Topological Insulators and Topological Semi-metals

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Outline

1. Introduction:

   TIs, Chern insulators, Chern semi-metal

2. Topological Insulators:

   Bi_2Se_3 & Bi_2Te_3, Ag_2Te, $NaCoO_2$ surface

3. Topological Semi-metals:

   Spinel **$HgCr_2Se_4$,**

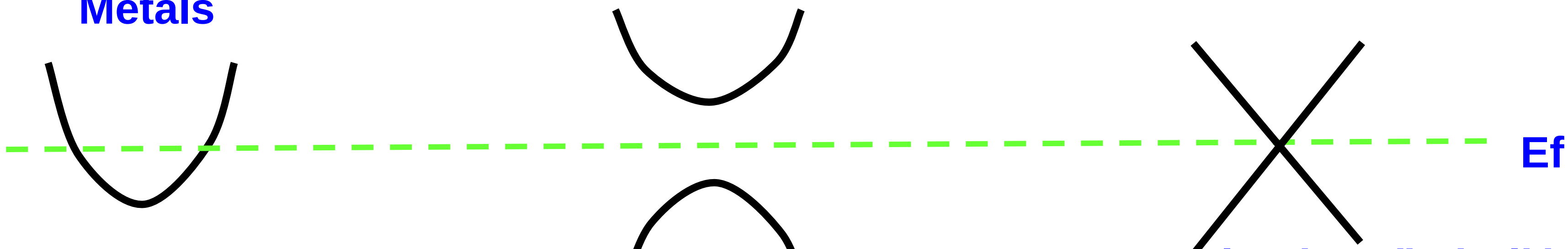
4. Magnetic Monopoles, Fermi Arcs,

   and Quantized AHE

1. Introductions: Momentum Space Topology

Three distinct universality classes in 3D:

Metals | **Insulators** | **Topological Semi-metal**



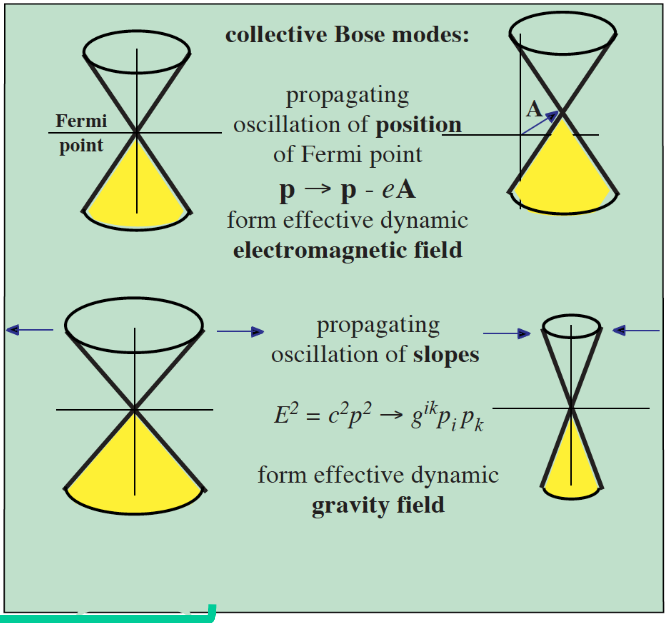
Metals: Fermi surface

Insulators: No fermi surface

Normal Insulators
+
Topological Insulators
(Weyl points at Boundary)
Separation in Real-Space

Topological Semi-metal:
Weyl points (in bulk)
Fermi arcs (on surface)

Standard Model + gravity



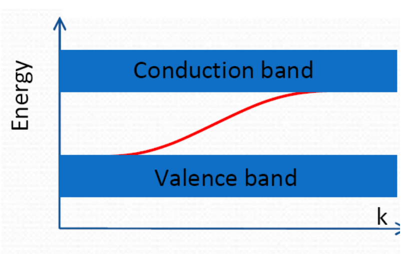
From Volovik

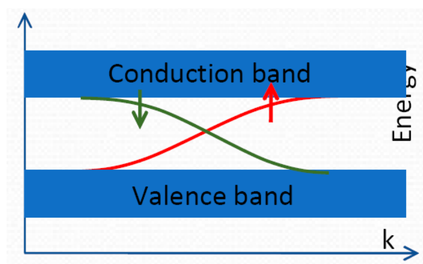
Graphene is not TS!

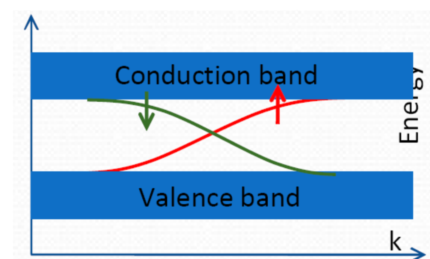
Our Subjects

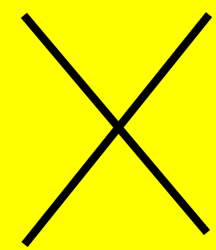
1. Introductions: Family of TIs?

2D		3D	
T-broken	T-invariant	T-invariant	T-Broken
QHE QAHE	QSHE	Kondo Topological Band Insulator Anderson Mott	Semi-metal









Edge States

TKNN
Chern number

Z2

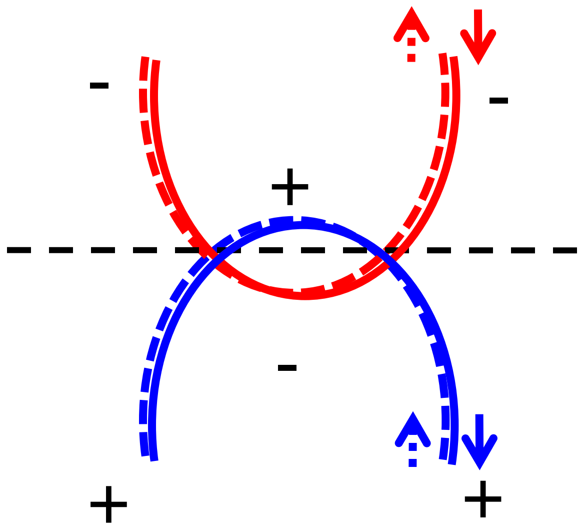
Surface States

Weyl points
(in bulk)

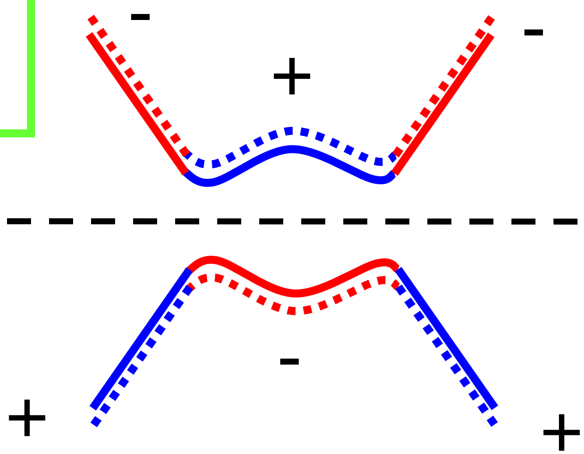
2. Topological Insulators: **Materials.**

Guidelines:

1. Semiconductor with inverted band structure
2. Strong SOC



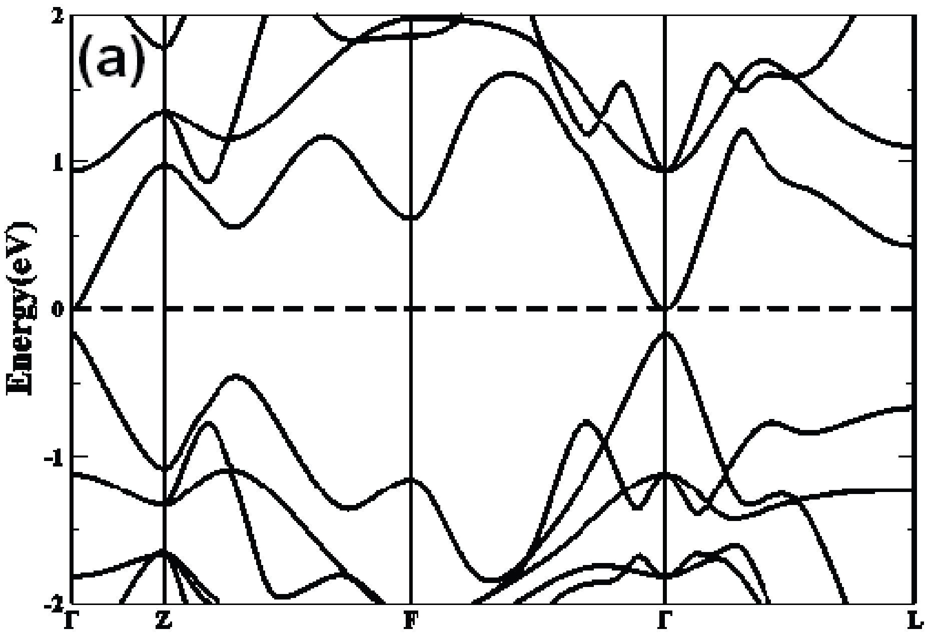
Gap opening due to SOC



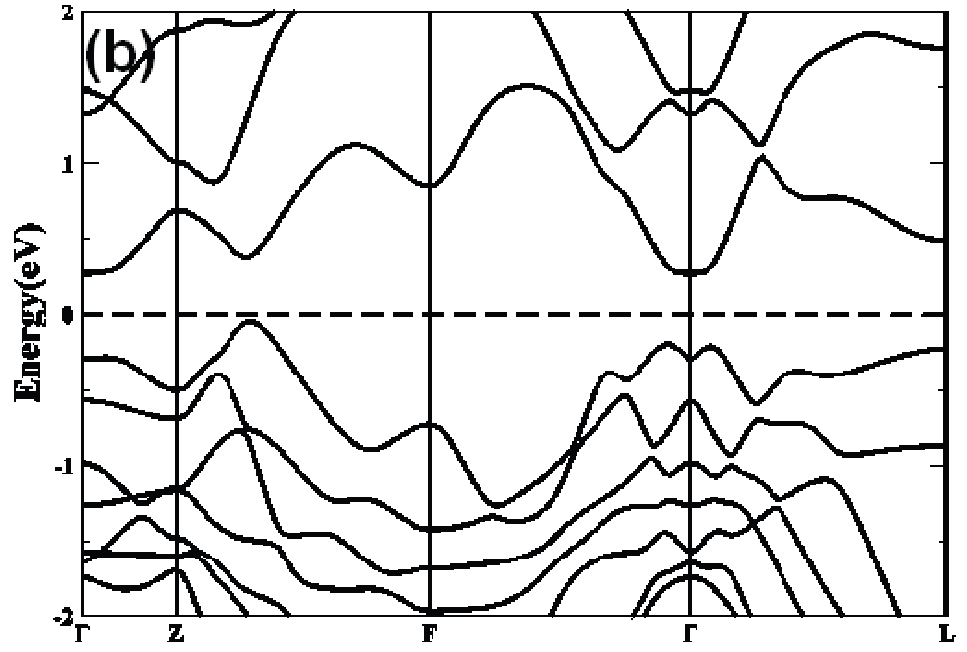
Real materials for 3D TI?

"twisted band"

Band Structure Bi2Se3

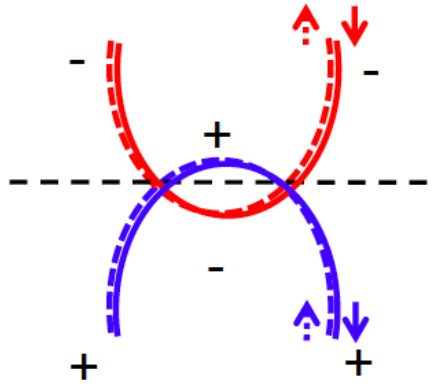


Without SOC



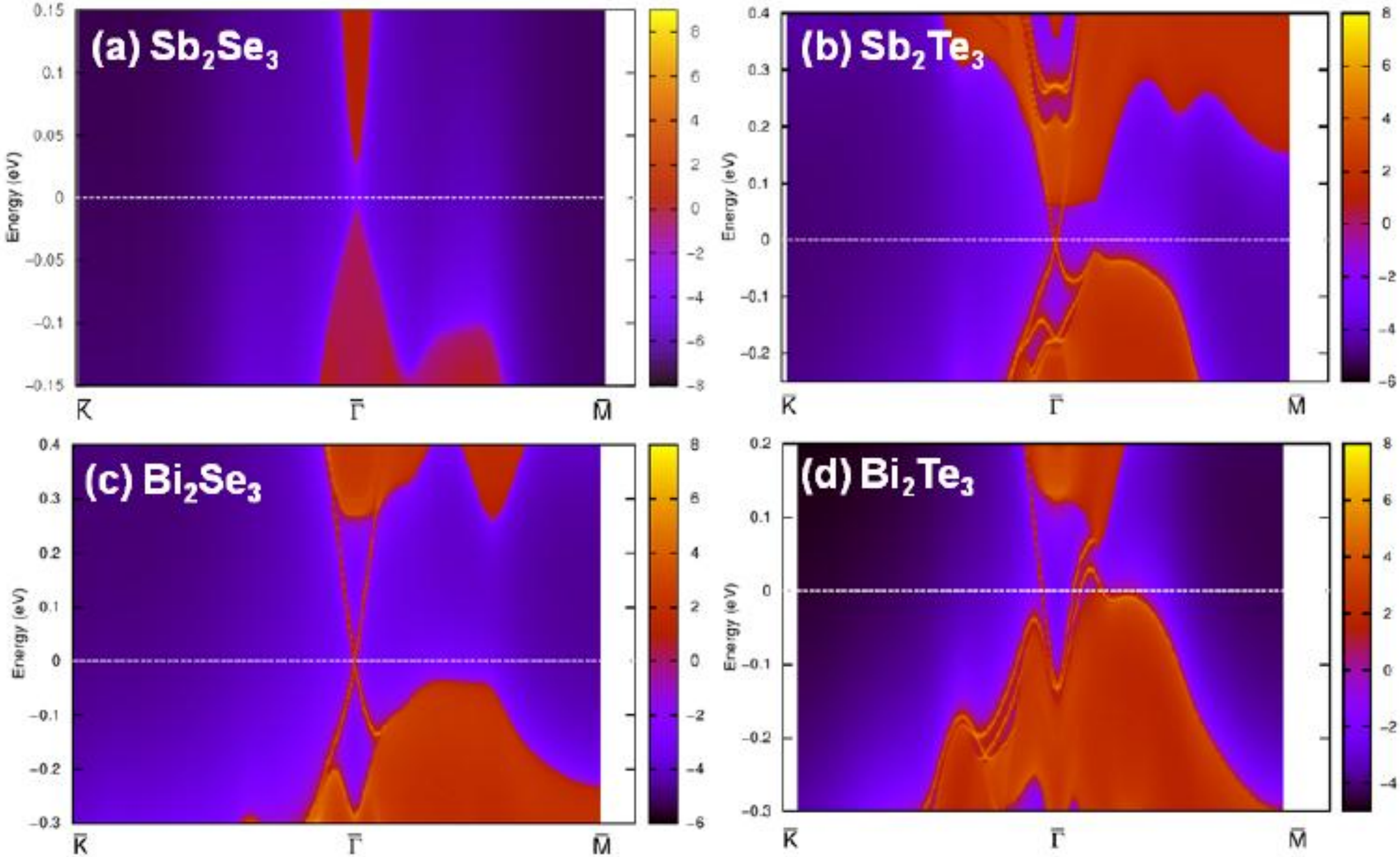
With SOC

1. Only Gamma Point is relavant.
2. SOC will invert the bands at Gamma.
3. Gap is around 0.3 eV.



ab-initio Surface States:

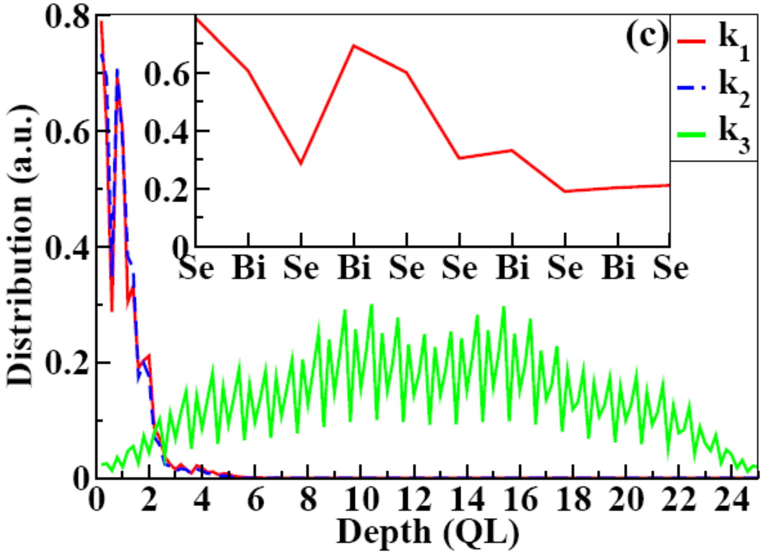
Bi_2Se_3 has the biggest Gap around 0.3eV



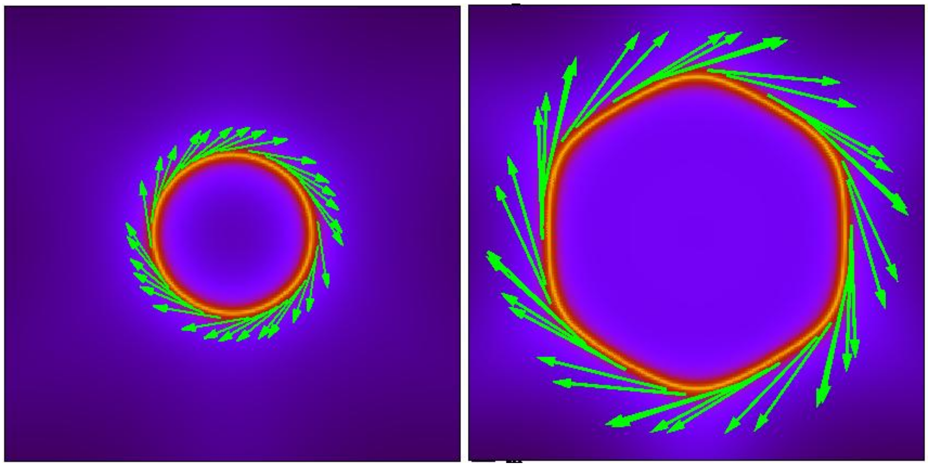
H. J. Zhang, et.al., Nature Phys. (2009)

2. Materials: Bi_2Te_3, Bi_2Se_3, Sb_2Te_3

Penetration Depth
of Surface state, 2nm



Chiral Spin texture



W. Zhang, et.al., New J. Phys, **12**, 065013 (2010)

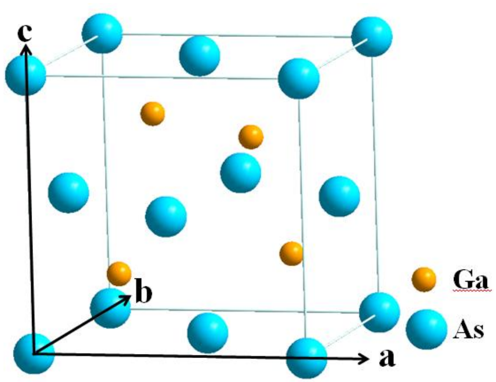
2. Materials: Ag_2Te

Crystal Structure:

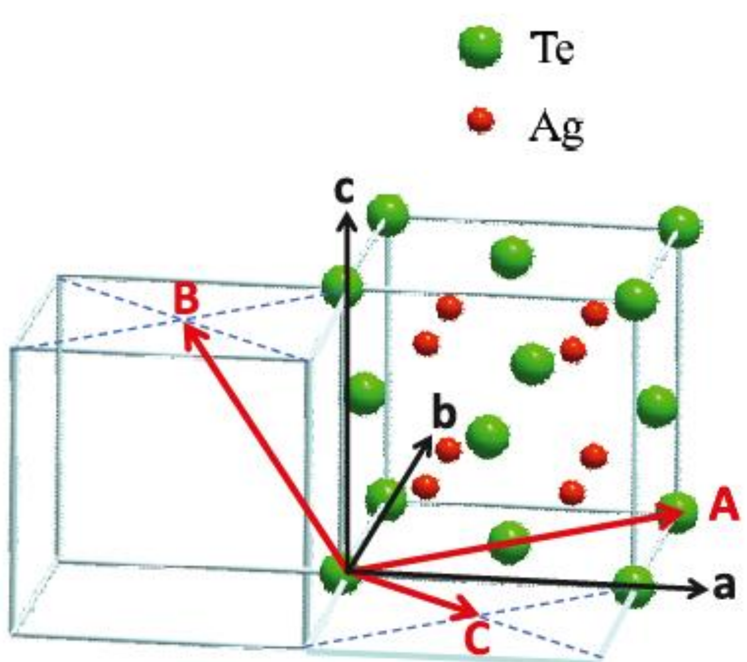
T > 417 K, α-Ag_2Te, anti-fluorite (Fm3m)

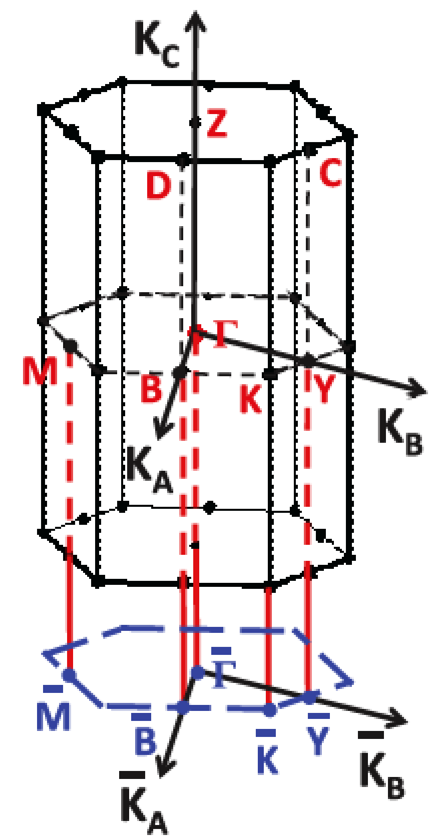
T < 417 K, β-Ag2Te, distorted ($P2_1/c$)

Cubic: a,b,c



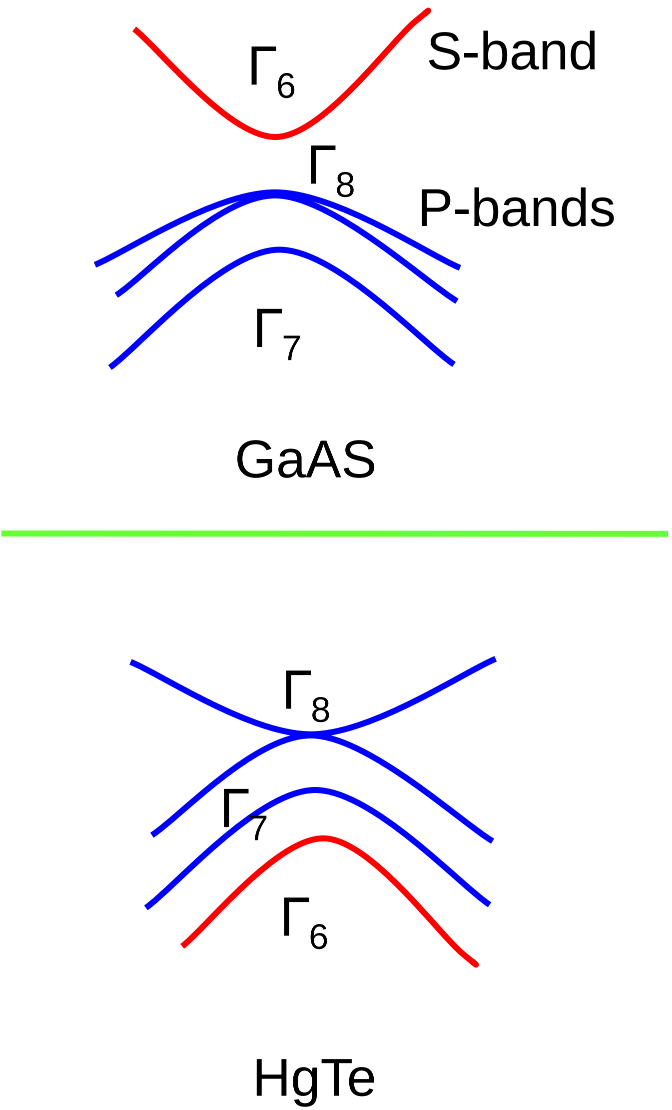
GaAs

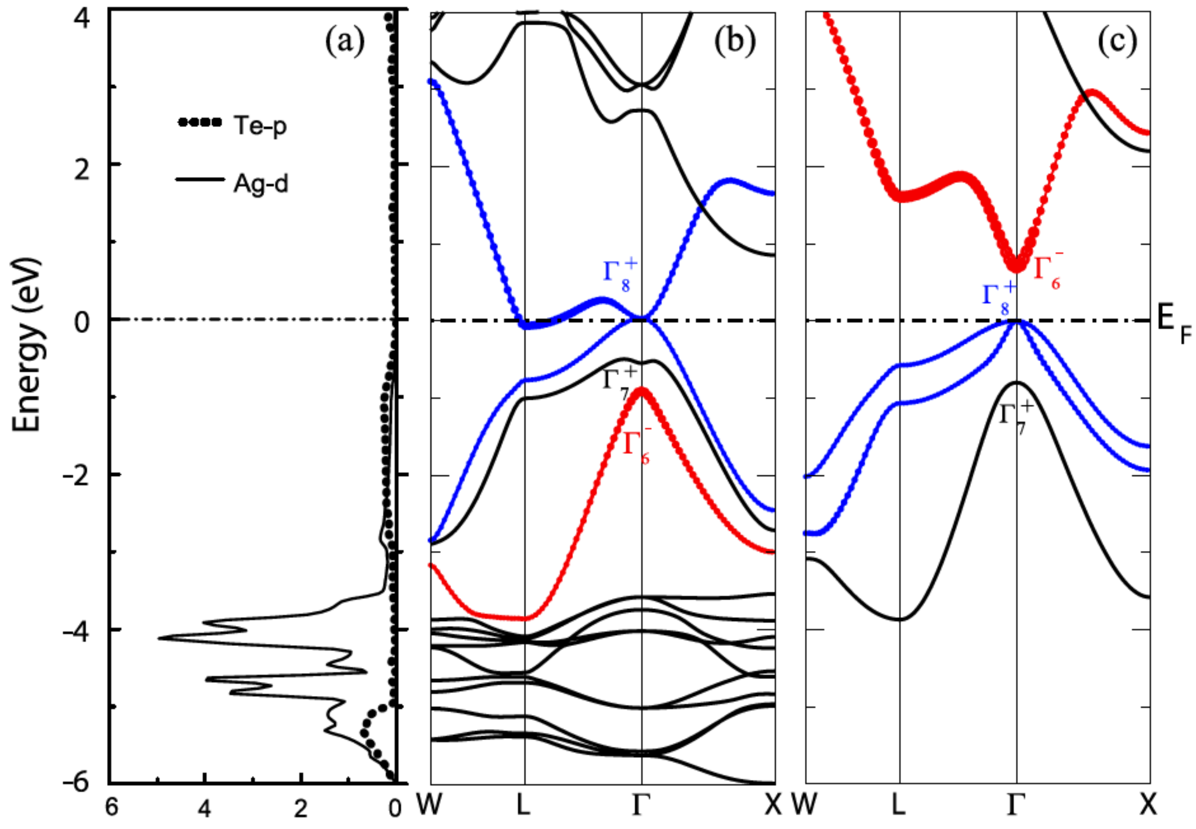




2. Materials: Ag_2Te

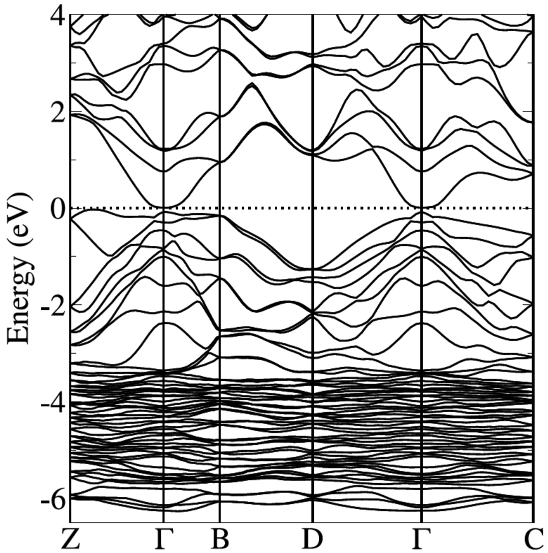
Inverted Band Structure of α-Ag_2Te Similar to HgTe

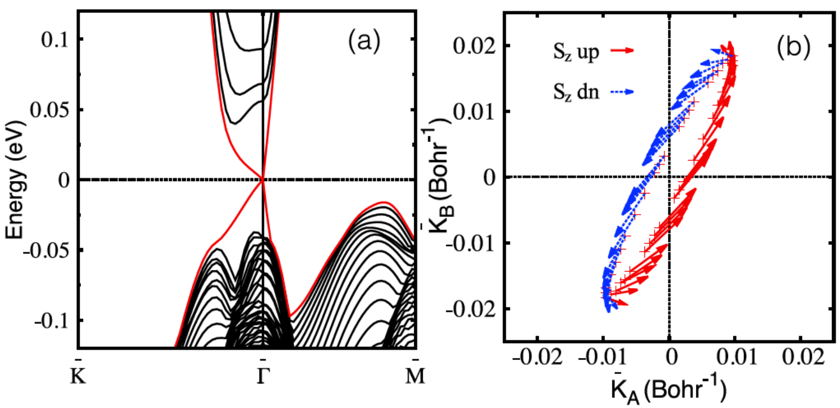




2. Materials: Ag_2Te

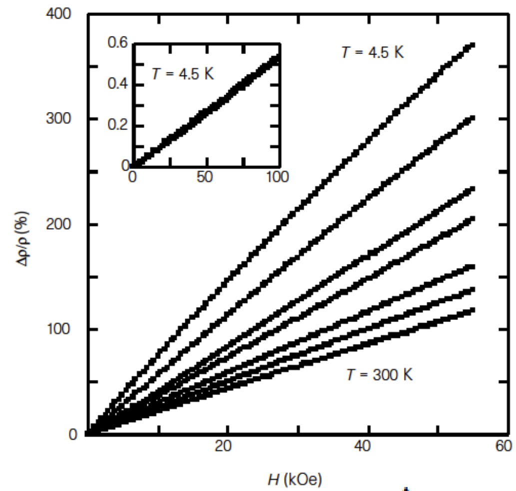
β-Ag_2Te, gap=80meV





W. Zhang, et.al., PRL **106**, 156808 (2011).

Quantum Magneto-resistance in $Ag_{2+\delta}Te$?



Super-linear MR
R. Xu, et.al., Nature (1997).

Conventional MR: $$\frac{\Delta\rho}{\rho} \propto \begin{cases} (\mu H)^2, & \mu H < 1 \\ C, & \mu H > 1, \end{cases}$$

Abrikosov's Quantum MR:

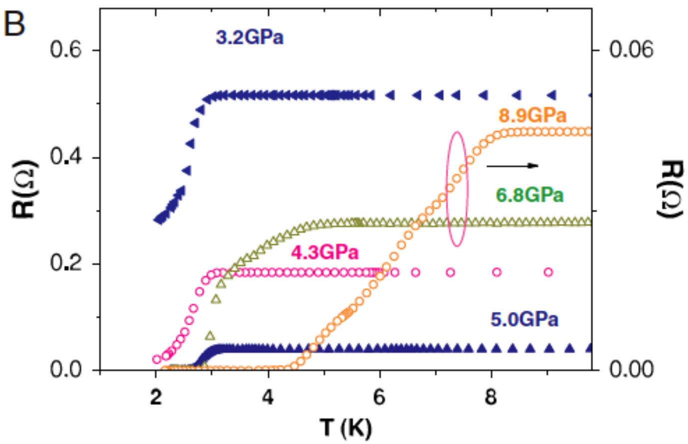
$$\rho_{xx} = \rho_{yy} = \frac{N_i H}{\pi n^2 ec}, \quad \rho_{xy} = RH = \frac{H}{nec},$$

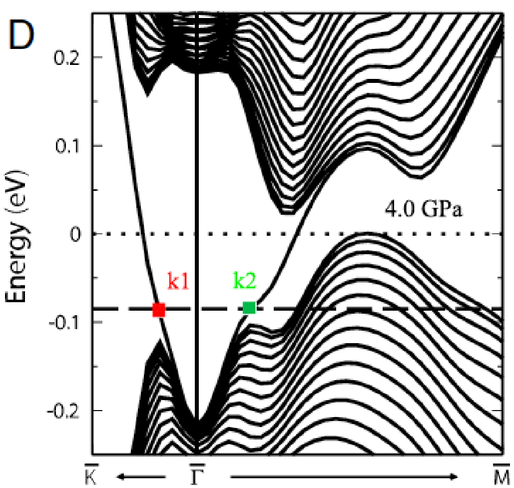
Linear Dispersion is Important!

Landau Level Spacing. $\propto \sqrt{B}$

2. TI materials：Other Recent Progresses

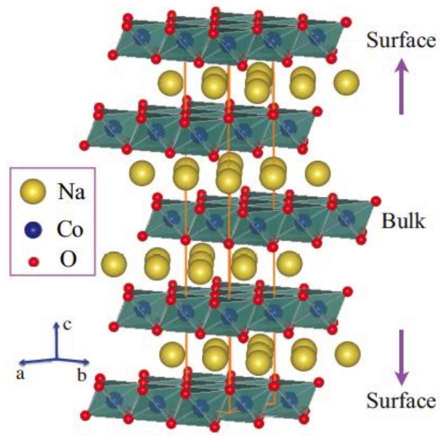
SC in Bi_2Te_3 under pressure

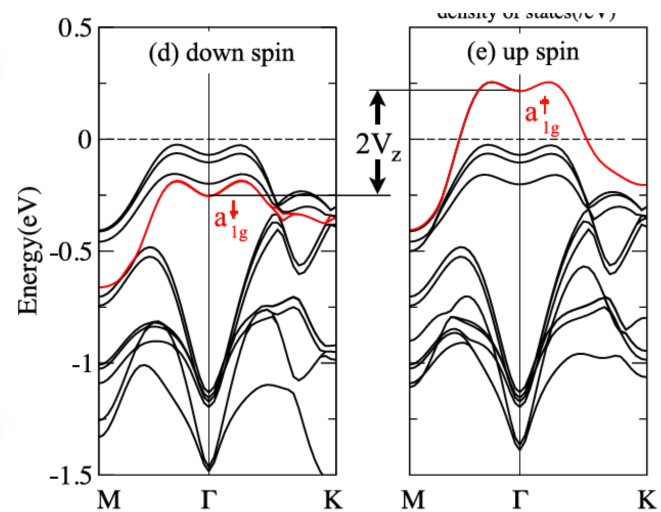


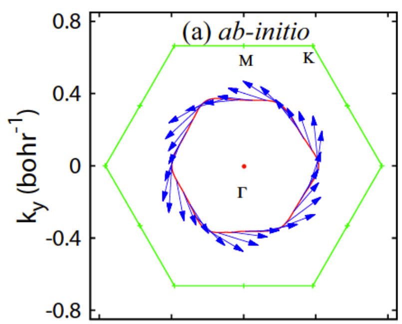


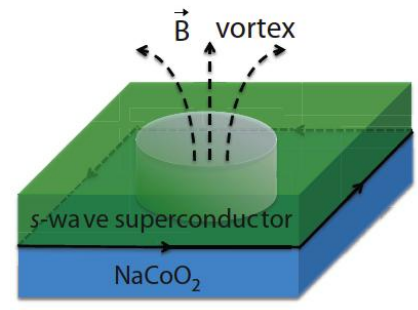
Jin,et.al，PNAS（2011）

Proximity：$NaCoO_2$ surface





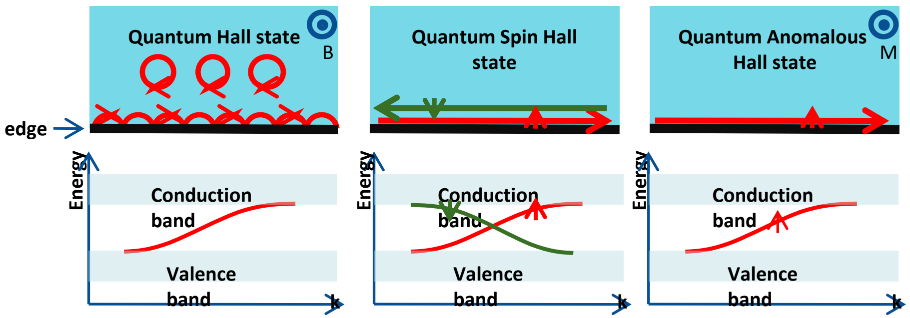


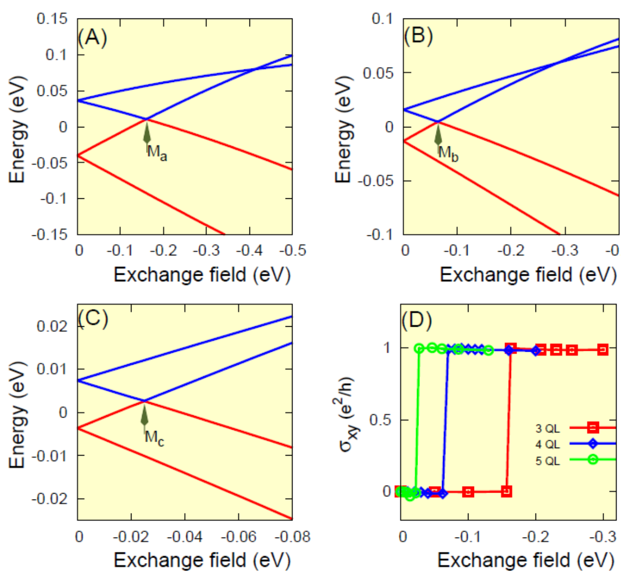


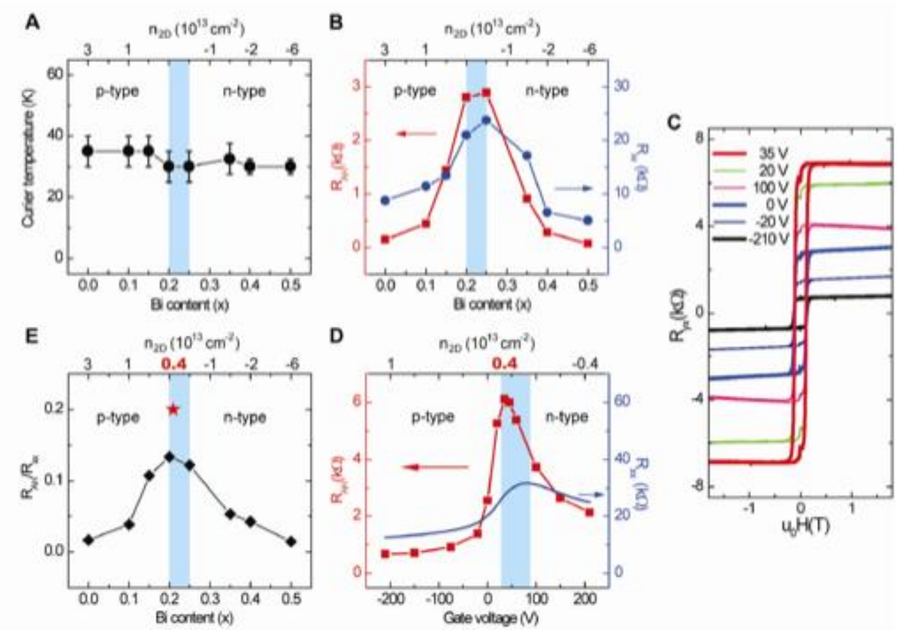
$$E_g = \sqrt{\frac{2m^*\alpha^2}{V_z}}(1+\frac{\mu}{V_z})\Delta \approx 0.22\Delta,$$

Weng, et.al, PRB 84, 060408 (2011).

2. TI materials：Other Recent Progresses







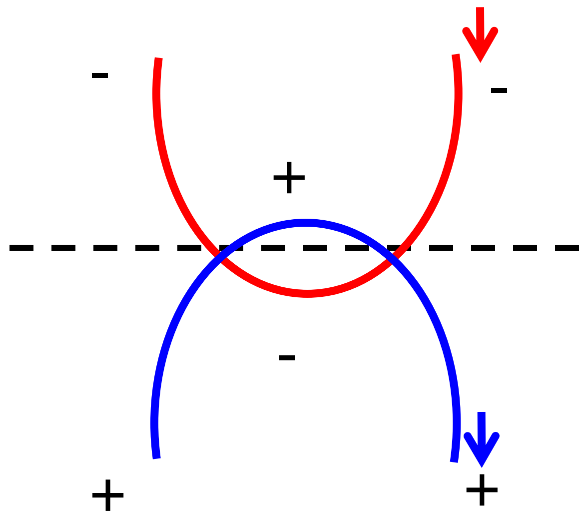
$R_{AH} \approx 6K\Omega$，约1/4个 e^2/h (25KΩ)

QAHE in Bi_2Se_3 film doped with Cr or Fe, Dai & Fang，Science(2010)

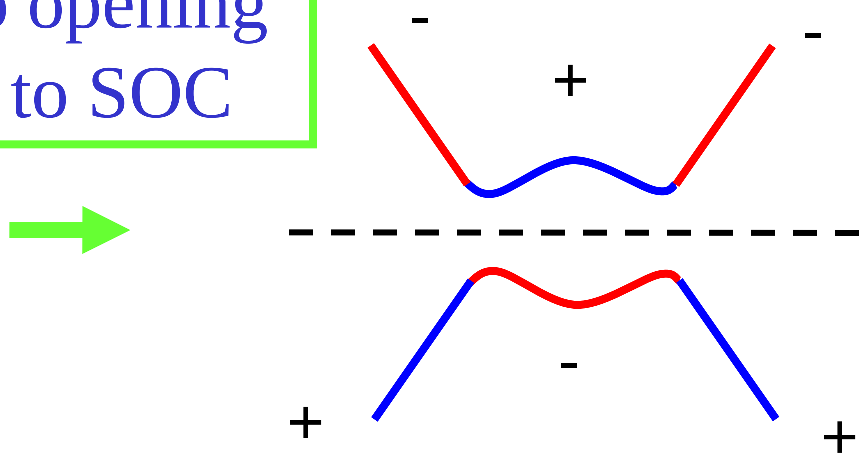
Cr-Bi_2Te_3-Sb_2Te_3 film，arxiv：1108.4754(2011).

3. Semi metals: From 2D to 3D without TRS?

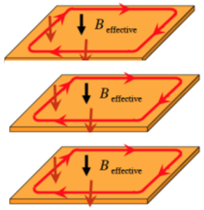
2D Chern Insulators:



Gap opening due to SOC



3D: (1) Weak 3D Chern Insulators:

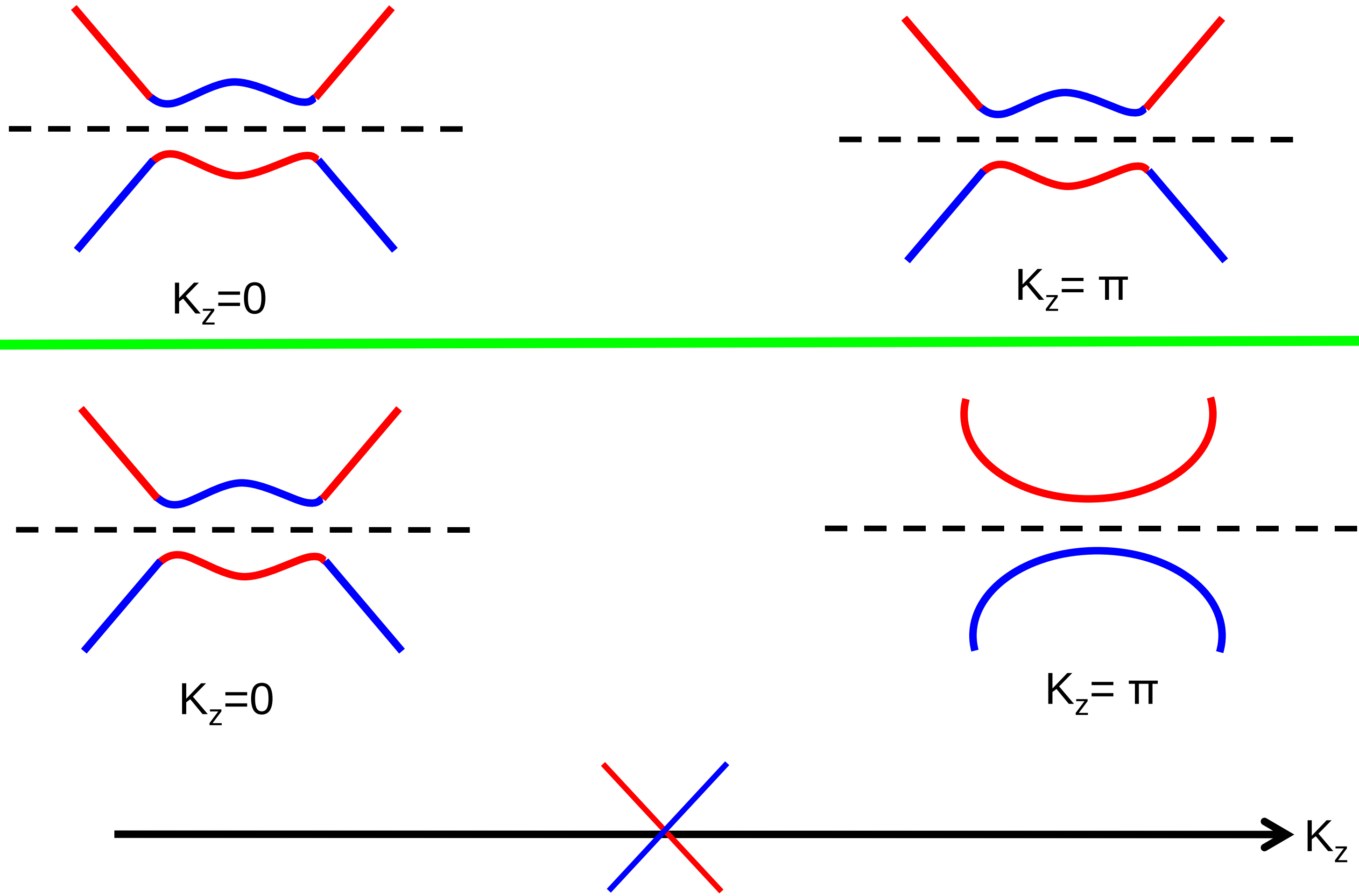


(2) Strong 3D--Any analogy? Chern semi-metal:

Time Reversal Polarization in momentum space!

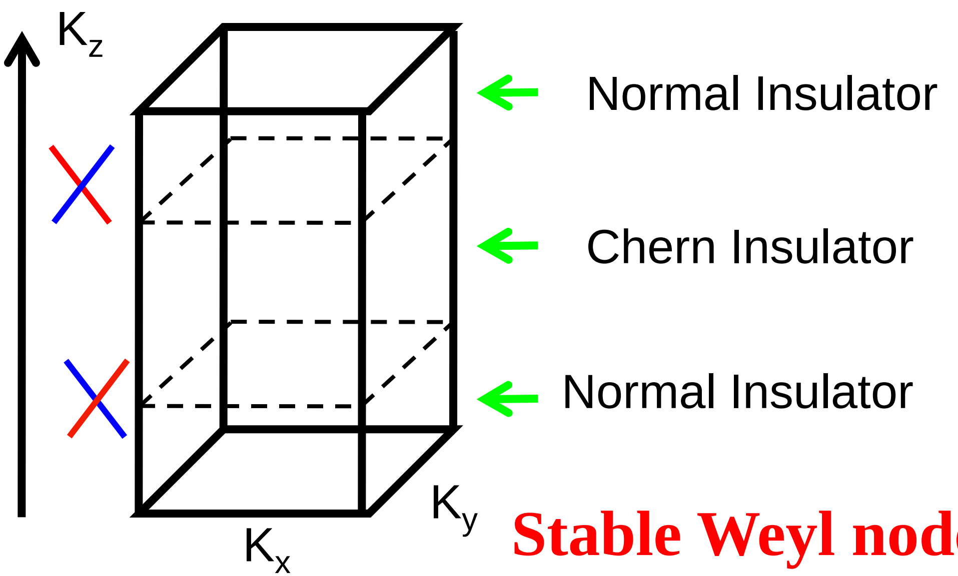
3. Semimetals: Chern Insulators and semi-metal?

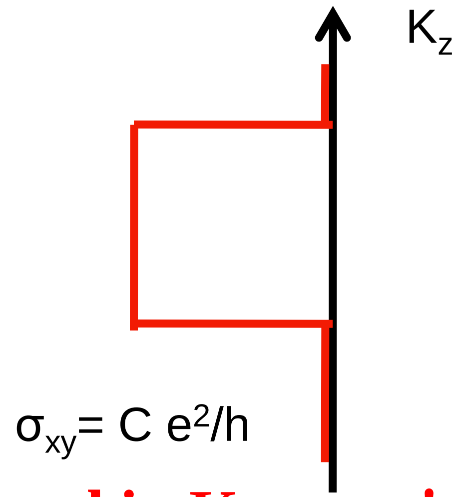
Weak Chern Insulators:



Topological Phase Transition

3. Semimetal: Chern semi-metal?





Stable Weyl nodes separated in K-space!

2x2 Hamiltonian in Bulk (not 4x4):

$$\varepsilon_{\pm} = \pm|\vec{f}(\vec{k})|$$

$$H(\vec{k}) = \vec{f}(\vec{k}) \cdot \vec{\sigma} = \begin{bmatrix} f_z & f_x - if_y \\ f_x + if_y & -f_z \end{bmatrix}$$

Weyl nodes at: $|\vec{f}| = 0$

Berry's connection: $$\vec{A}(\vec{k}) = -i\langle u_{\vec{k}}|\nabla_{\vec{k}}|u_{\vec{k}}\rangle$$

Berry's curvature: $$\vec{\Omega}(\vec{k}) = \nabla_{\vec{k}} \times \vec{A}$$

1. Introduction: Chern semi-metal?

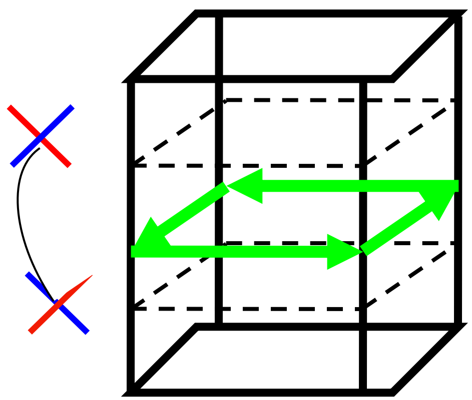
(1) It is topologically unavoidable. (not accidental)

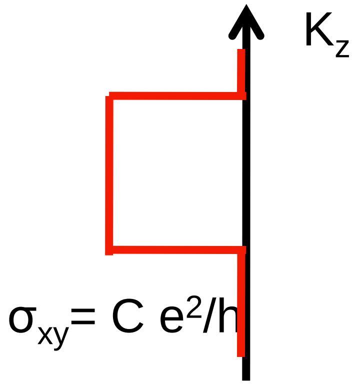
(2) Time-reversal polarization & Magnetic Monopoles in the K-space.

$$\vec{\Omega} = \pm \frac{\vec{f}}{|\vec{f}|^3} \quad \text{around} \quad |\vec{f}| = 0$$

(See, Z. Fang, Science (2003))

(3) Fermi arcs on the side surface.



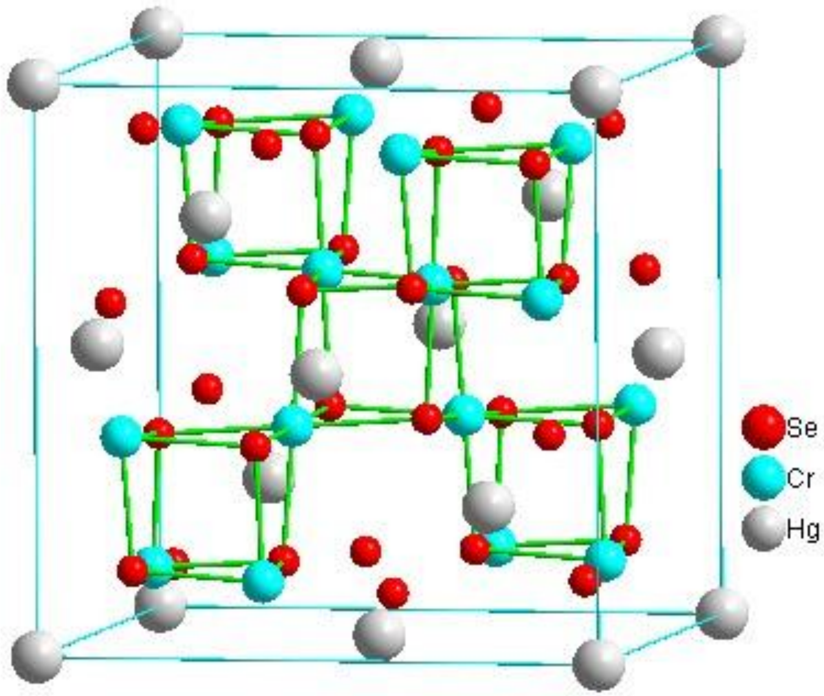


**(See, X. G. Wan & Savaraso, PRB (2011), on AF Pyrochlore iridates
See also, K. Y. Yang, et.al, PRB (2011); A.A.Burkov, et.al, PRL (2011).)**

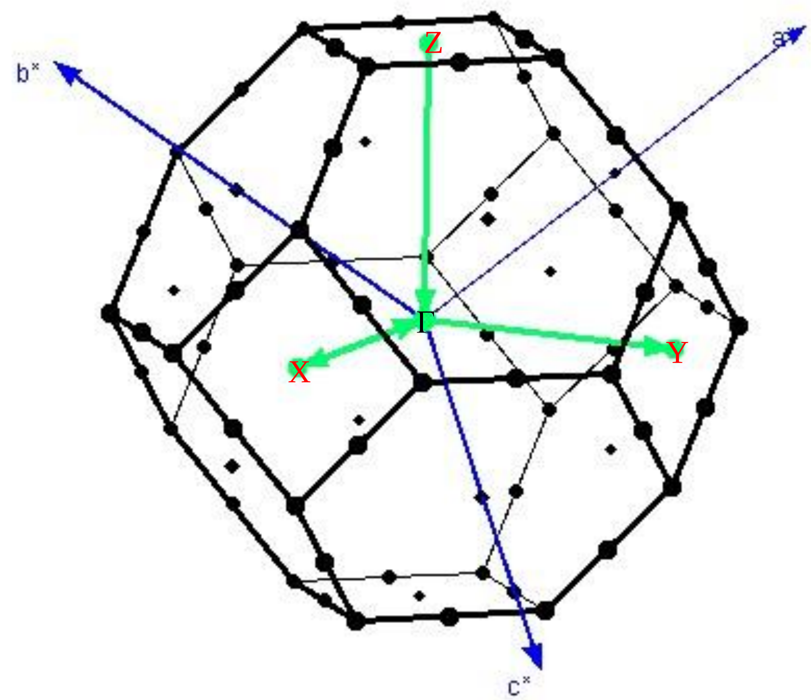
(4) QAHE in quantum well structure.

Crystal structure of $HgCr_2Se_4$

Crystal structure



BZ



HgX sublattice is zinc-blende

Two HgX sublattice are connected by Inversion, like Diamond.

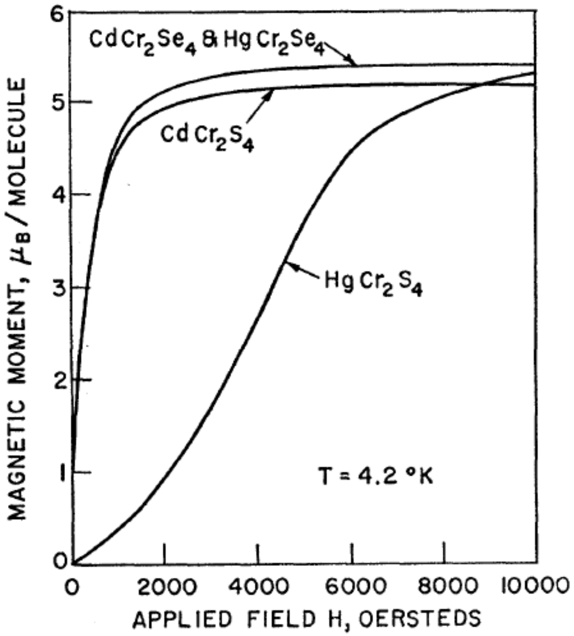
Space group Fd-3m (point group O_h).

Each Cr atom is octahedrally coordinated by 6 nearest Se atoms.

$HgCr_2Se_4$

TABLE II. Magnetic and crystallographic properties of ferromagnetic spinels.

Composition	Lattice parameter Å	u parameter	Magnetic moment (4.2°K) μ_B/molecule	Curie temp. T_c, °K	Curie-Weiss θ, °K	Curie constant C_M	θ/T_c
$CdCr_2S_4$	10.244	0.390	5.15	84.5	152	3.70	1.80
$CdCr_2Se_4$	10.755	0.390	5.62	129.5	204	3.82	1.57
$HgCr_2S_4$	10.237	0.390	5.35	36.0	142	3.62	3.94
$HgCr_2Se_4$	10.753	0.390	5.64	106	200	3.79	1.89



MAGNETIZATION CURVES AT 4.2° K

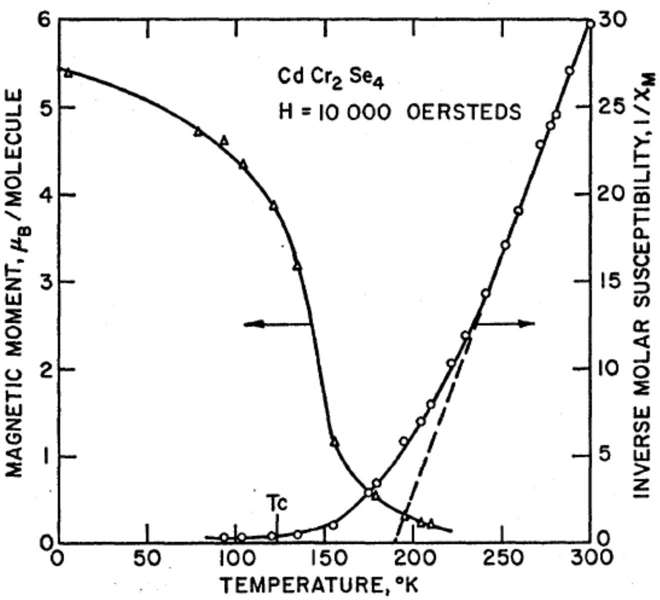
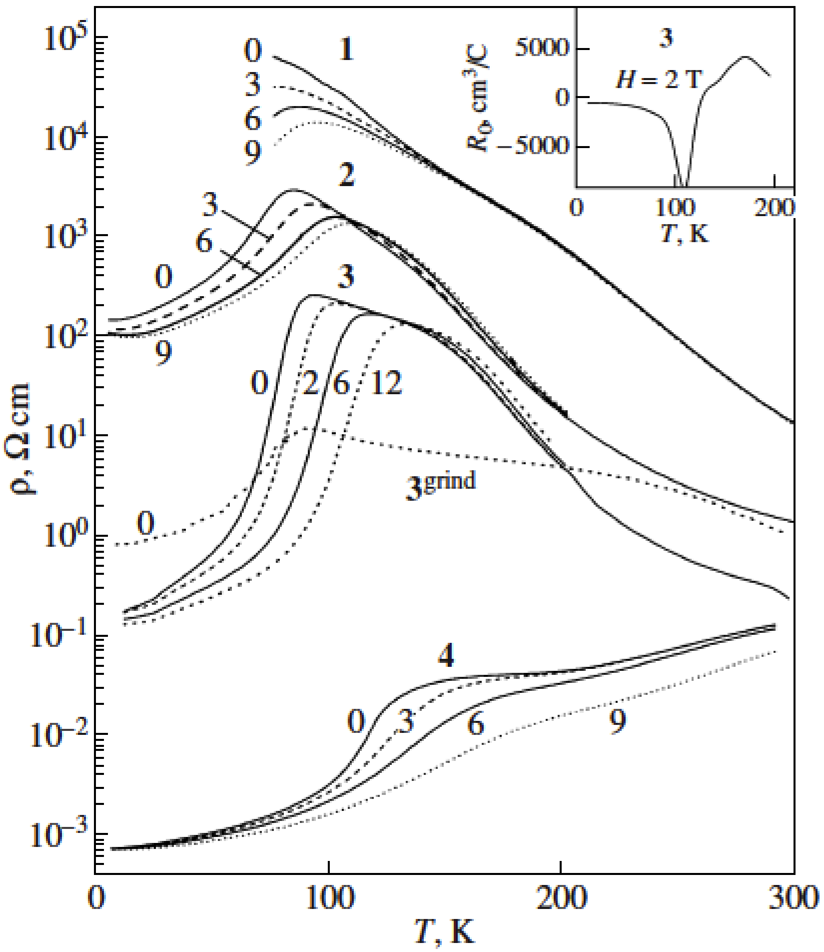


FIG. 3. Magnetic moment and inverse susceptibility as a function of temperature for $CdCr_2Se_4$ in an applied field of 10 000 Oe.

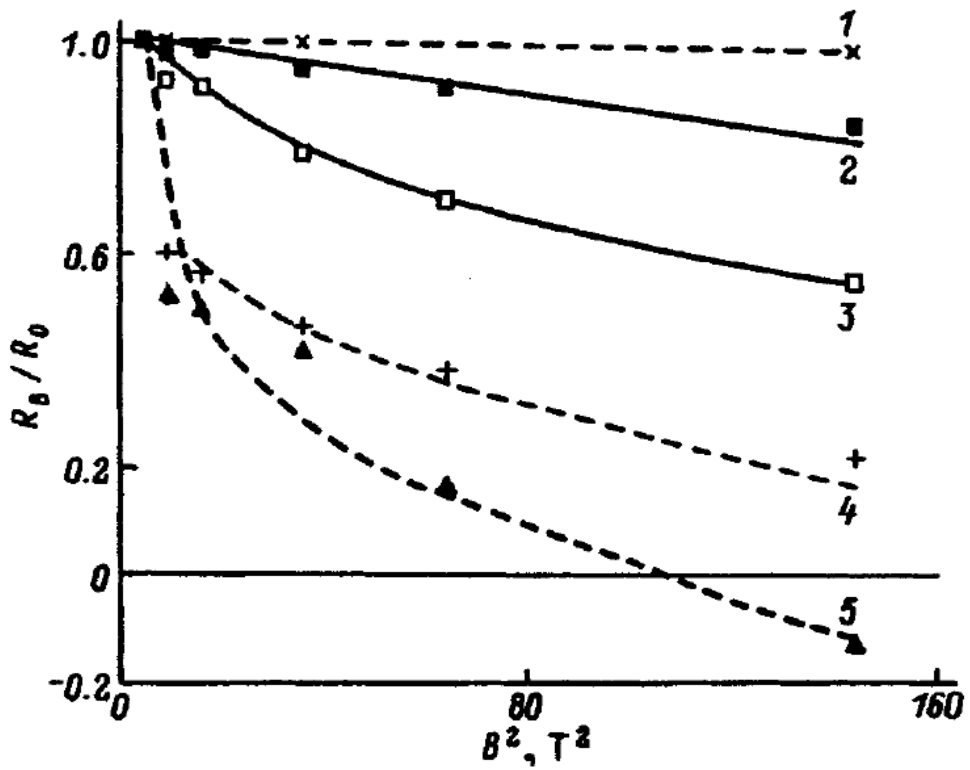
P. K. Baltzer, et.al, PRB (1966)

$HgCr_2Se_4$



Metallic

N. I . Solin, et.al, PRB (2008)



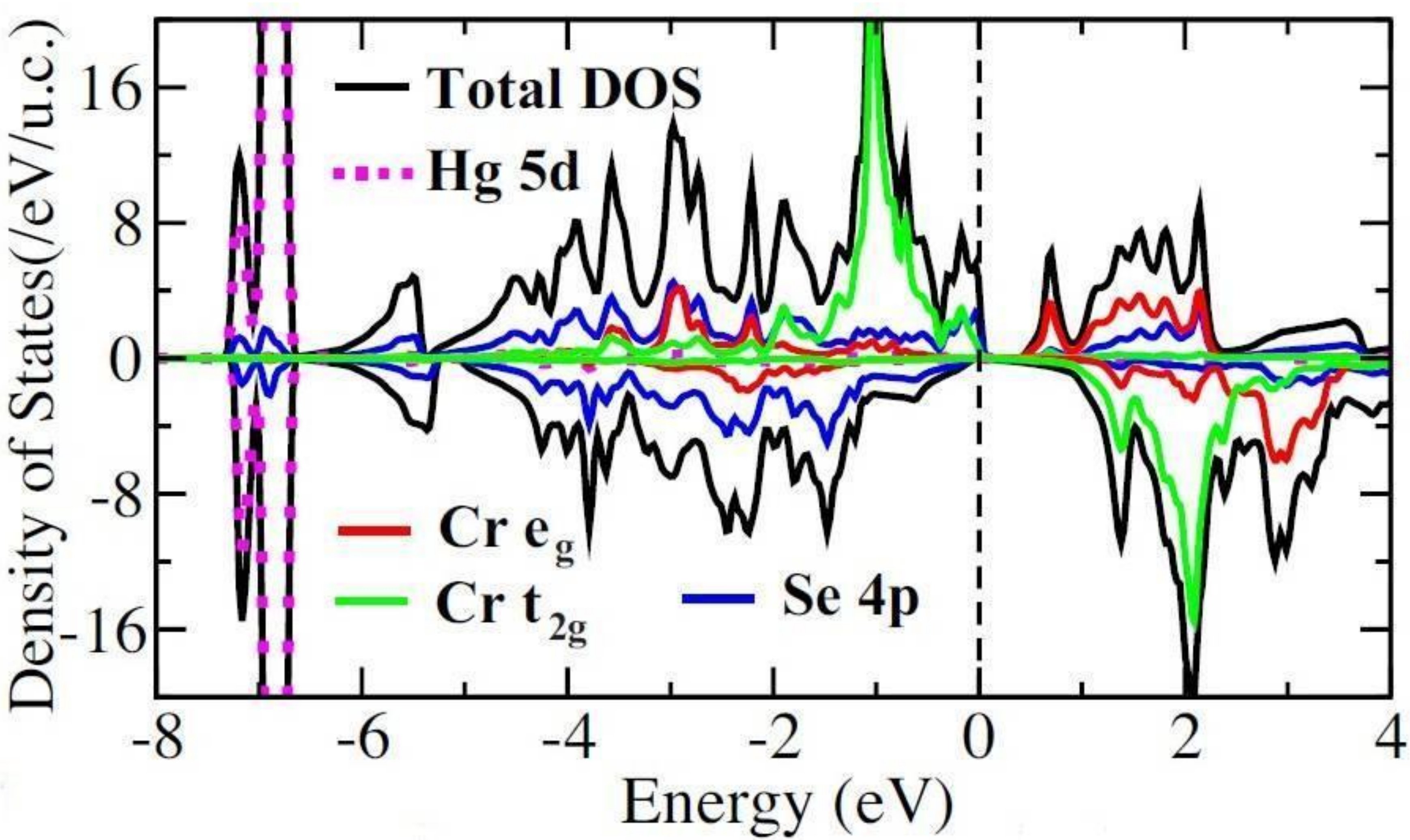
AHE

N. I . Solin, et.al,

Phys. Solid State (1996)

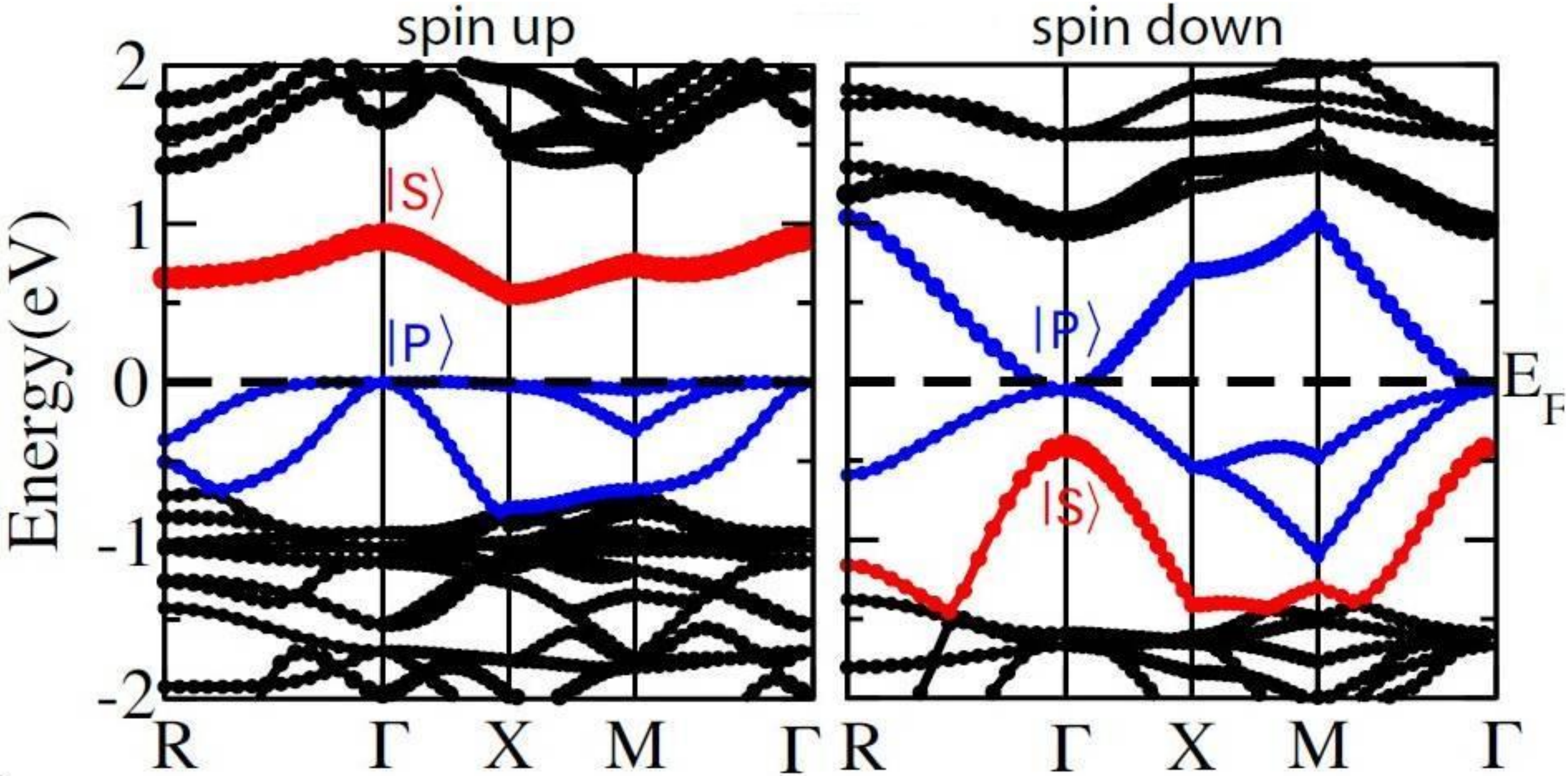
Electronic structure without SOC

DOS

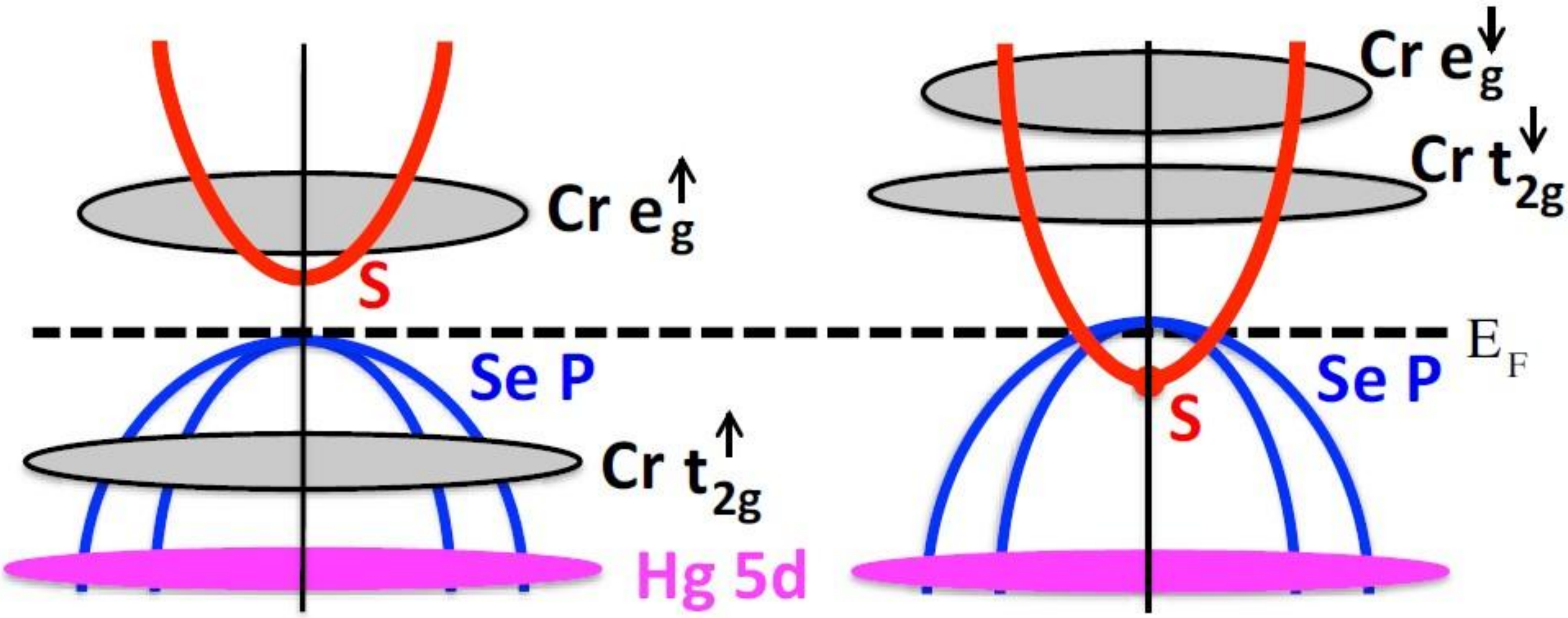


Electronic structure without SOC

Band

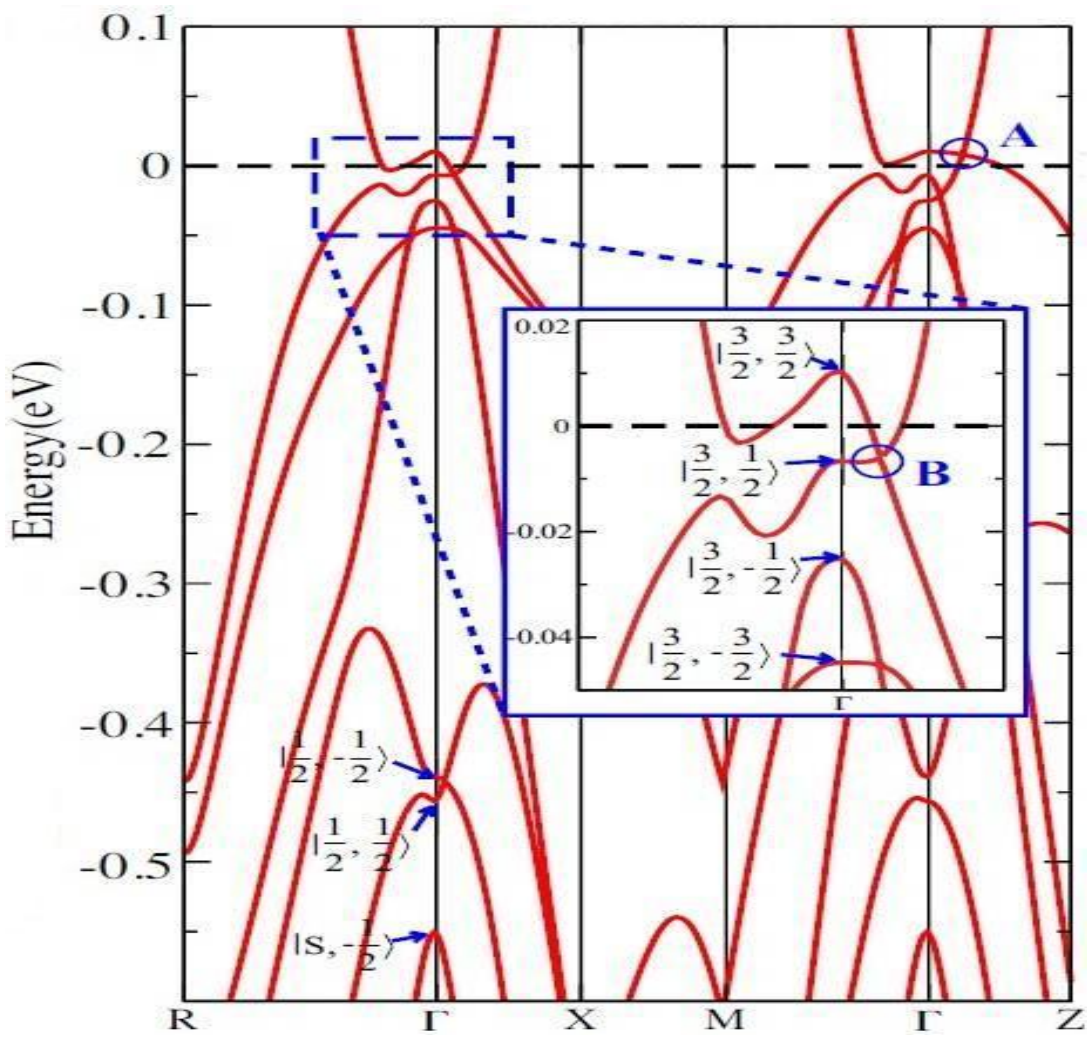


Schematic diagram for the band-inversion



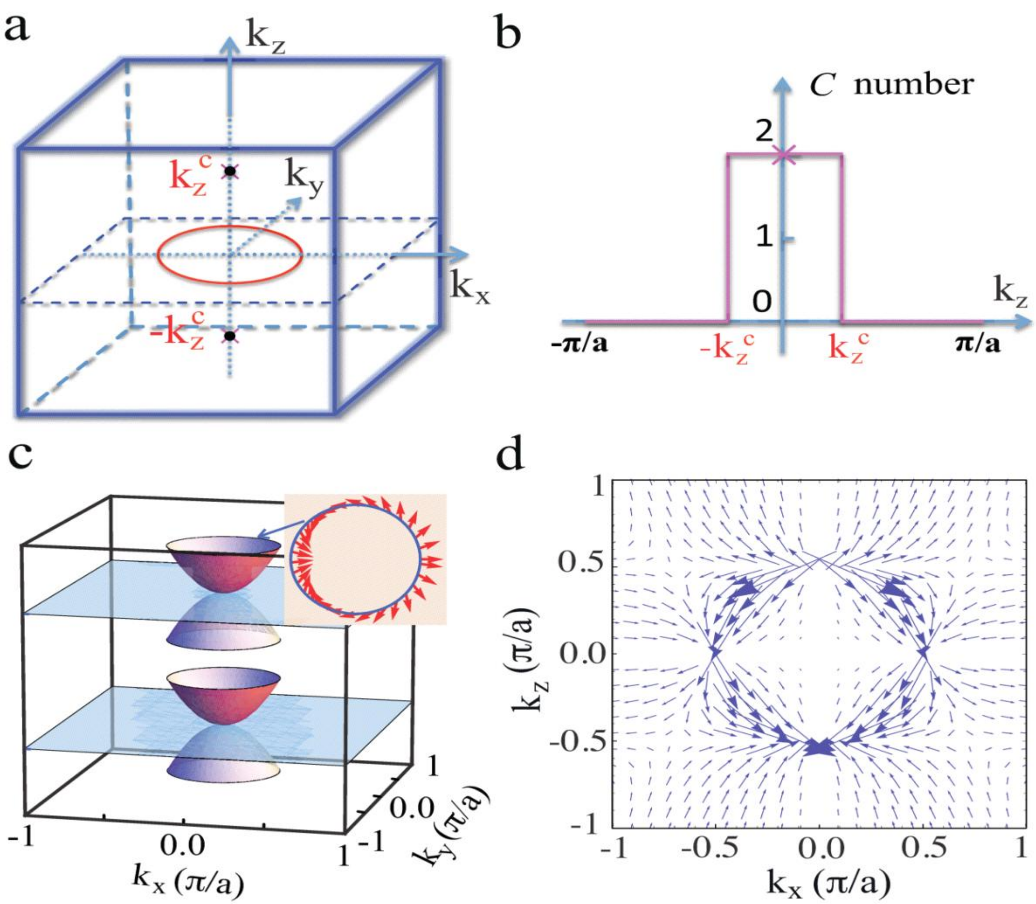
Electronic structure with SOC

low energy band with SOC



Weyl fermions and magnetic monopoles

Due to the presence of $k_{\pm}$ in the off-diagonal element, it is easy to check that Chern number C equals to 2 for the planes with $-k_z^c < k_z < k_z^c$ and $k_z \neq 0$



The in-plane band dispersions near the Weyl nodes $k_z = \pm k_z^c$ are thus quadratic rather than linear, with a phase of 4π for the chiral spin texture. The two Weyl nodes form a single pair of magnetic monopoles carrying gauge flux in k-space.

8-band model for HgCr2Se4

2-band effective model

Two basis: |3/2, 3/2> , |S, -1/2> with band-inversion

$$H_{eff} = \begin{bmatrix} M & Dk_z k_-^2 \\ Dk_z k_+^2 & -M \end{bmatrix}$$

Here $k_\pm = k_x \pm i k_y$, and $M = M_0 - \beta k^2$ is the mass term expanded to the second order, with parameters $M_0 > 0$ and $\beta > 0$ to ensure band inversion.

$$\mathrm{E}(\boldsymbol{k}) = \pm\sqrt{\boldsymbol{M}^2 + \boldsymbol{D}^2 \boldsymbol{k}_z^{\ 2}(\boldsymbol{k}_x^{\ 2} + \boldsymbol{k}_y^{\ 2})}$$

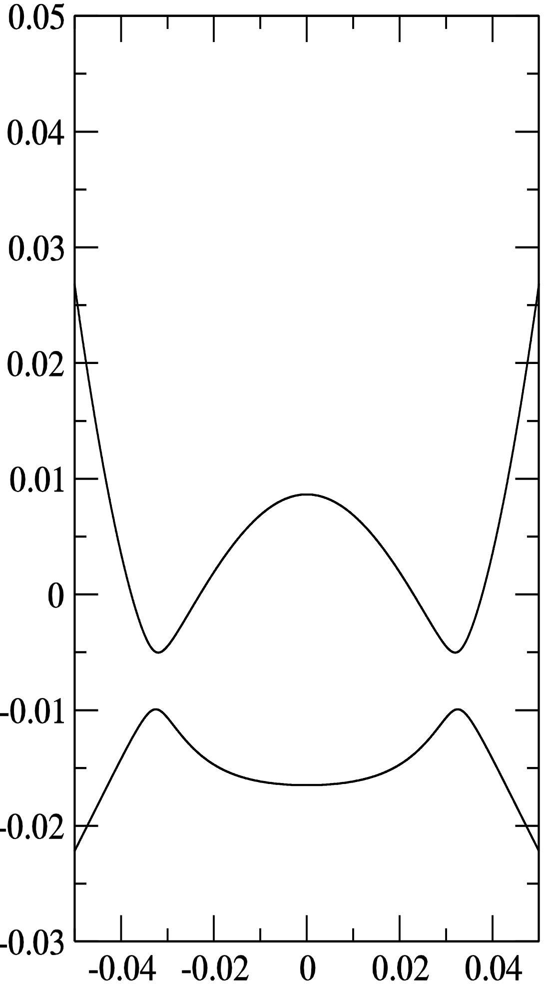
two gapless solutions:

$$\boldsymbol{k}_z = \pm \boldsymbol{k}_z^{\ c} = \pm\sqrt{\boldsymbol{M}_0 / \beta}$$

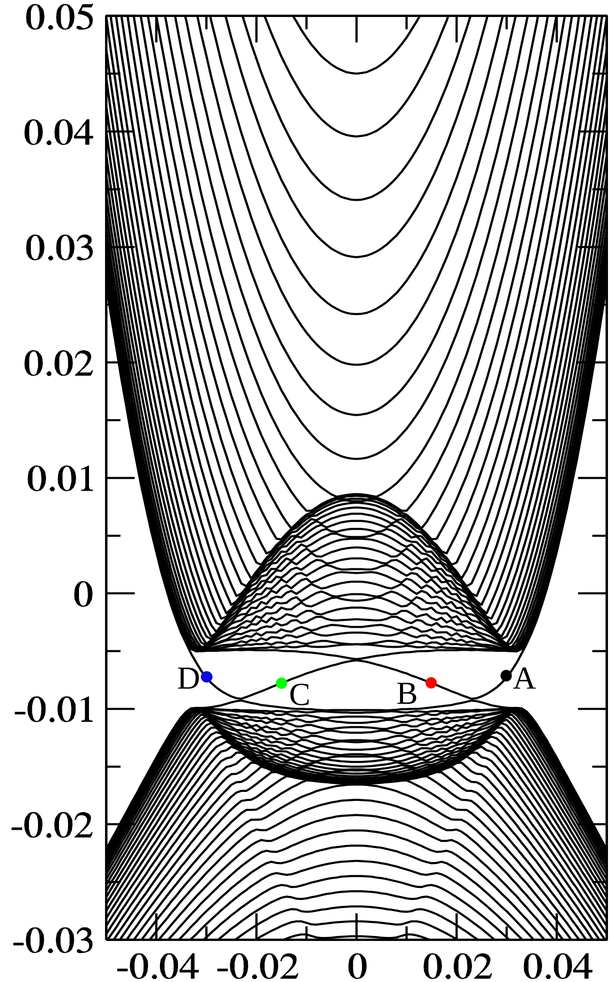
$$\boldsymbol{k}_x^{\ 2} + \boldsymbol{k}_y^{\ 2} = \boldsymbol{M}_0 / \beta$$

Edge states and fermi arcs on surface

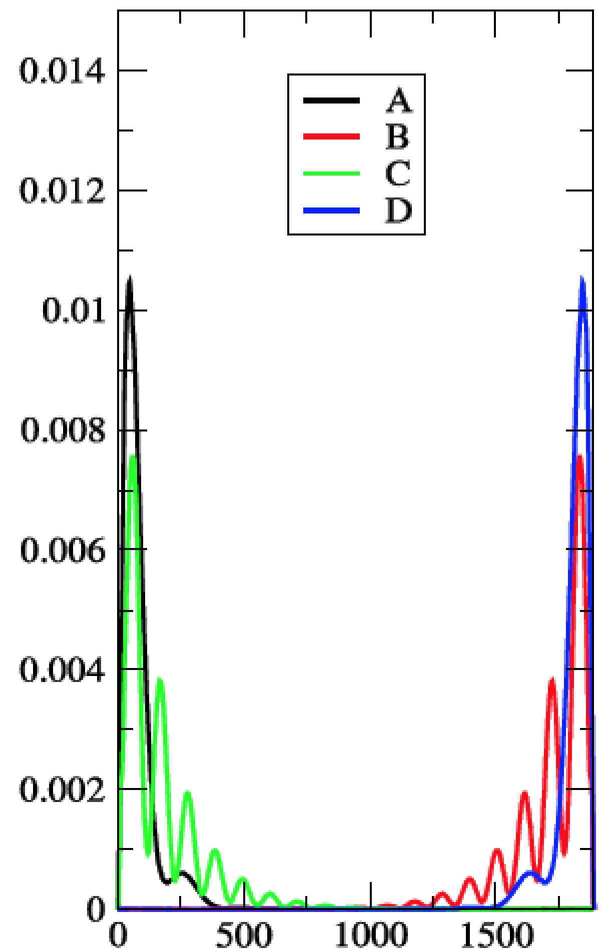
Edge state in $k_z=0.06\pi$ plane



Band of bulk



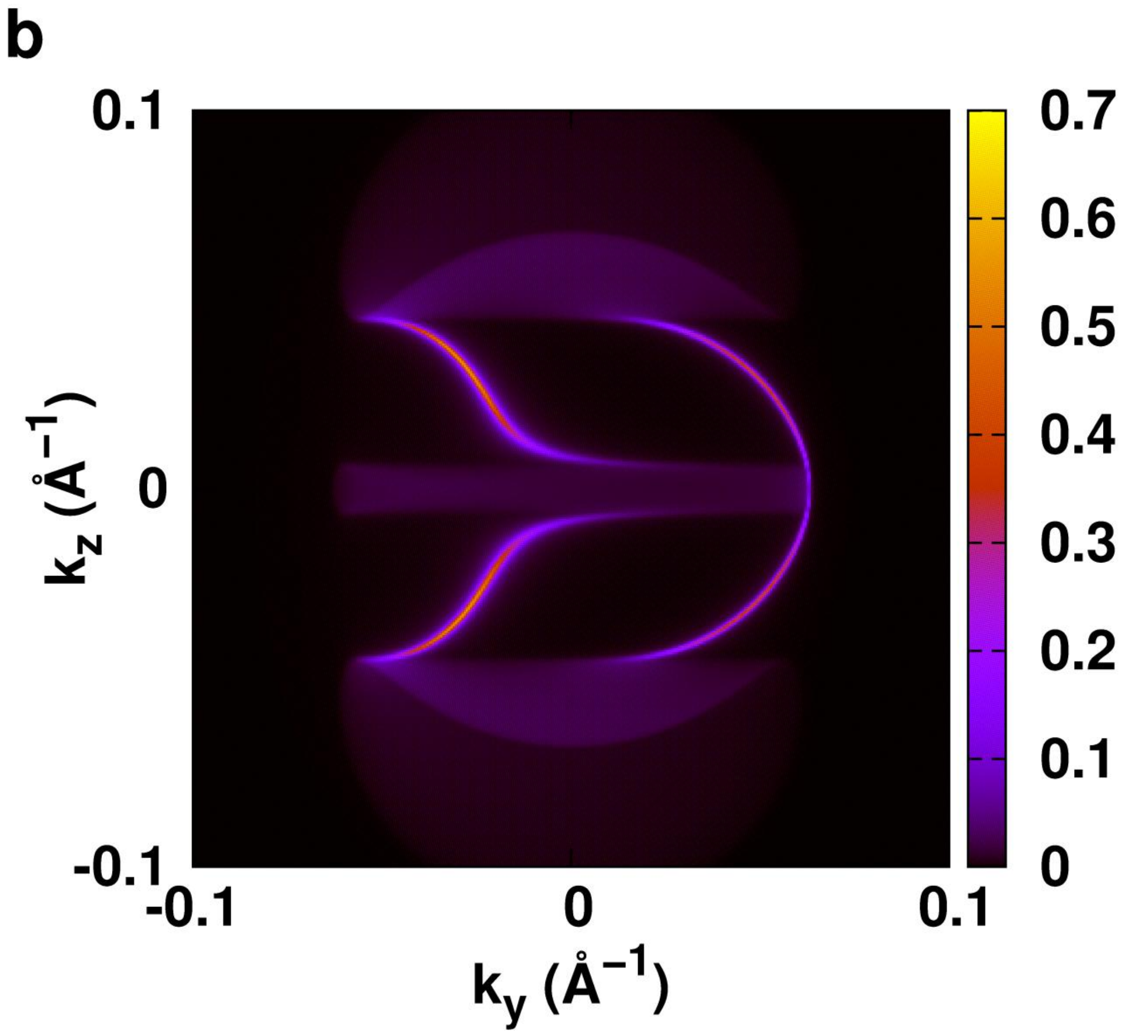
Edge state



Distribution along x

Edge states and fermi arcs on surface

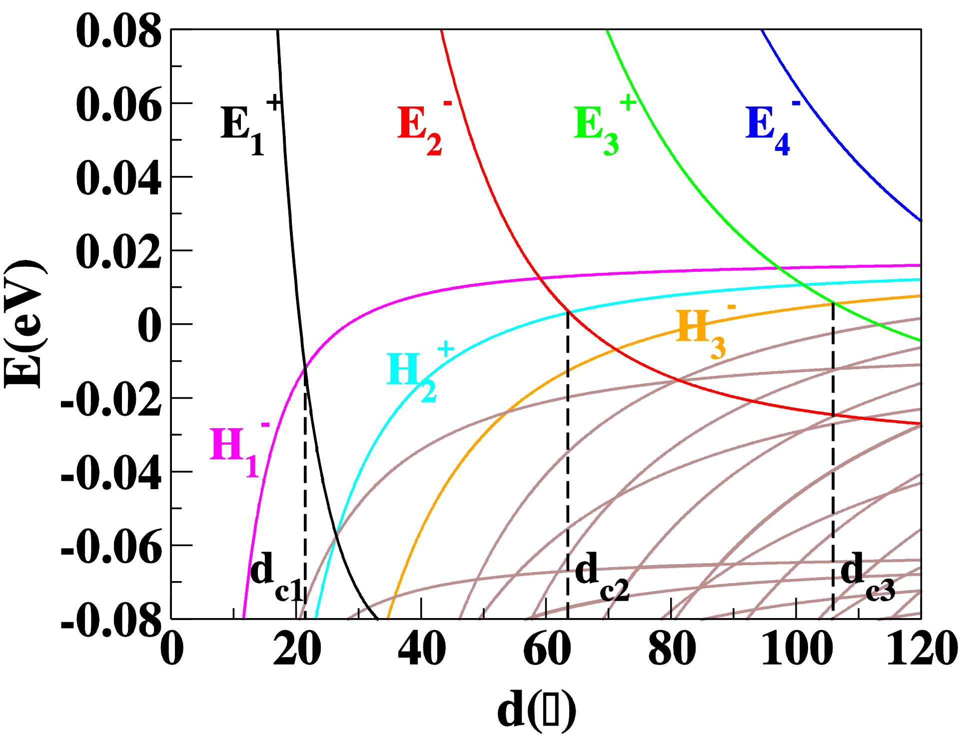
Fermi arcs for the (k_y, k_z) side surface

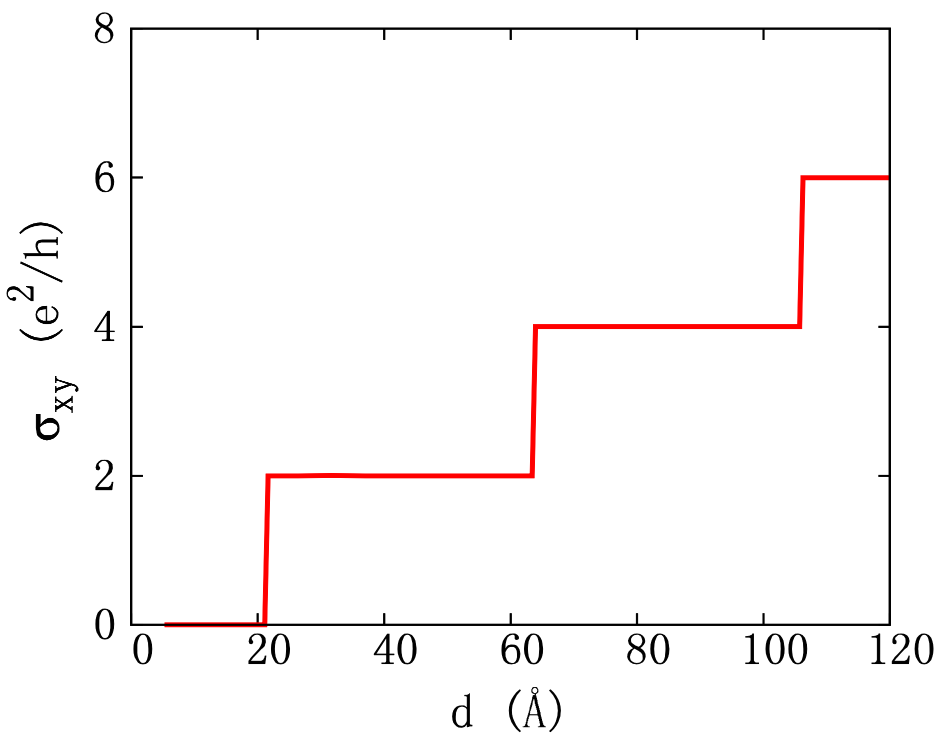


G. Xu, et.al, PRL 107, 186806 (2011)

QAHE in the quantum well structure

If we consider the open boundary condition along z direction, and replace k_z by $-i\hbar\partial_z$,we can evaluate the Hall conductance in the quantum well structure.





Energy gap at Γ vs. d **Hall conductance vs. d**

Our Early Proposal: Bi2Se3-doped by Cr, Fe. Science (2010)

Summary:

✓1. Strong 3D TIs in Bi_2Se_3, Bi_2Te_3, Sb_2Te_3.

✓2. Topological aspect and Quantum MR in Ag_2Te.

✓3. Superconductivity in Bi_2Te_3 under pressure.

✓4. Proximity effect and Majorana at $NaCoO_2$ /SC interface.

✓5. QAHE in Bi_2Se_3 and Bi_2Te_3 doped with Cr or Fe.

✓6. $HgCr_2Se_4$ is a topological Chern semi-metal with a single pair of magnetic monopoles in the bulk, and Fermi arcs on the surface.

✓7. Possible QAHE in $HgCr_2Se_4$ quantum well structure.

Thank you!