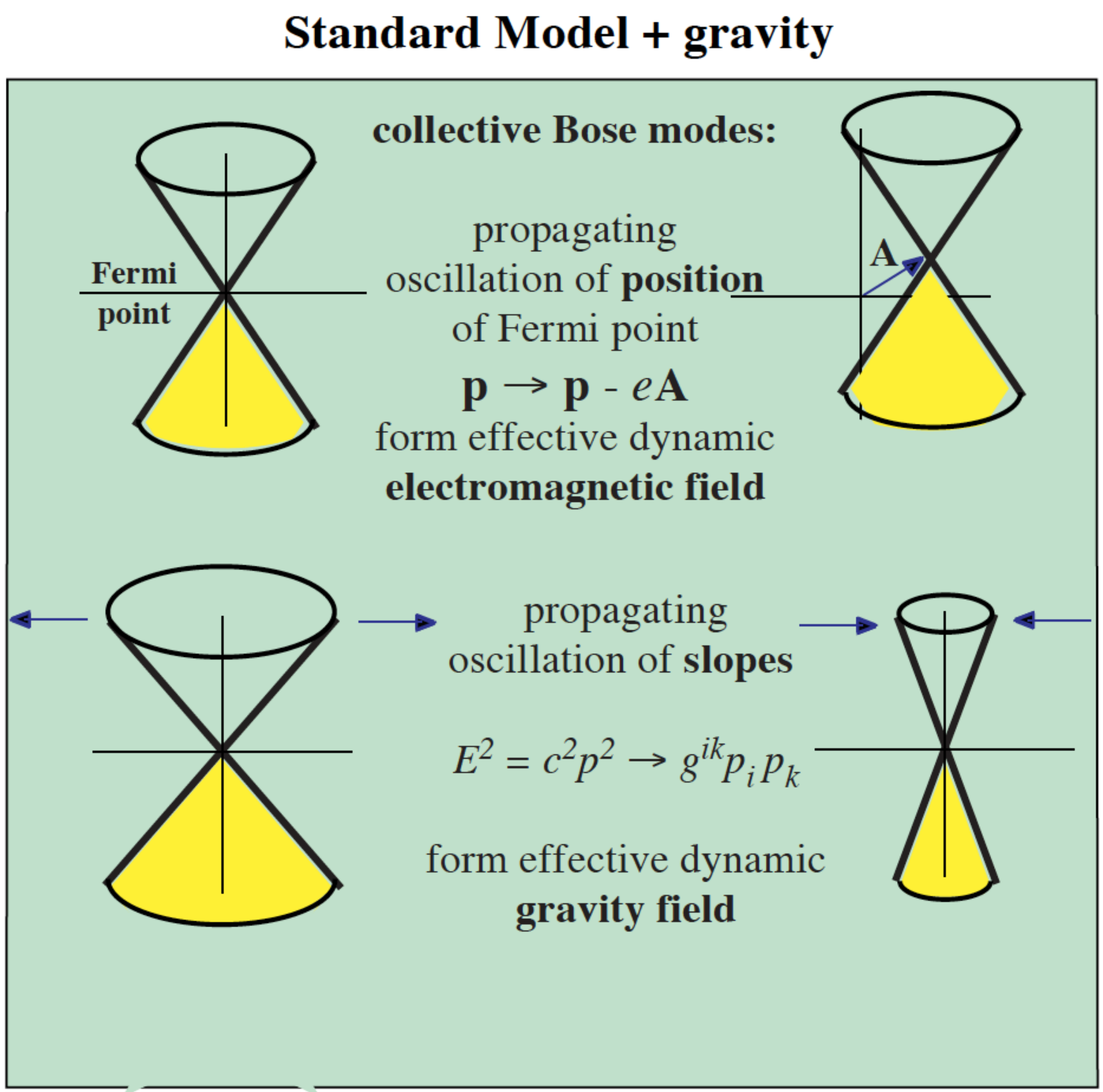
Negative MR is observed for E∥B.

Summary:

1. **Definition of Topological Metals**
2. **Novel Properties of TSM.**
3. **Dirac SM: Na_3Bi, Cd_3As_2**
4. **Weyl SM: $HgCr_2Se_4$, TaAs, NbAs, TaP, NbP**

2D		3D	
T-broken	T-invariant	T-invariant	T or I−Broken
QHE QAHE	QSHE	Kondo Topo. Band Insu. Anderson Mott …	Semi-metal Weyl nodes (in bulk)
			
Edge States, TKNN, Chern Num. $Z \neq 0$	Edge States, $Z_2 \neq 0$	Surface States $Z_2 \neq 0$	Surface Fermi arcs $C_{FS} \neq 0$
✔	✔	✔	New State

Summary:


Standard Model + gravity
collective Bose modes:
Fermi
point
propagating
oscillation of **position**
of Fermi point
$\mathbf{p} \to \mathbf{p} - e\mathbf{A}$
form effective dynamic
electromagnetic field
A
propagating
oscillation of **slopes**
$E^2 = c^2p^2 \to g^{ik}p_i p_k$
form effective dynamic
gravity field