拓扑绝缘体与拓扑半金属

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1. 简介：拓扑有序态

有序态是凝聚态物理研究的基本内涵之一

例如：磁有序态、电荷有序态、超导态等

局域有序态：

对称性破缺导致有序态
（朗道对称性破缺理论）

1.物态可以用局域序参量描写
如：铁磁态的磁化强度 M(r)

2.相变伴随着对称性破缺
如：M(r)的出现破坏了
旋转对称性

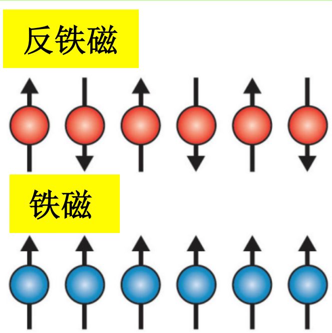
宏观有序态：

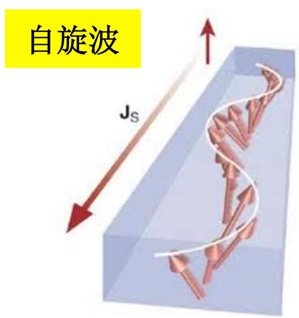
拓扑有序态
（量子物理与几何的完美结合）

1. 具有拓扑性质的“量子态”

2. 不能用局域序参量描写，而要用全局拓扑不变量描写

3. 相变过程并不伴随对称性破缺





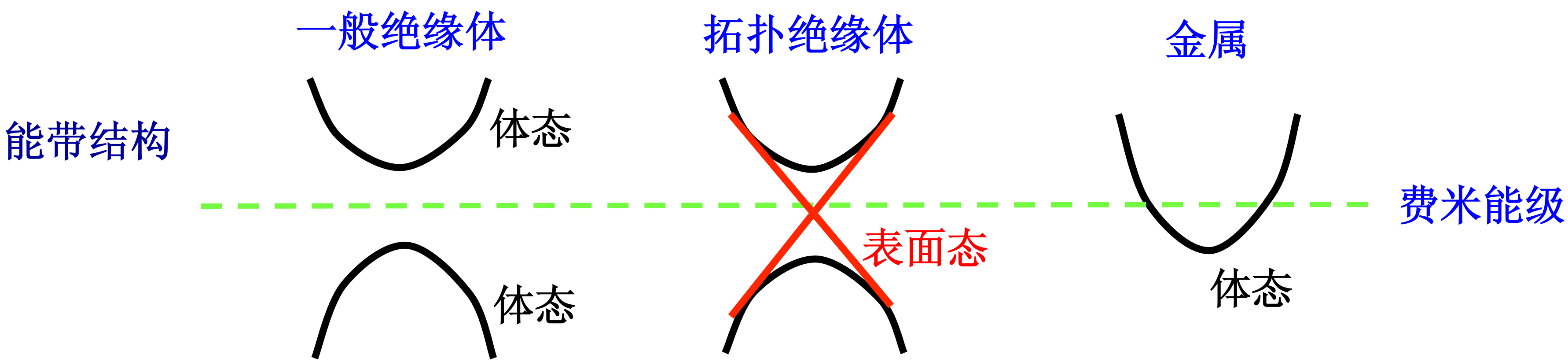
拓扑“0”

拓扑“1”

1. 简介：拓扑绝缘体简介

拓扑绝缘体：一种全新的拓扑有序态：受时间反演性保护

要考虑 相对论+量子力学



理论模型：

1. C. L. Kane，PRL (2005)
2. S. C. Zhang，PRL (2006)

材料实现：

1. 二维材料： L. Molenkamp, Science (2007)
2. 三维材料： 方忠 等，Nature Phys. (2009) (Bi_2Te_3, Bi_2Se_3, Sb_2Te_3)

与一般表面态区别：

无论如何切样品，表面态总是存在

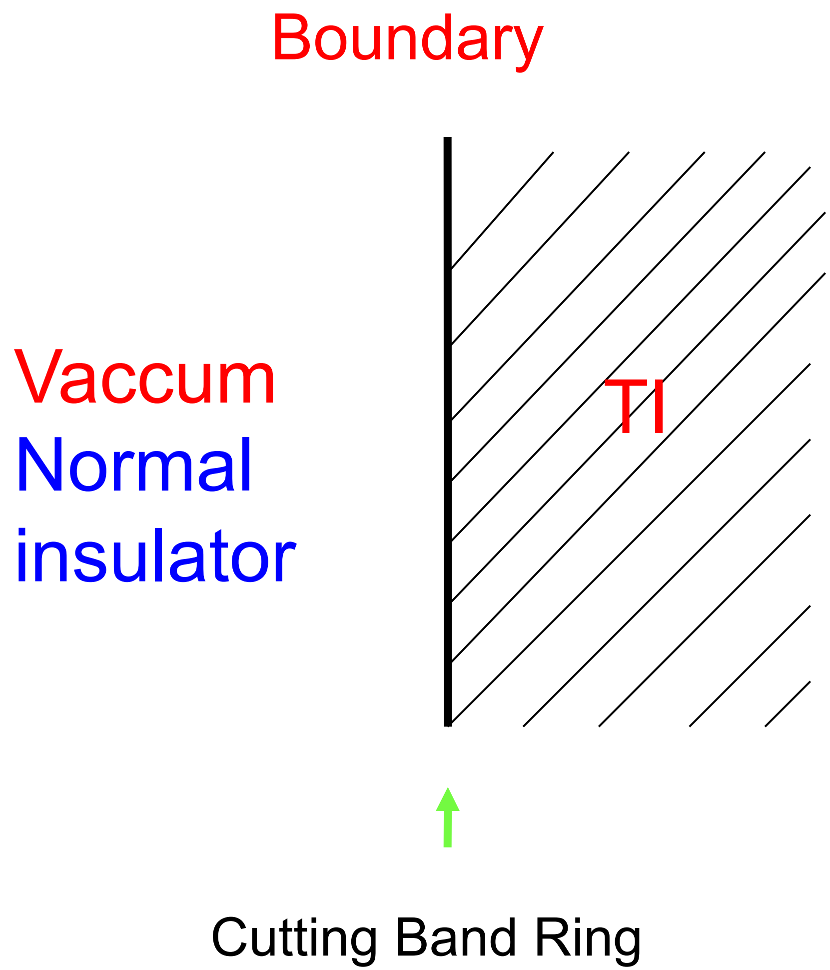
1．简介：Why edge states？

"Band twist"

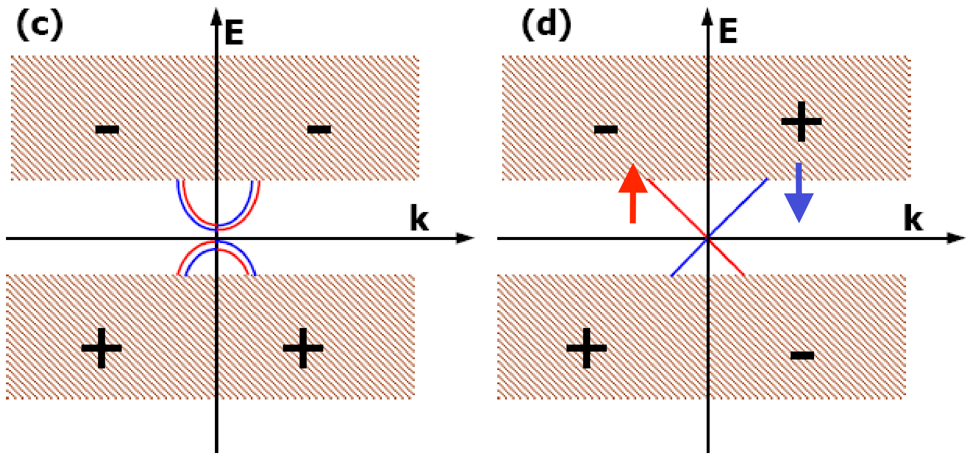
Defined by the Z2 number
(or parity for inversion system)

Ref:

[1] Kane & Mele, PRL (2005).
[2] Fu, Kane, Mele, PRL (2007)
[3] Fu, Kane, PRB (2007).



1．简介：Different Surface states



Surface State
ordinary Insulator

Surface State
Topological Insulator

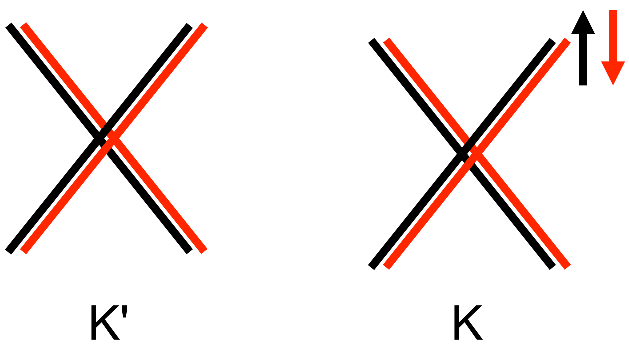
Topological Insulators:

1. Insulating bulk
2. Conducting surface
3. Defined by the Z2 quantum number
4. Surface state is protected by T reversal symmetry
5. Robust against none-M disorders

"能带 twist"

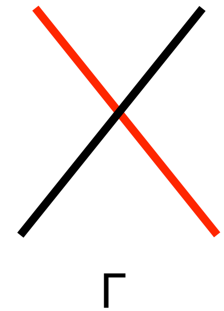
1. 简介：Surface state vs Graphene

Graphene



（1） psudo-spin
（2） Klien Paradox
（3） linear n~E，
linear σ~E，
linear m~E
（4） Localization？
（5） Universal σ？
（6） ……

Surface state of TI



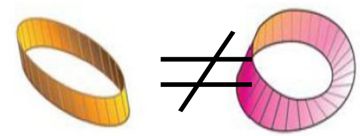
（1） 1/4 of Graphene，
spin splitting，
T-invariant
（2） 2DEG without mass
（3） Klien Paradox
（4） linear n~E，
linear σ~E，
linear m~E
（5） QHE？ Localization？
（6） Multi-ferroic？

1. 简介：拓扑有序态 → 新奇量子现象

拓扑有序量子态的优点：

1. “0” 与 “1” 严格区分，

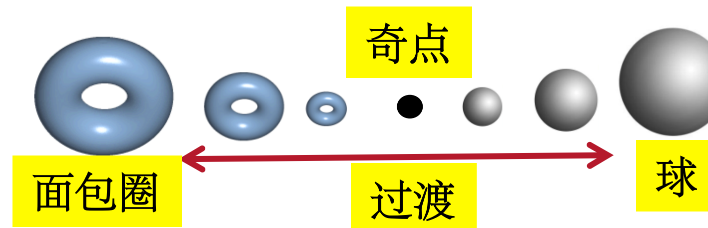
无微扰过程，不怕干扰、噪声



除非破坏性剪断

2. 与“奇点”密切相关，

在边界上会有特殊量子态



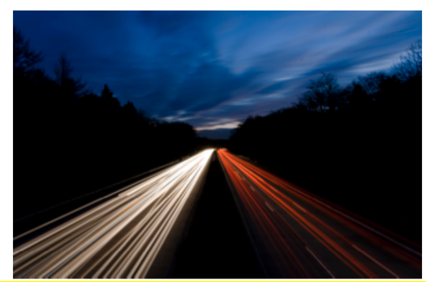
信息高速公路：极低电阻、极低能耗

普通态

鱼目混杂，杂乱无章

遇到杂质，会被散射

拓扑有序态



各行其道，永不混杂

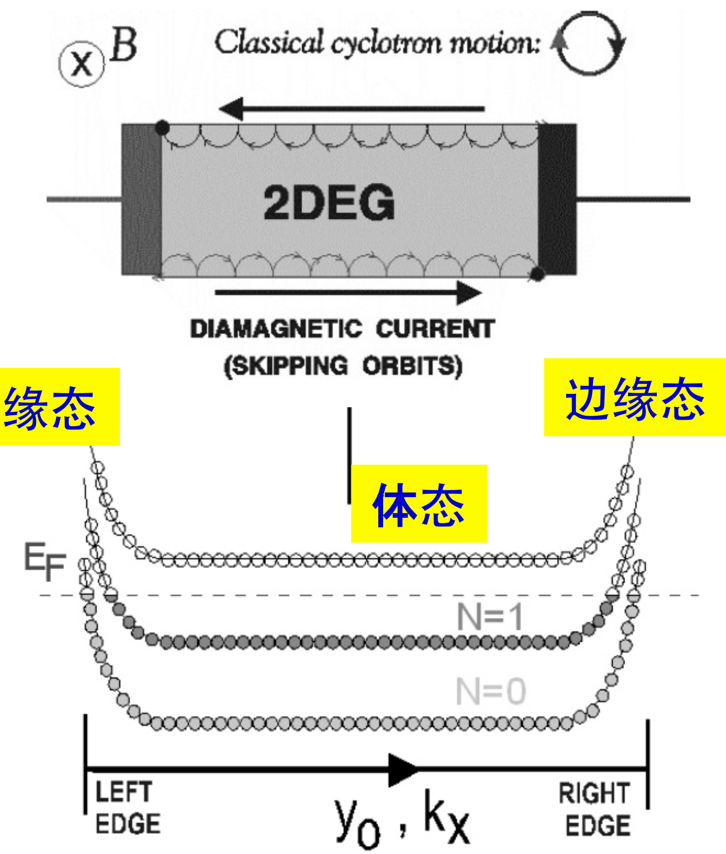
遇到杂质，自动绕行

1.简介：量子霍尔效应（IQHE）

最早认识的拓扑有序态是----量子霍尔效应

中间绝缘边界导电

朗道能级



$$\Psi_{N,y_0} \propto e^{ik_x x}\cdot\Phi_N(y-y_0),\quad y_0=\frac{\hbar k_x}{eB}$$

量子Hall效应

1. **Very Stable**
2. **No backscattering**

   (Edge state can not localize)

问题:

1. 需要强磁场、极低温
2. 破坏了时间反演对称性
3. 只存在于二维系统
4. 不是拓扑绝缘体

   （需要借助于外磁场）

1. 简介：拓扑绝缘体简介

重要性：

（1）基础科学发展：**全新的物理概念、现象、效应**

1. 新奇量子效应
2. 基本物理常数的确定

（2）下一代电子技术：**革新性的进步**

1. 准零能耗电子器件：无电阻的“理想导线”
2. “电”与“磁”交叉调控，巨大响应
3. 能源器件：热电效应、 非线性光学
4. 拓扑催化
5. 核燃料问题：高熔点、高热导

（3）国际发展的趋势：**是当前国际发展的前沿**

1. 欧美已投入巨资
2. 日本正在启动

1. 简介： Family of TIs?

2D		3D	
T-broken	T-invariant	T-invariant	T-Broken

QHE

QAHE

QSHE

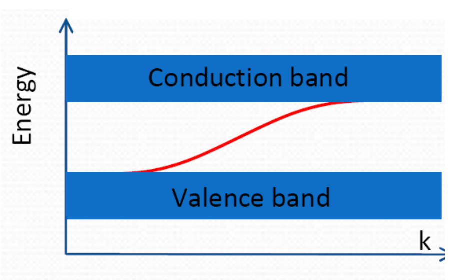
Kondo

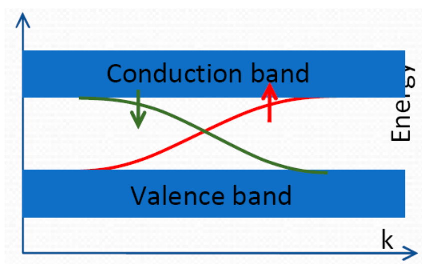
Topological Band Insulator

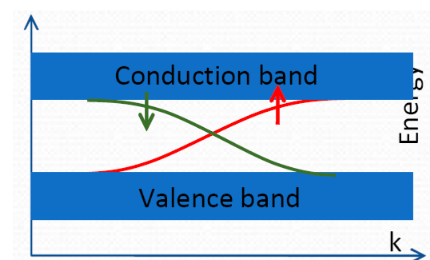
Anderson

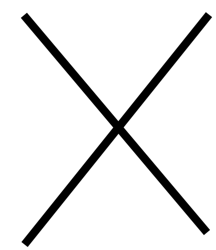
Mott ......

Semi-metal









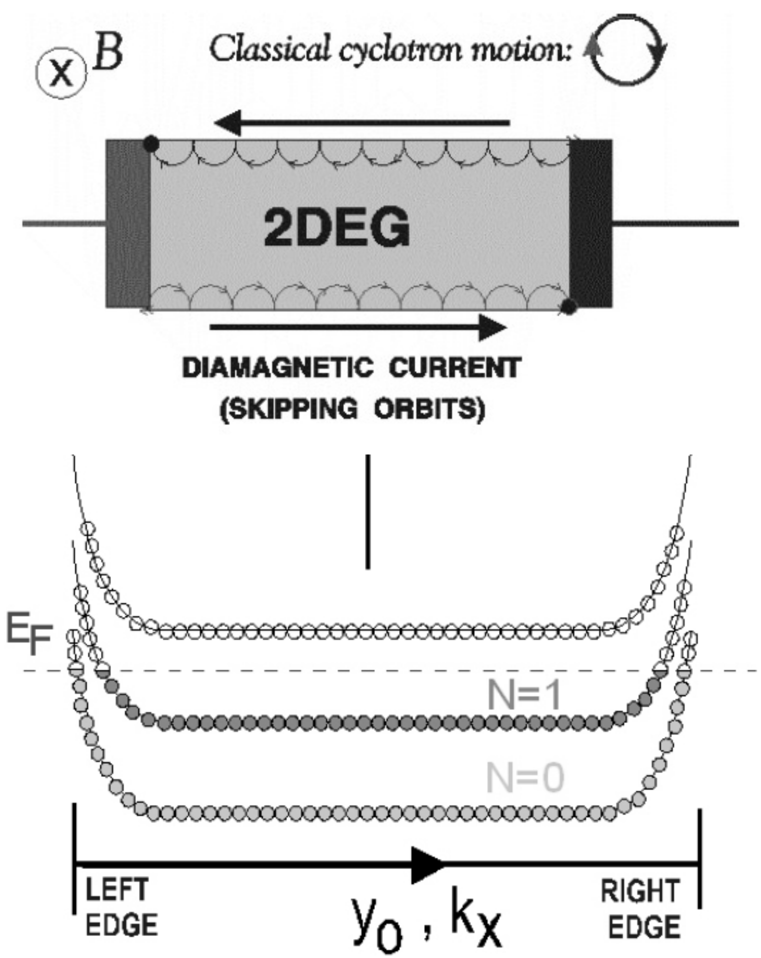
Edge States
TKNN
Chern number

Z2

Surface States

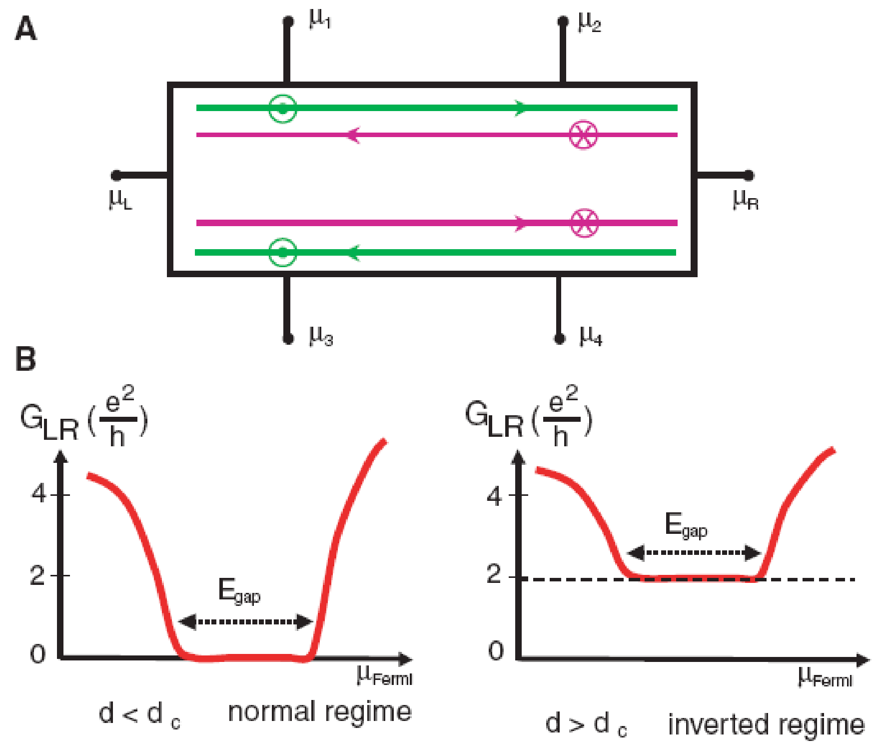
Femi points (in bulk)

2. 拓扑绝缘体：T-broken vs T-Invariant



$$\Psi_{N,y_0} \propto e^{ik_x x} \cdot \Phi_N(y-y_0), \quad y_0 = \frac{\hbar k_x}{eB}$$

QHE



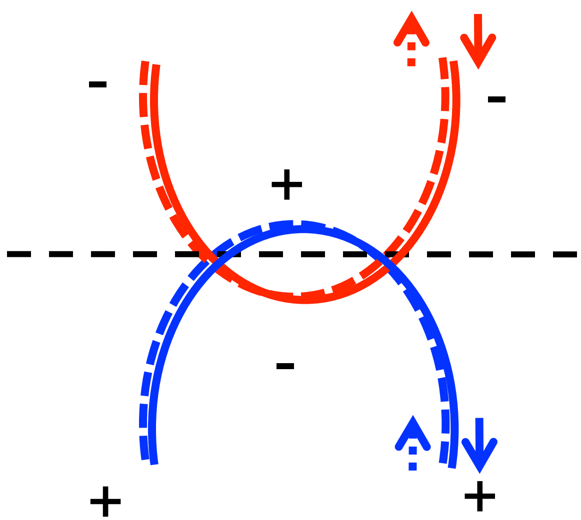
QSHE in HgTe/CdTe

(S. C. Zhang, SCIENCE 2006)

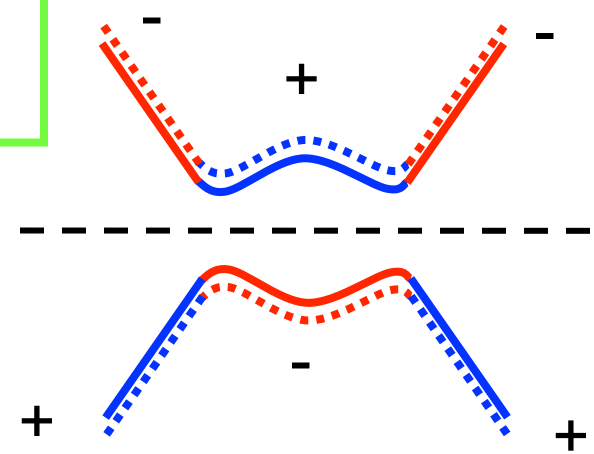
2. 拓扑绝缘体：Materials.

Guidelines:

1. Semiconductor with inverted band structure
2. Strong SOC



Gap opening due to SOC



困难：Real materials for 3D TI?

"twisted band"

2. 拓扑绝缘体：Bi2Te3，Bi2Se3，Sb2Te3

Predictions for Bi2Te3 family: Basic Properties

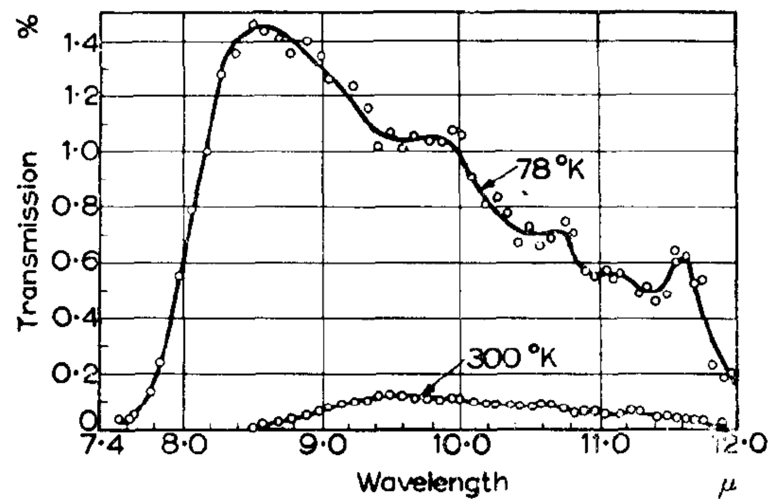
1. Found 70 years ago.
   Naturwissenschaften,
   27, 133 (1939)

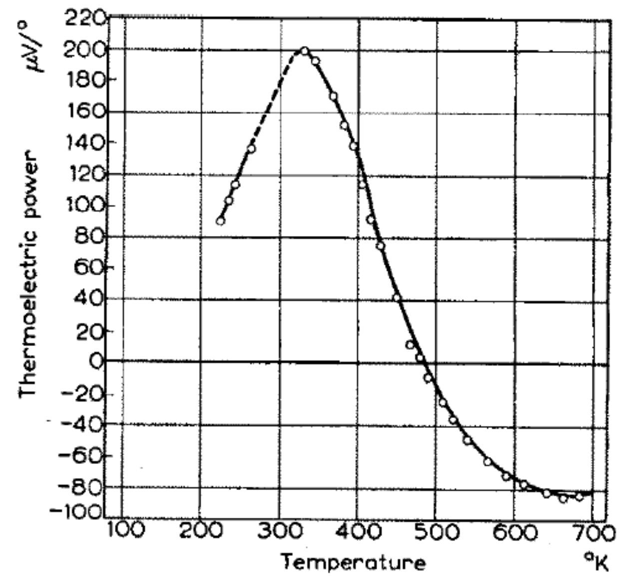
2. Semi-conductor.
   Optical Gap ~ 0.2 eV
   J. Phys. Chem. Solids, 2, 240 (1957)

3. One of the best thermoelectic materials.
   ZT ~ 1 at room T

4. Easy to be synthesized

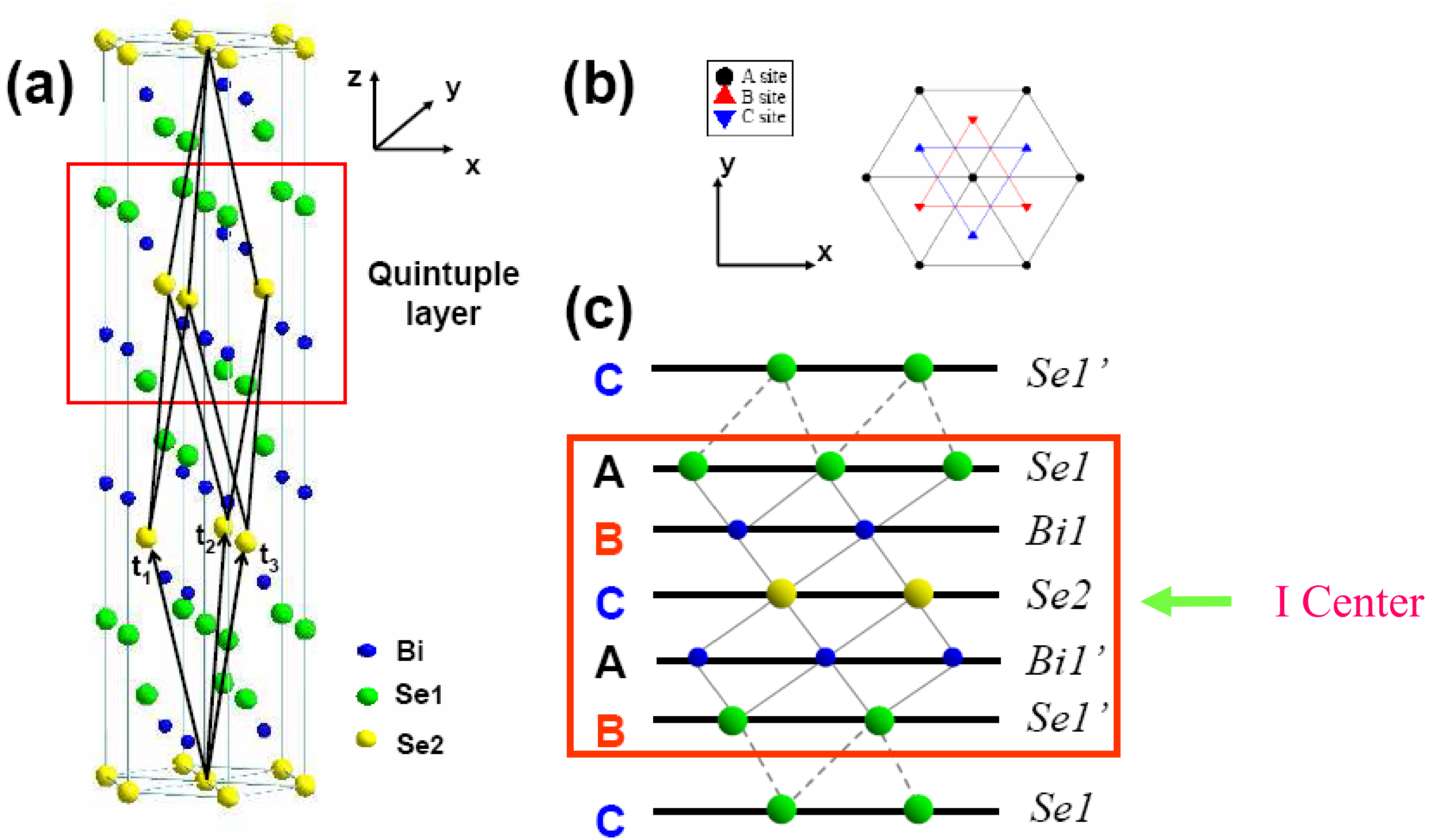
5. Whole Family:
   Bi2Te3, Sb2Te3
   Bi2Se3, Sb2Se3



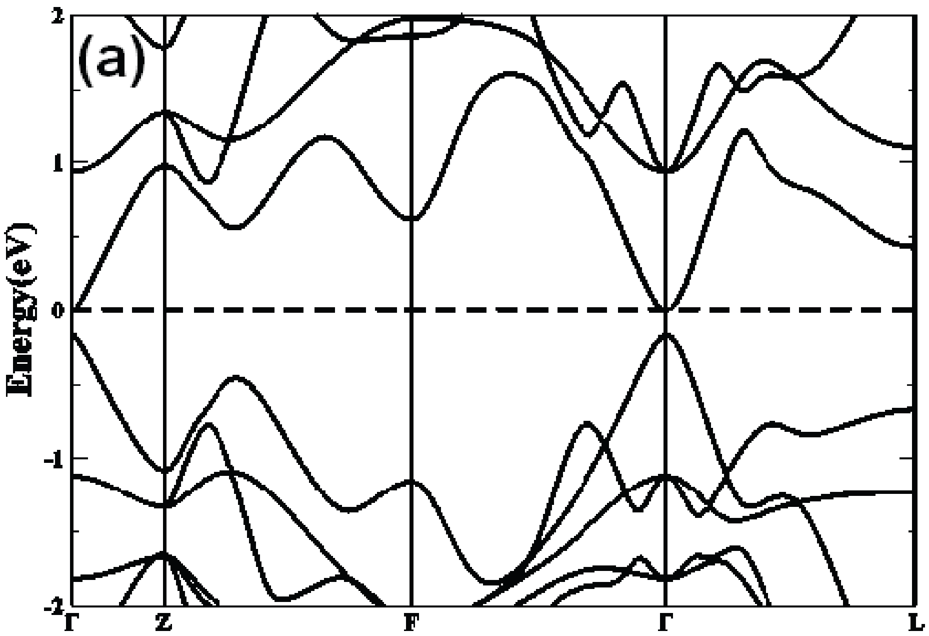


2. 拓扑绝缘体：Bi2Te3，Bi2Se3，Sb2Te3

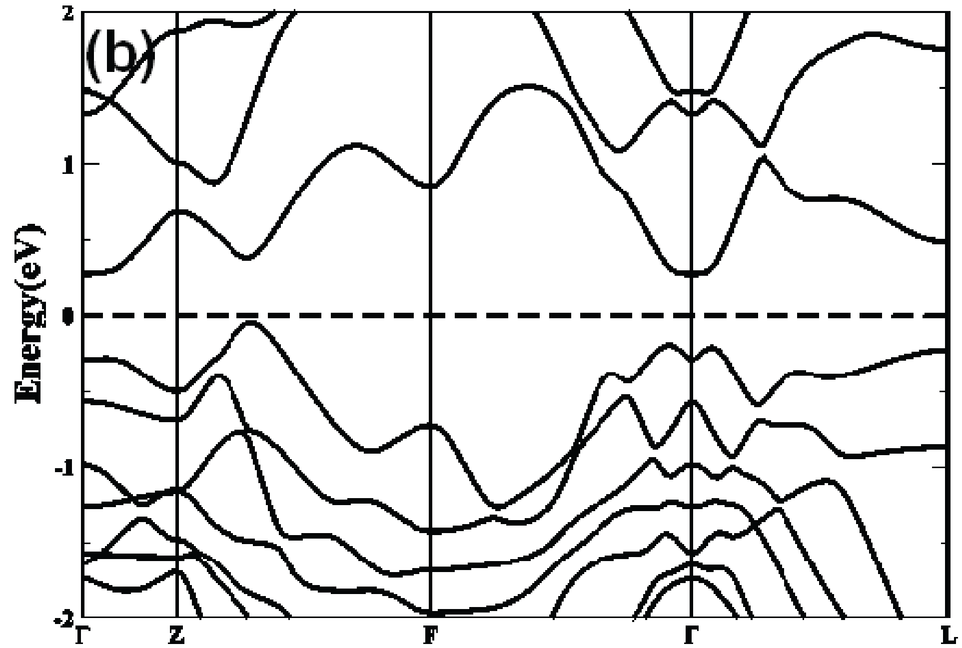
Crystal Structure D_{3d}^5 $(R\bar{3}m)$



Band Structure Bi2Se3

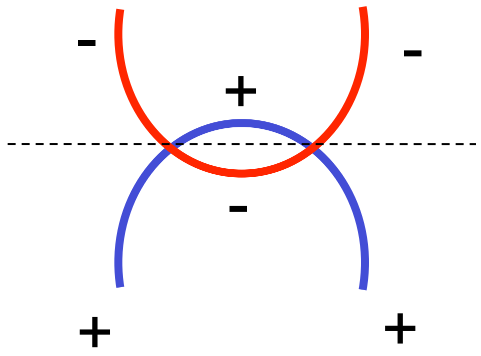


Without SOC



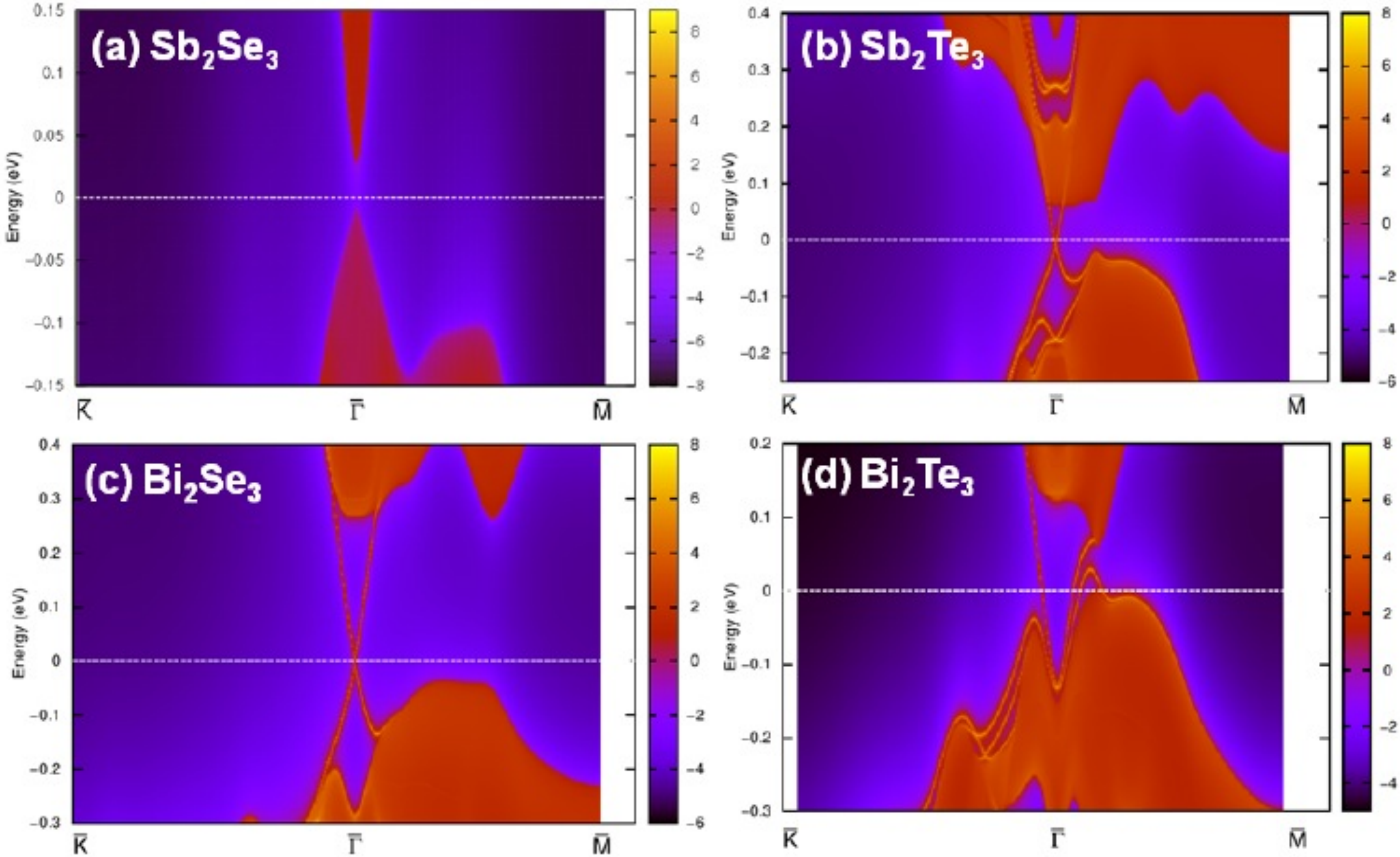
With SOC

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

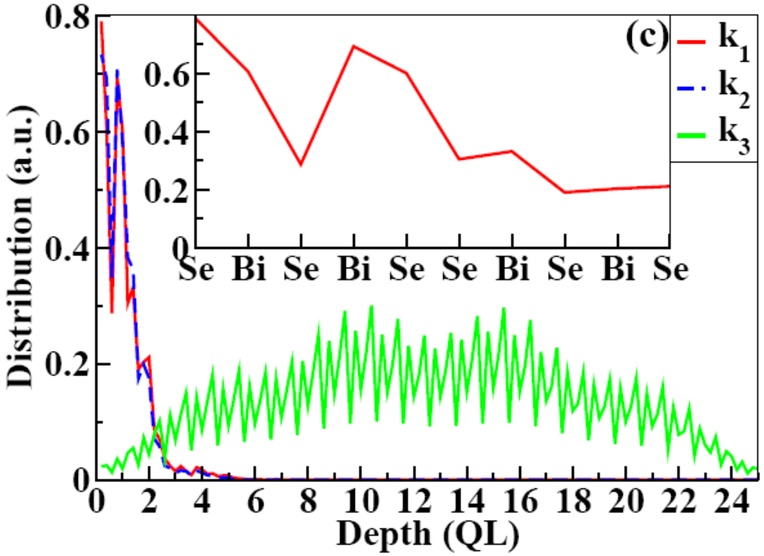


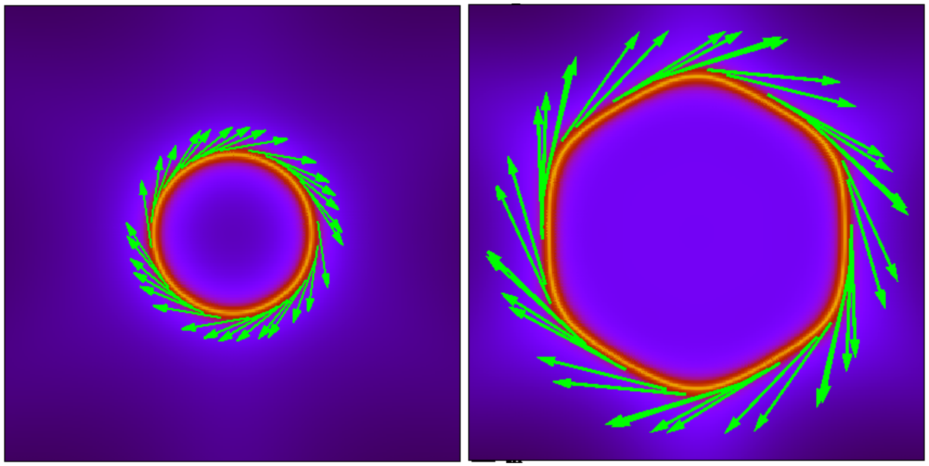
H. J. Zhang, et.al., Nature Phys. (2009)

2. Materials: Bi_2Te_3, Bi_2Se_3, Sb_2Te_3

Penetration Depth
of Surface state, 2nm

Chiral Spin texture

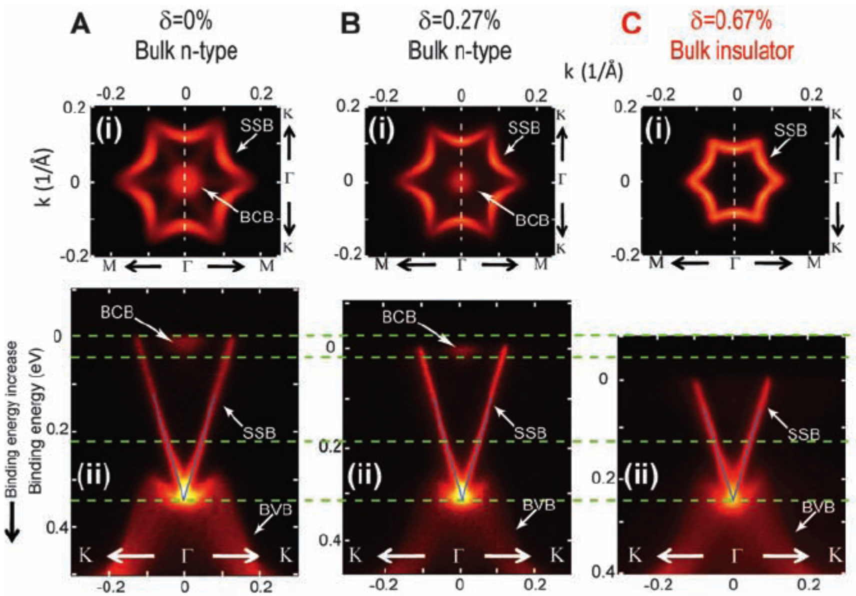


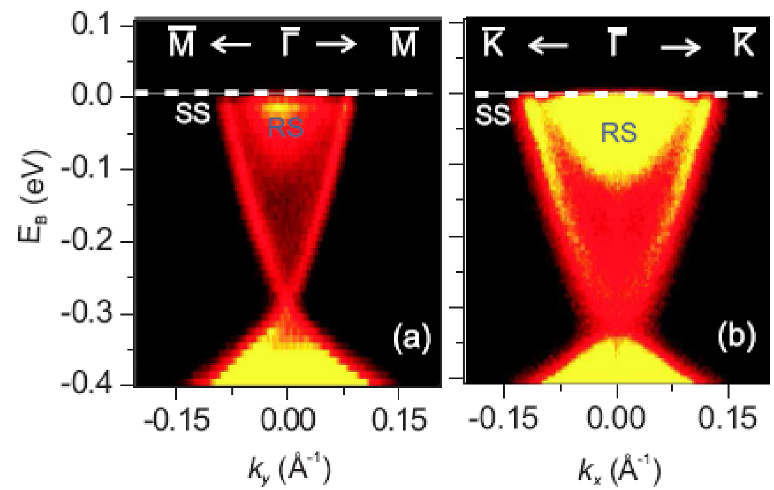


W. Zhang, et.al., New J. Phys, **12**, 065013 (2010)

2. TI Materials: Exp. evidence

ARPES



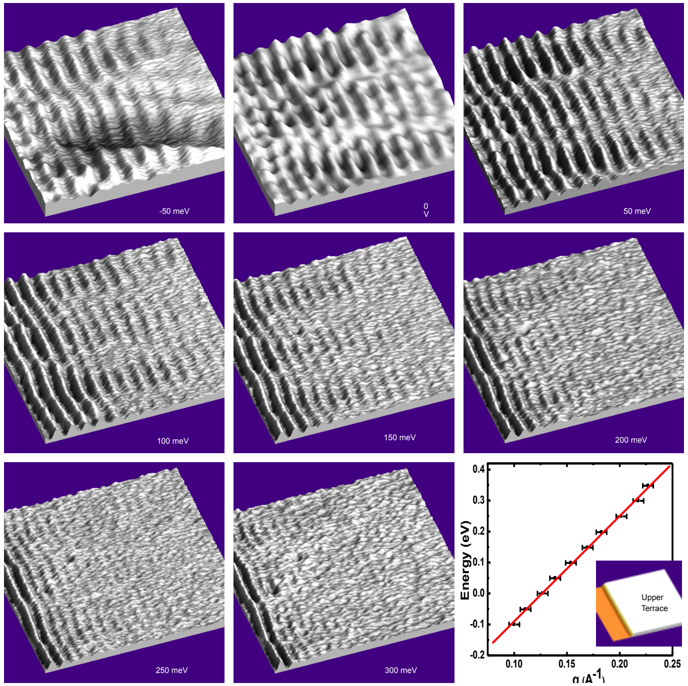


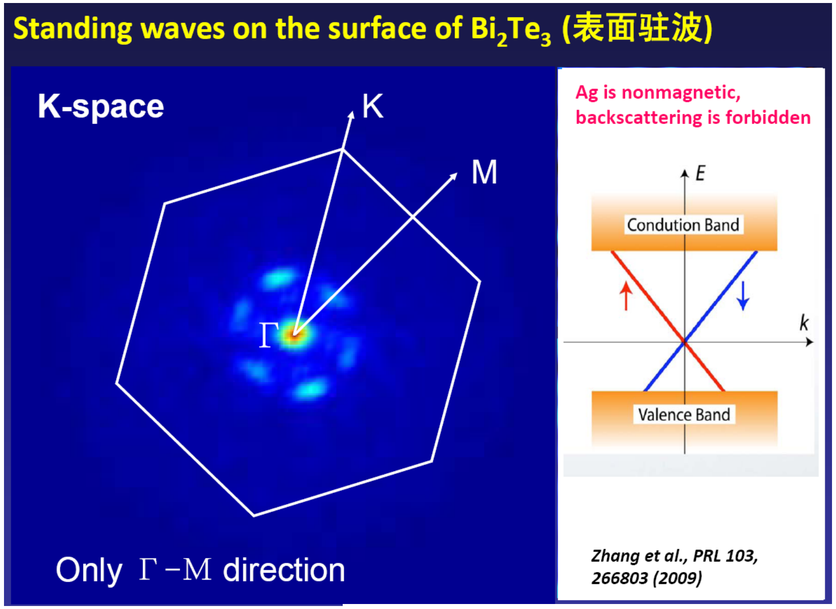
Y. L. Chen,et.al.
SCIENCE (2009)
Bi_2Te_3

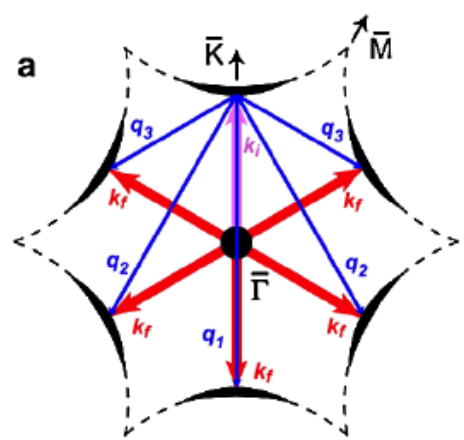
Y. Xia,et.al.
Nature Physics (2009)
Bi_2Se_3

2. TI Materials: Exp. evidence

Absence of back-scattering



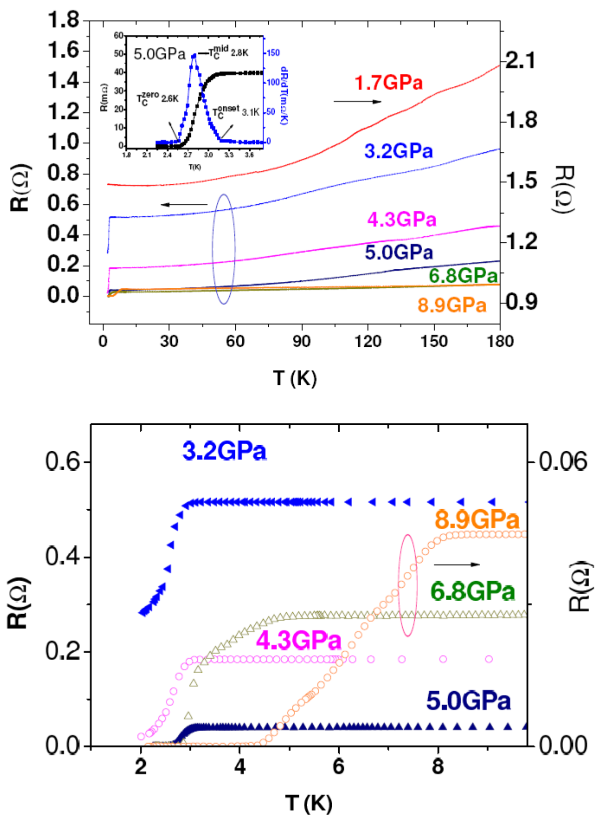


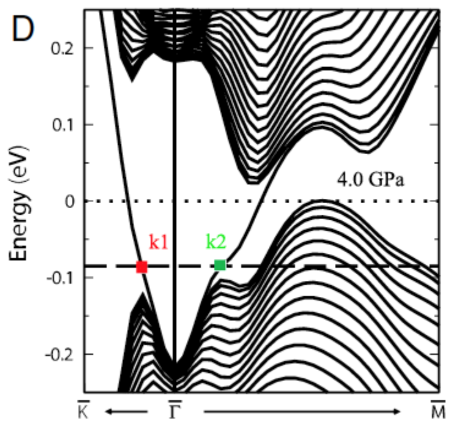


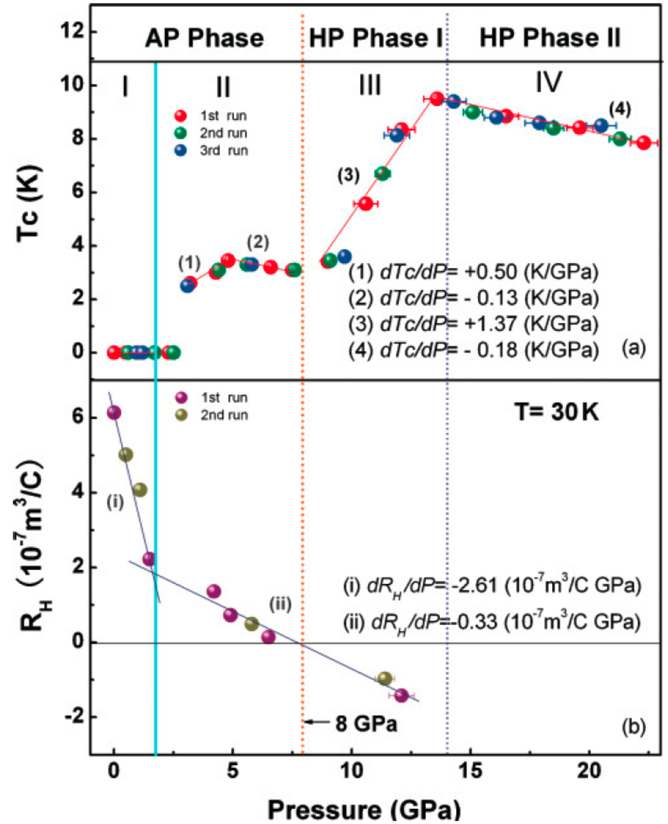
T. Zhang, et.al., PRL (2009).

2. TI materials：

拓扑绝缘体在压力下的超导态：







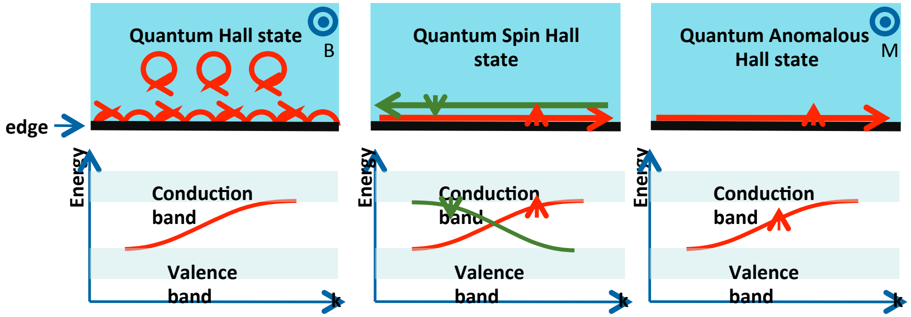
靳常青，PNAS（2011）

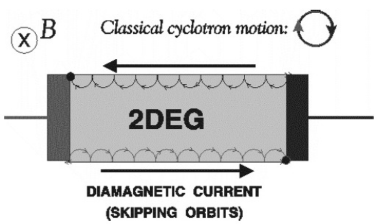
孙立玲，等，PRB(2011).
Editor's Suggestion

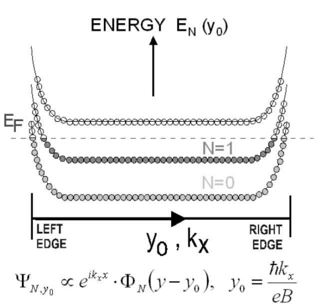
拓扑超导态？

2. 拓扑绝缘体：最新进展

磁性拓扑绝缘体----量子化反常Hall效应

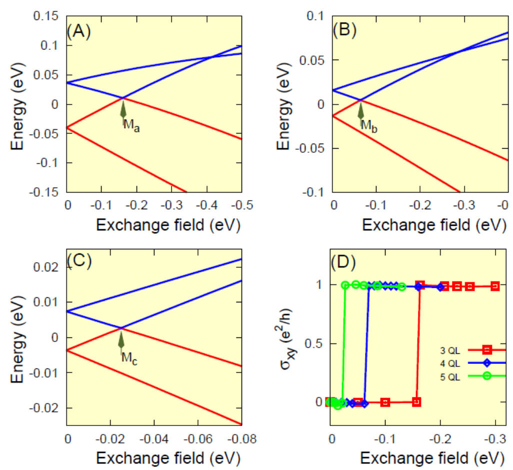






量子Hall效应

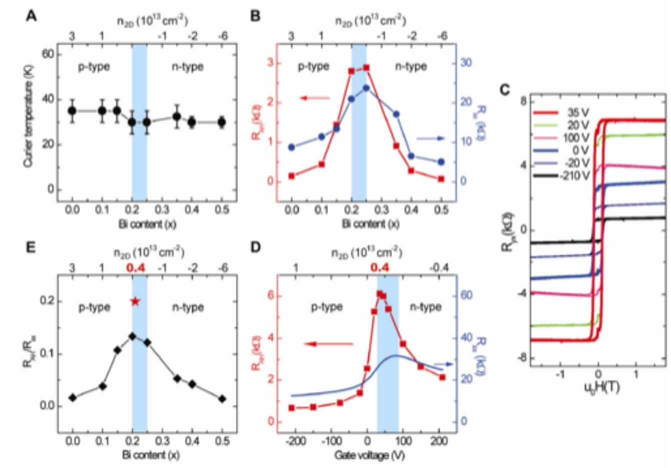
Bi_2Se_3 film doped with Cr or Fe



量子反常Hall效应

方忠、戴希等，SCIENCE(2010)

无需外加磁场实现量子Hall效应！



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

已获得初步实验证实：

何柯，马旭村，薛其坤等，

$Cr\text{-}Bi_2Te_3\text{-}Sb_2Te_3$ film，

arxiv：1108.4754(2011).

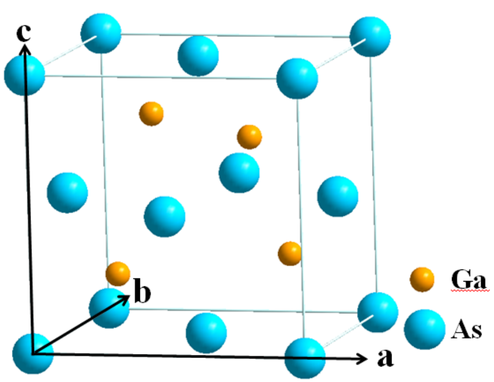
2. TI Materials: Ag_2Te

Crystal Structure:

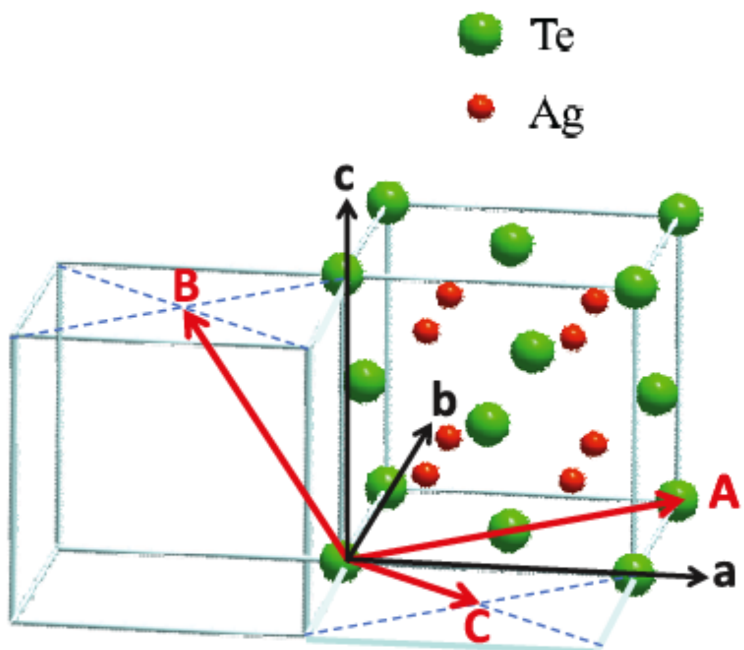
T > 417 K, α-Ag_2Te, anti-fluorite (Fm3m)

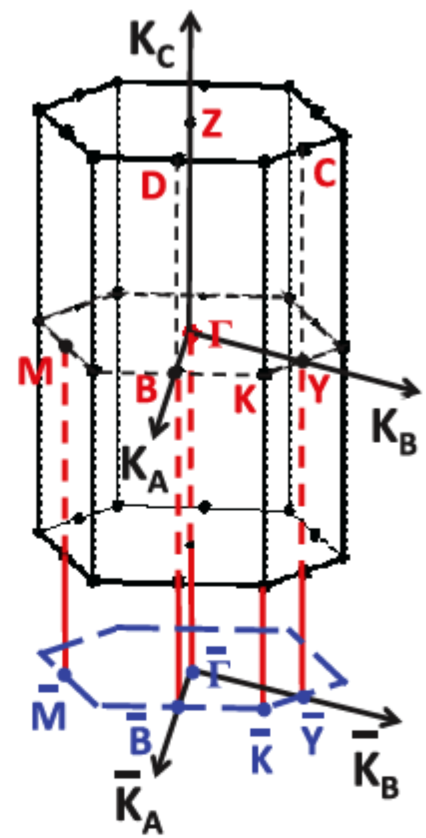
T < 417 K, β-Ag2Te, distorted ($P2_1/c$)

Cubic: a, b, c



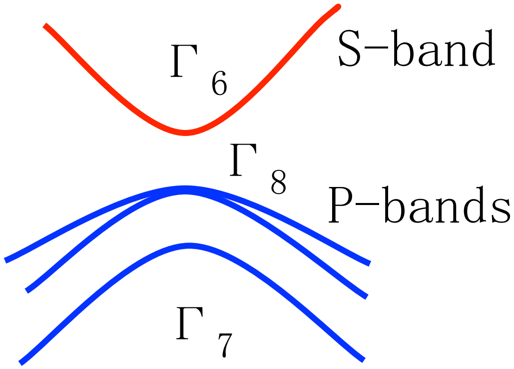
GaAs



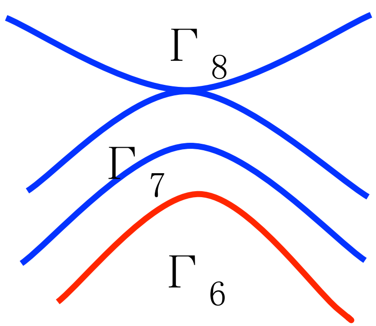


2. TI Materials: Ag_2Te

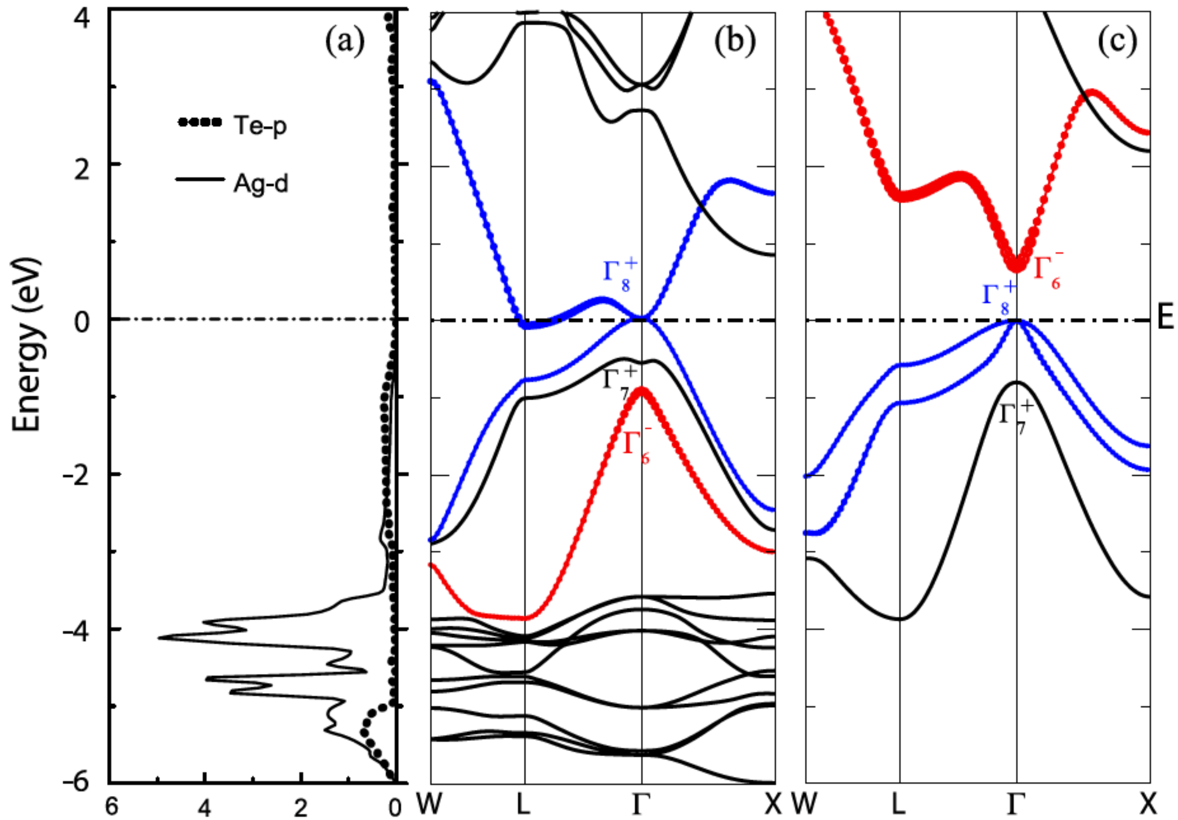
Inverted Band Structure of α-Ag_2Te Similar to HgTe



GaAS

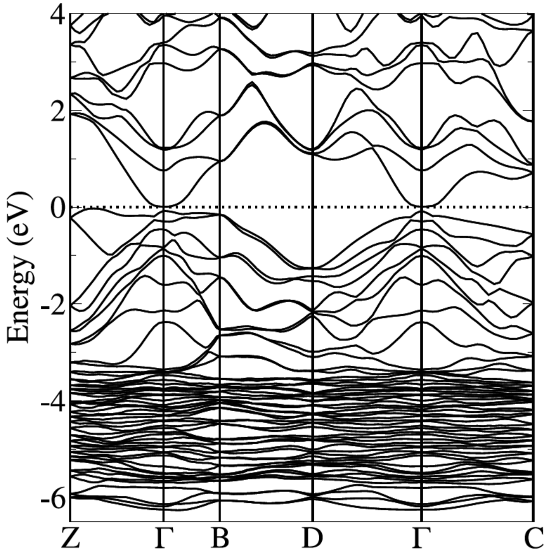


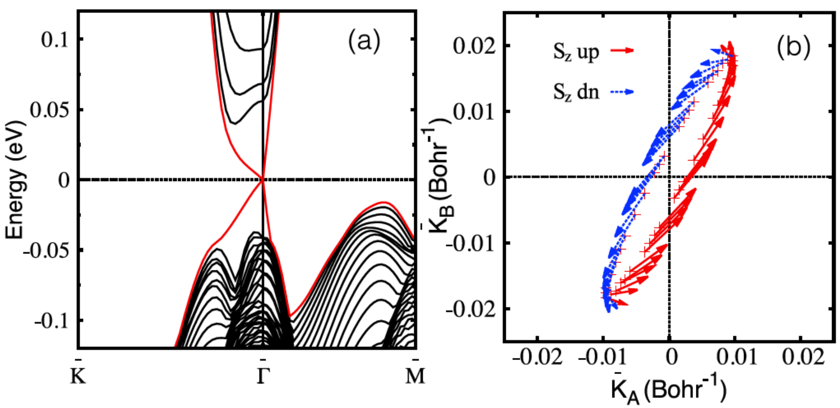
HgTe



2. TI Materials: Ag_2Te

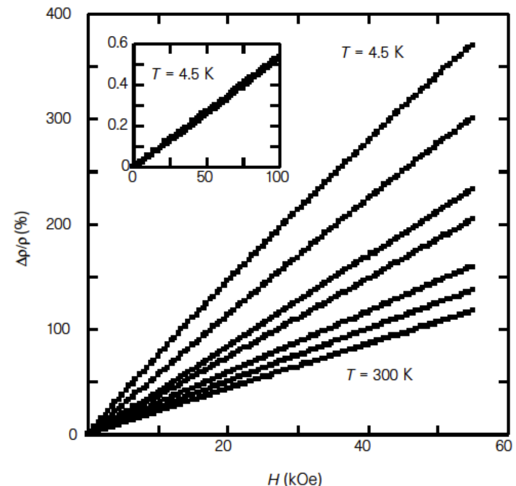
β-Ag_2Te, gap=80meV





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

Abrikosov's Quantum MR:

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

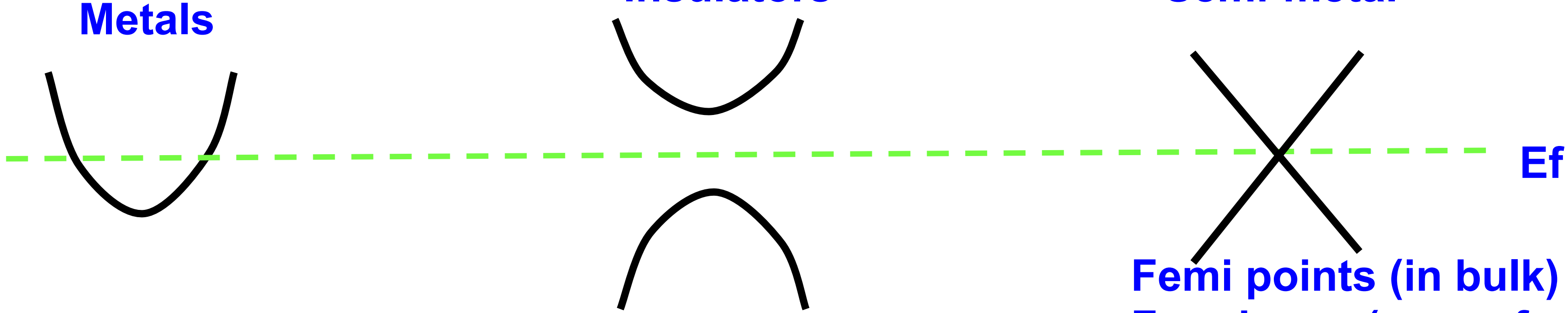
Linear Dispersion is Important!

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

3. 拓扑半金属： Momentum Space Topology

Three distinct stable classes in 3D:

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



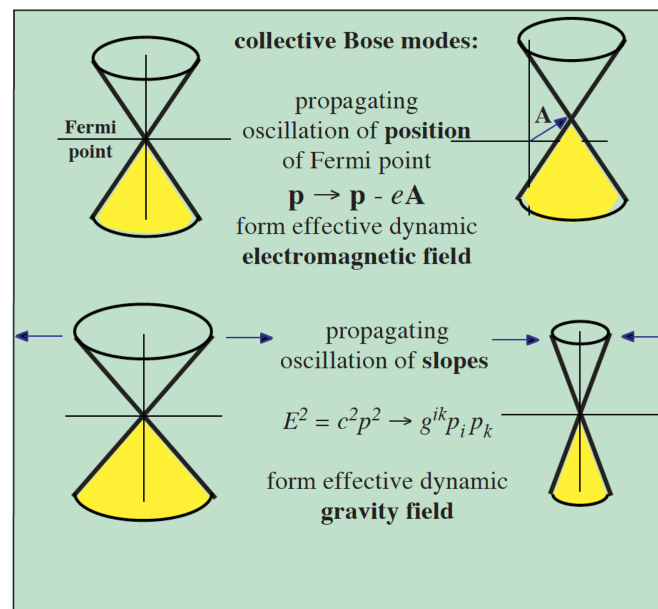
Fermi surface

No fermi surface

Normal Insulators
+
Topological Insulators
(Weyl points at Boundary)

Femi points (in bulk)
Fermi arcs (on surface)

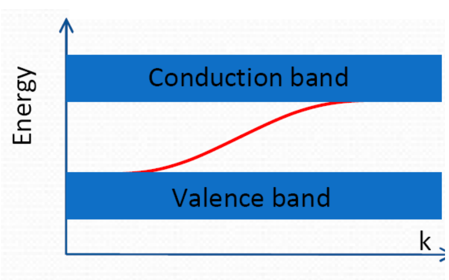
Standard Model + gravity

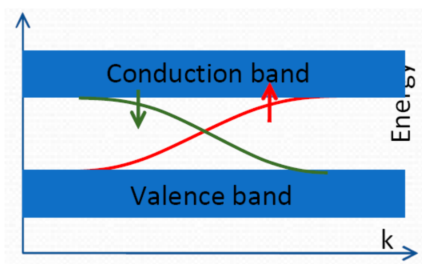


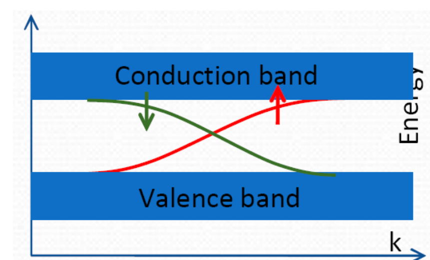
Our Subjects

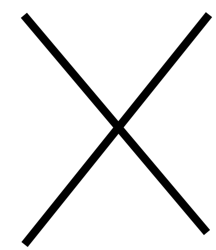
3. 拓扑半金属： Family of TIs?

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

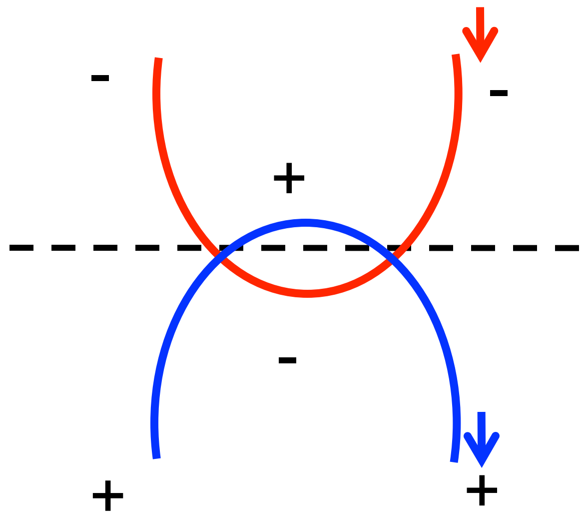
Z2

Surface States

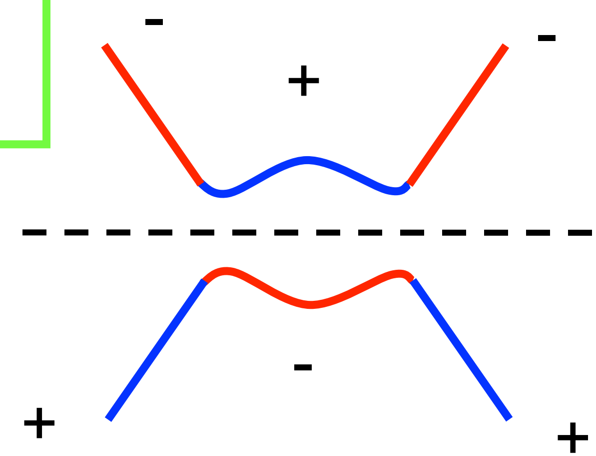
Femi points
(in bulk)

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

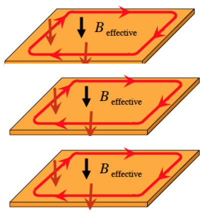
2D Chern Insulators:



Gap opening due to SOC



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

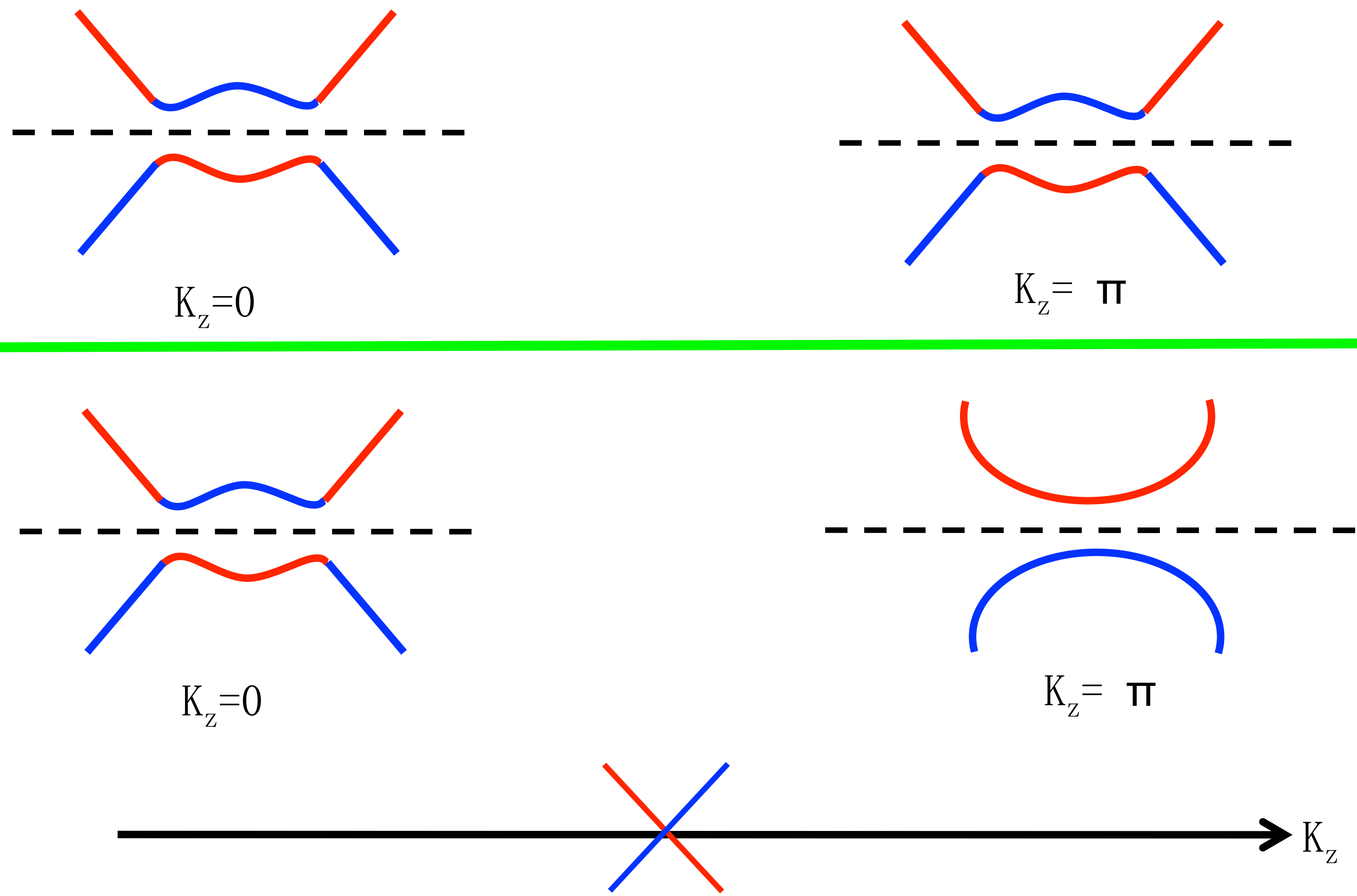


(2) Strong 3D--Any analogy? Chern semi-metal:

Time Reversal Polarization in momentum space!

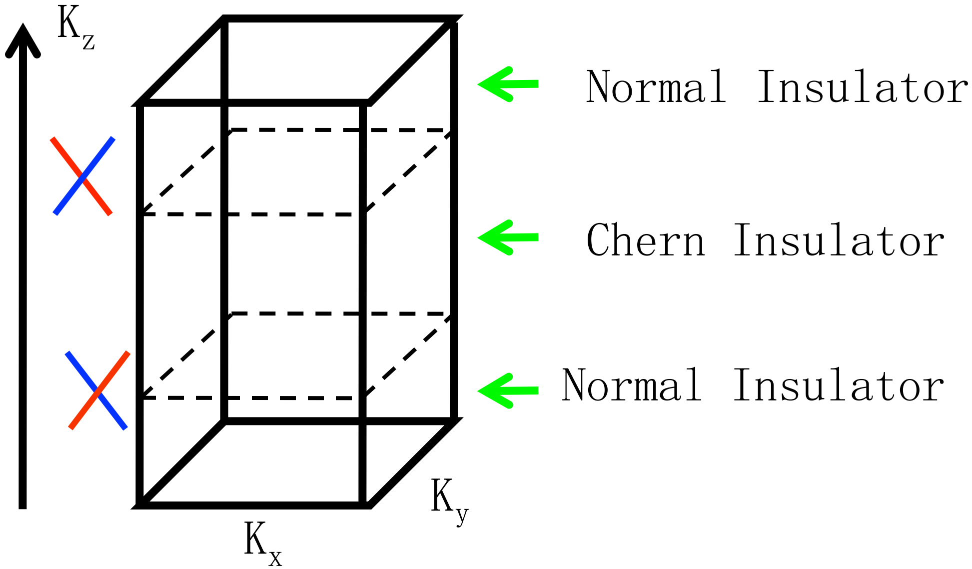
3. Semimetals: Chern Insulators and semi-metal?

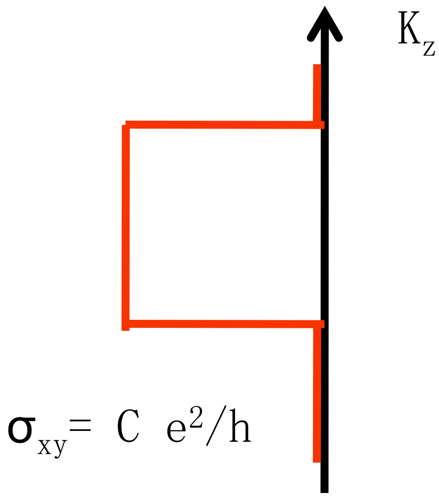
Weak Chern Insulators:



Topological Phase Transition

3. Semimetal: Chern semi-metal?





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: $\vec{\Omega}(\vec{k}) = \nabla_{\vec{k}} \times \vec{A}$

3. Semimetal: Chern semi-metal?

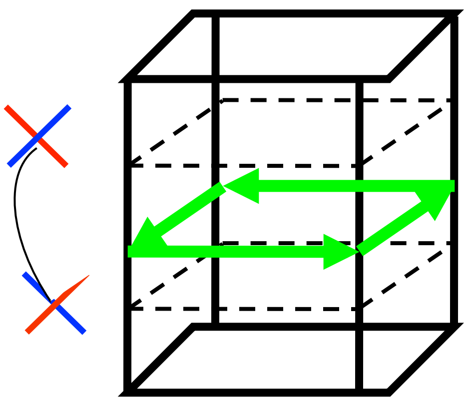
(1) It is topologically unavoidable. (not accidental)

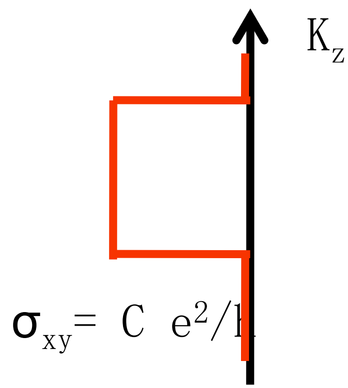
(2) Time-reversal polarization & Magnetic Monopoles in the K-space.

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

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

(3) Fermi arcs on the side surface.



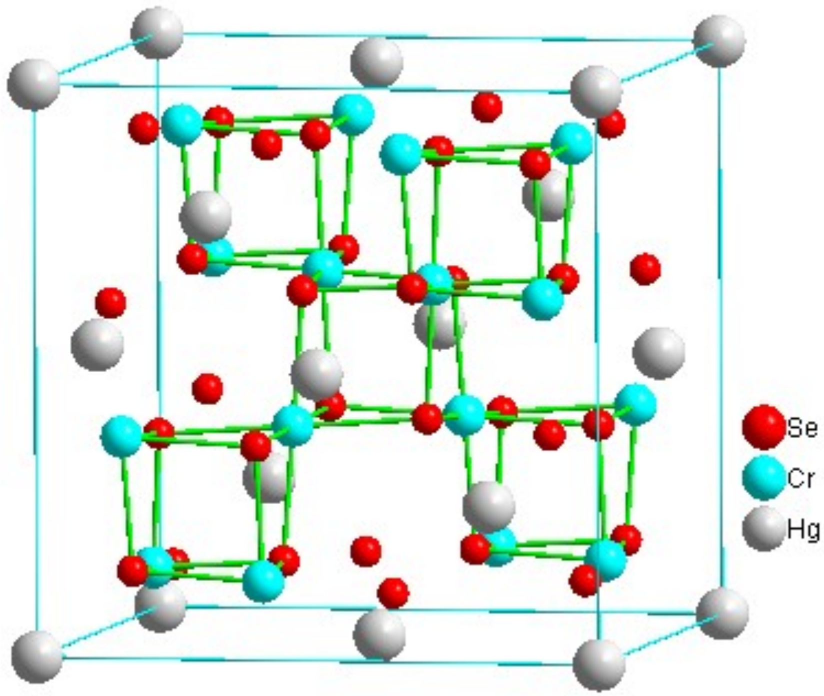


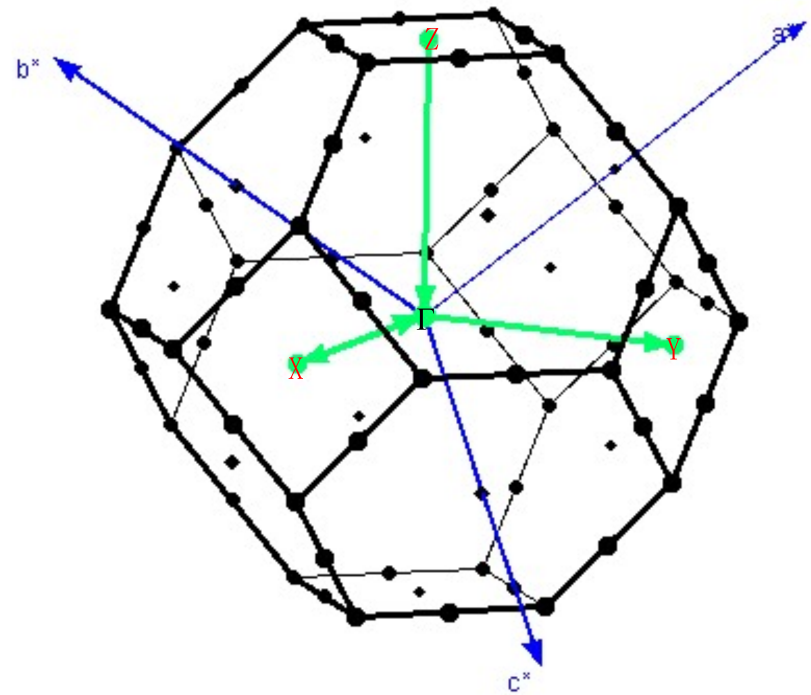
(See, X. G. Wan & Savaraso, PRB (2011), on AF Pyrochlore iridates)

(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.

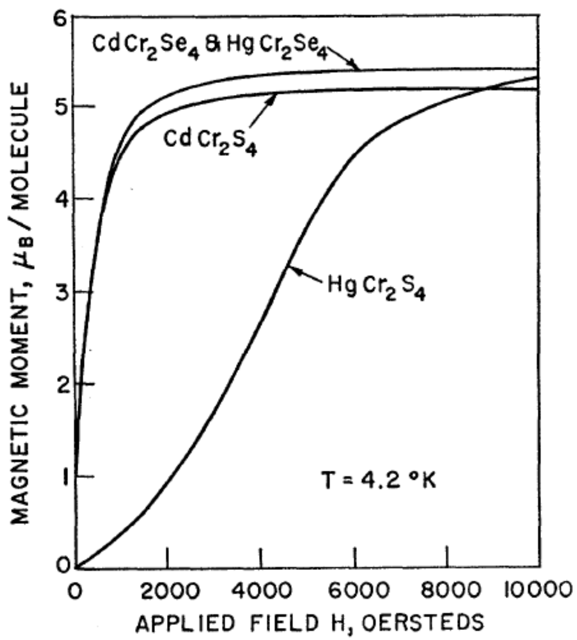
Space group Fd-3m (point group O_h).

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	$\frac{\theta}{T_c}$
$CdCr_2S_4$	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

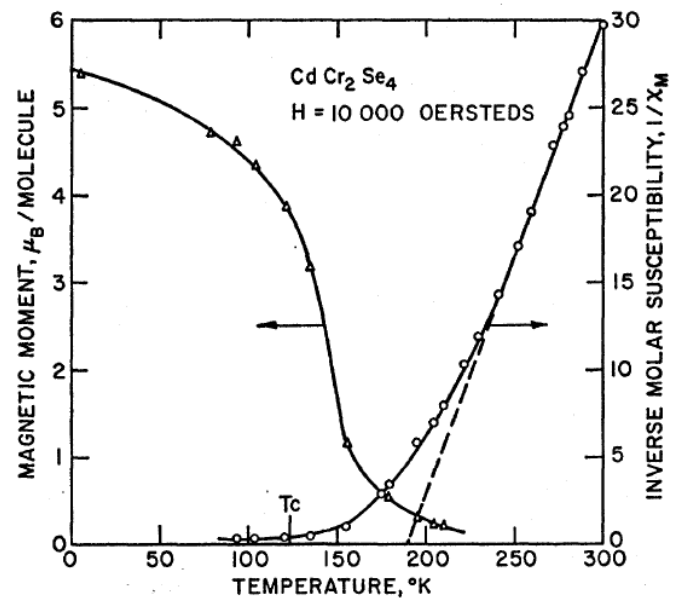
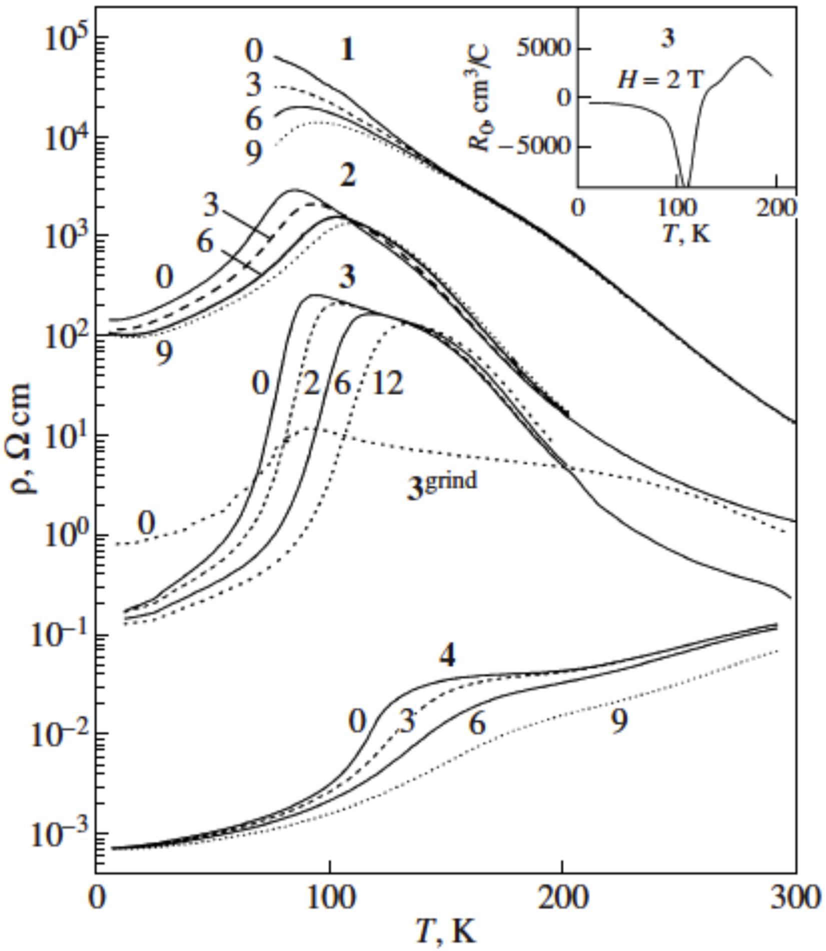
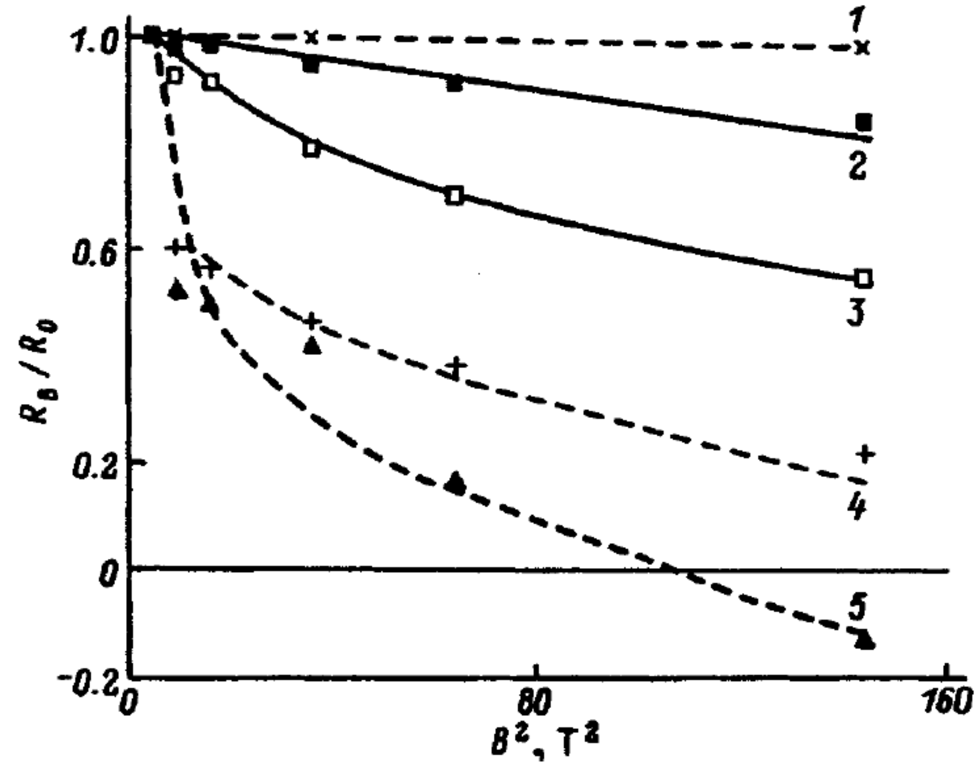


FIG. 3. Magnetic moment and inverse susceptibility as a function of temperature for $CdCr_2Se_4$ in an applied field of 10 000 Oe.

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

$HgCr_2Se_4$





Metallic

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

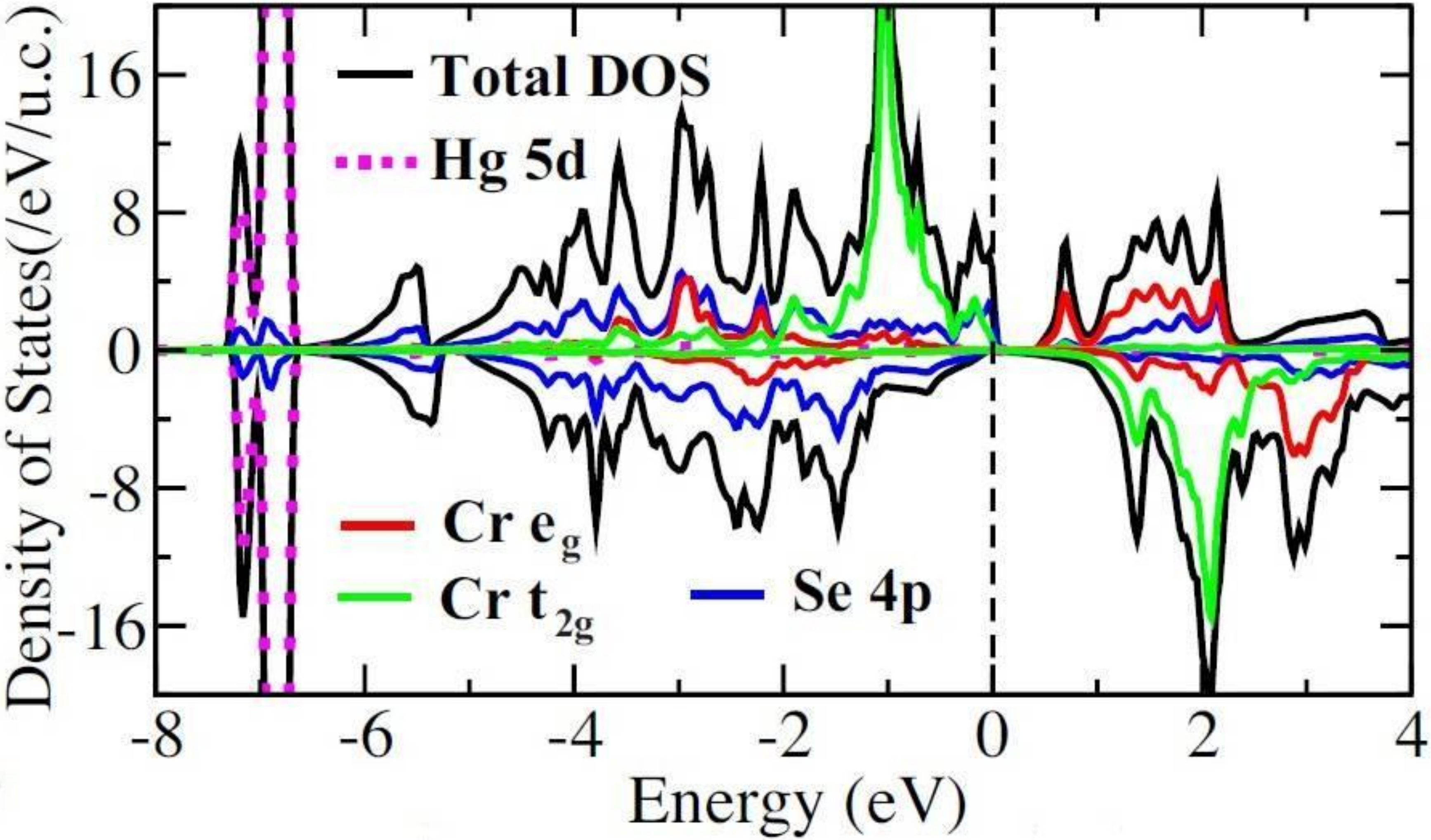
AHE

N. I . Solin, et.al,

Phys. Solid State (1996)

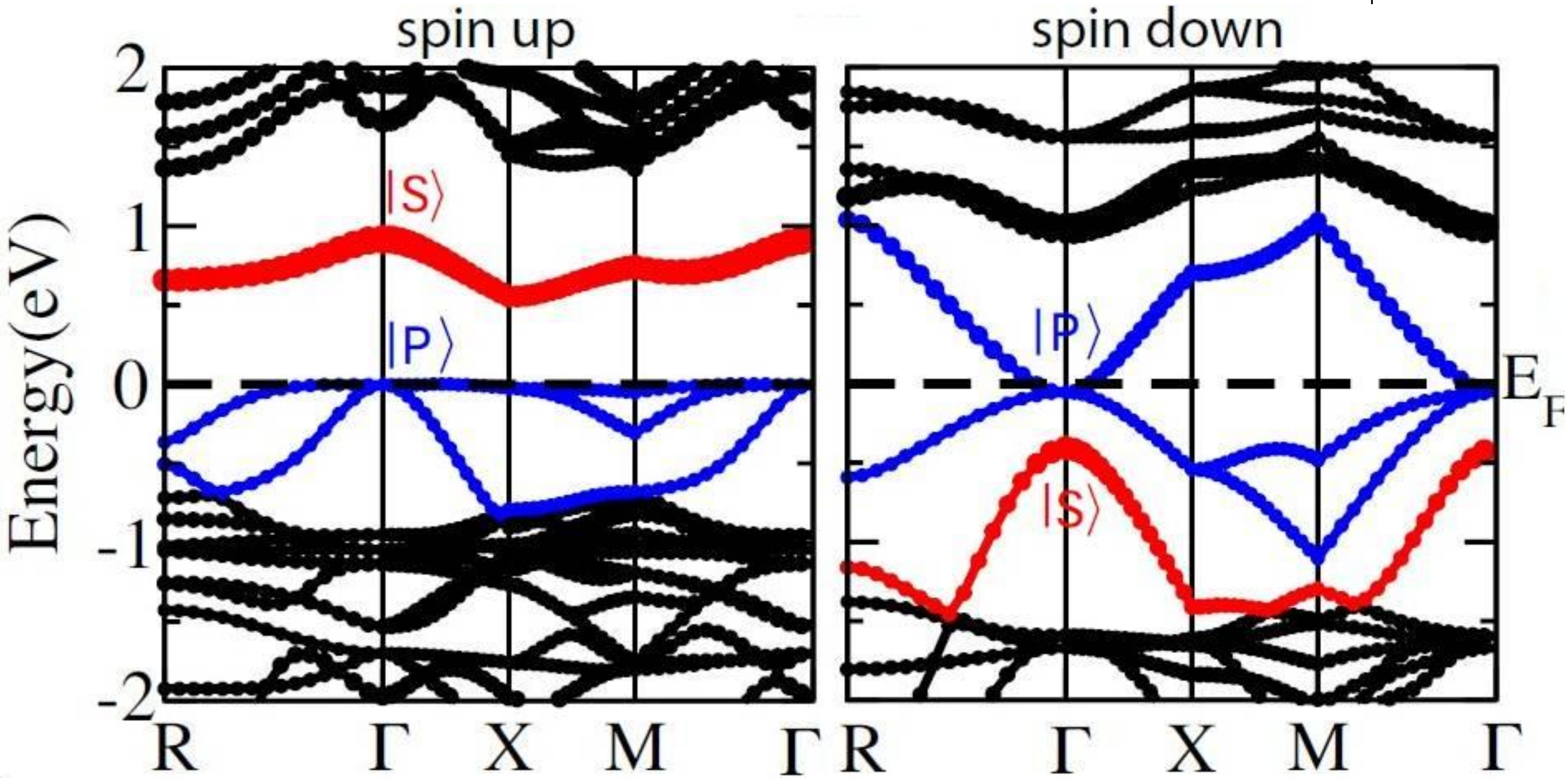
Electronic structure without SOC

DOS

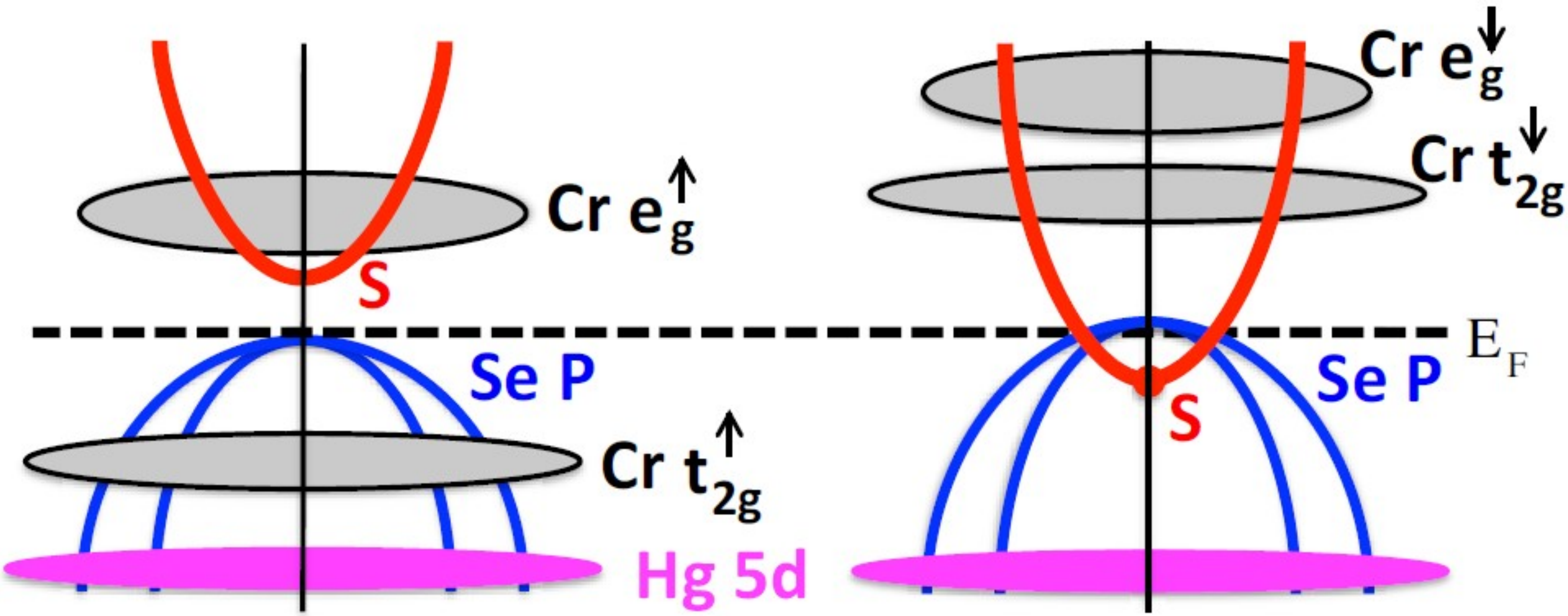


Electronic structure without SOC

Band

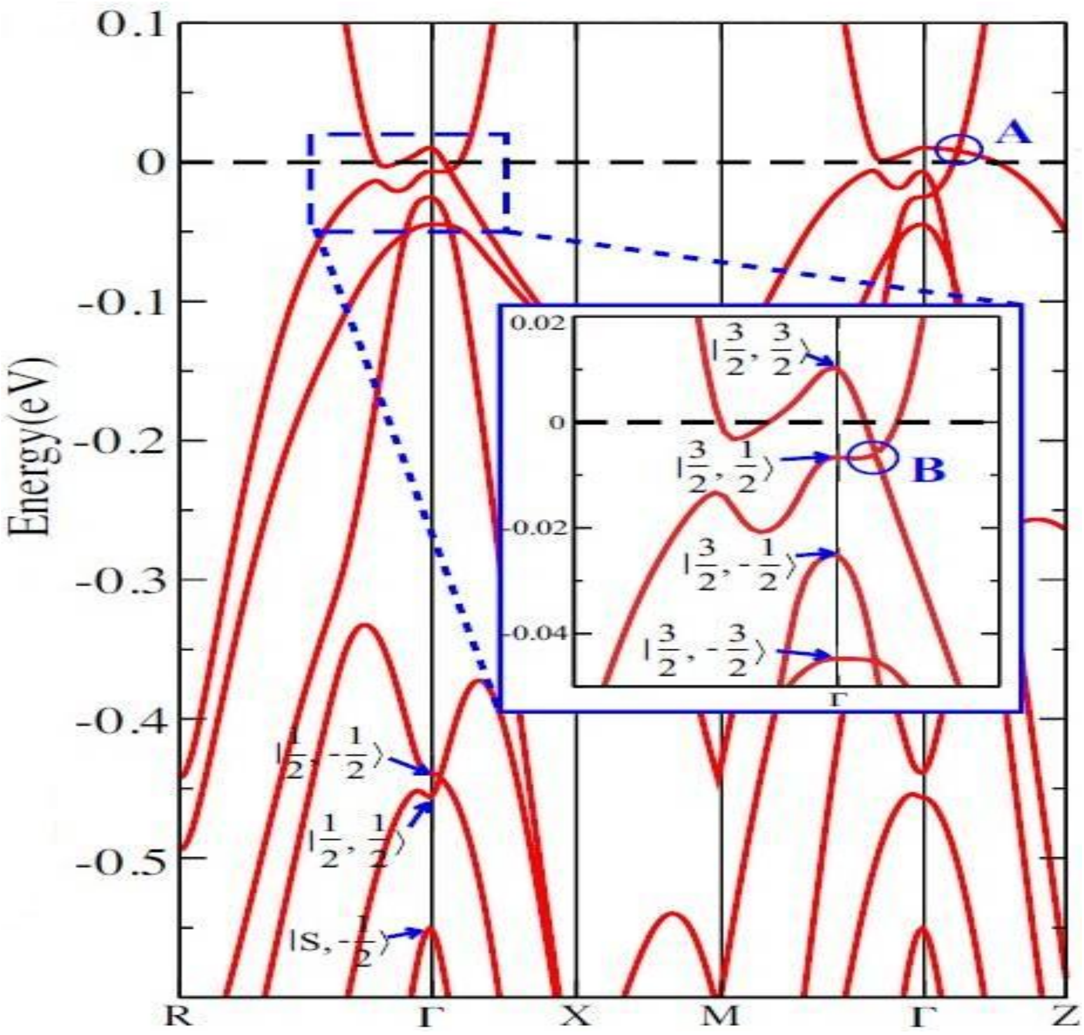


Schematic diagram for the band-inversion



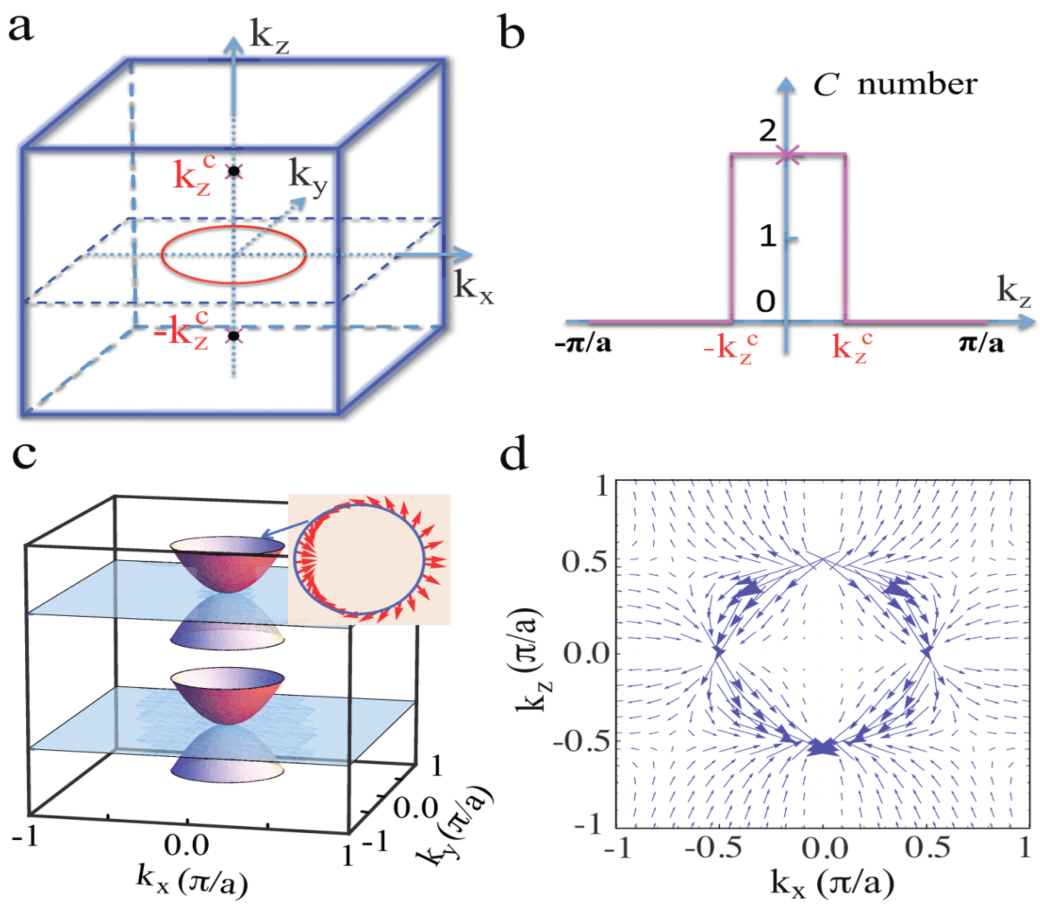
Electronic structure with SOC

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 $k_\pm = k_x \pm ik_y$, 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.

$$\mathrm{E}(\boldsymbol{k}) = \pm\sqrt{M^2 + D^2 k_z^{\ 2}(k_x^{\ 2} + k_y^{\ 2})}$$

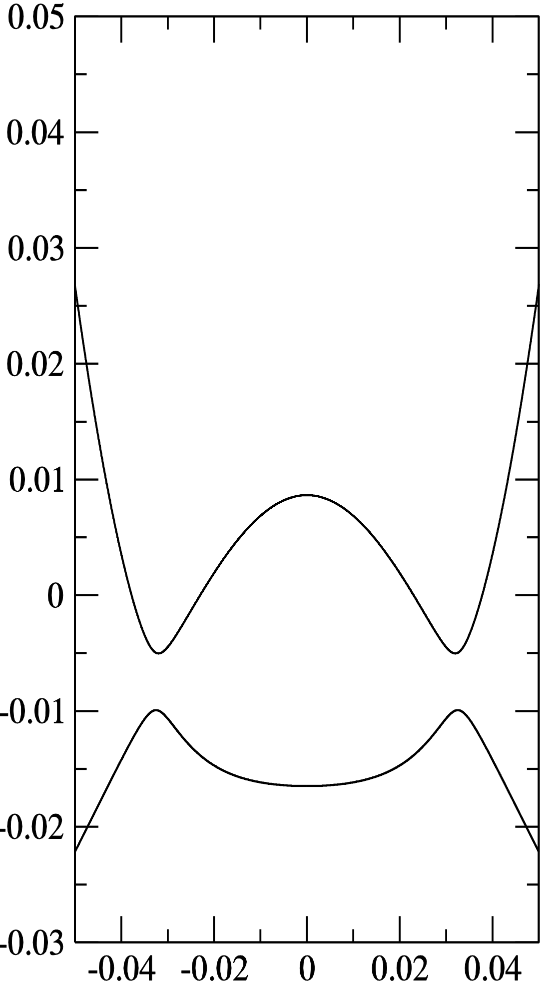
two gapless solutions:

$$k_z = \pm k_z^{\ c} = \pm\sqrt{M_0 / \beta}$$

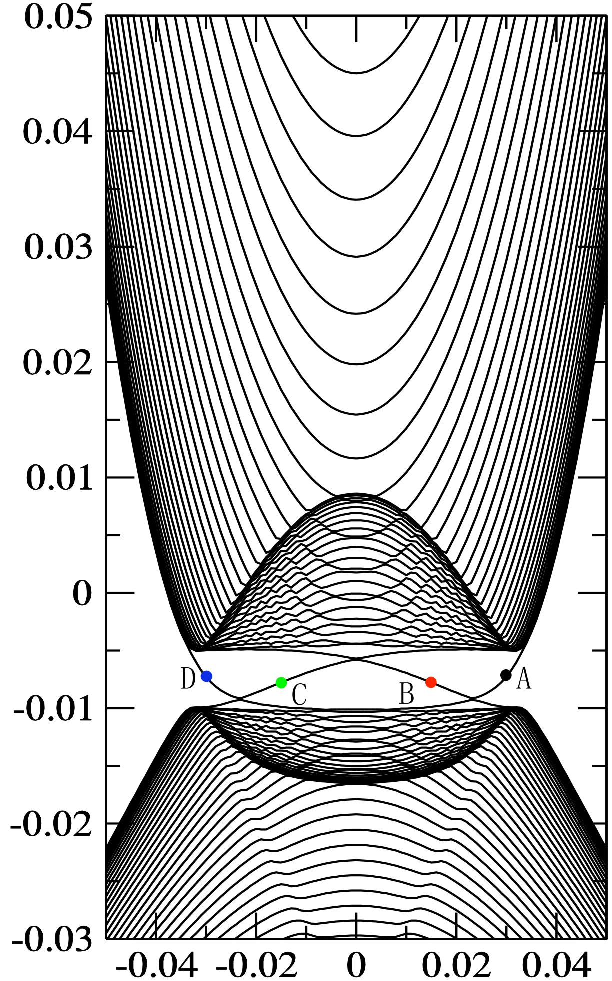
$$k_x^{\ 2} + k_y^{\ 2} = M_0 / \beta$$

Edge states and fermi arcs on surface

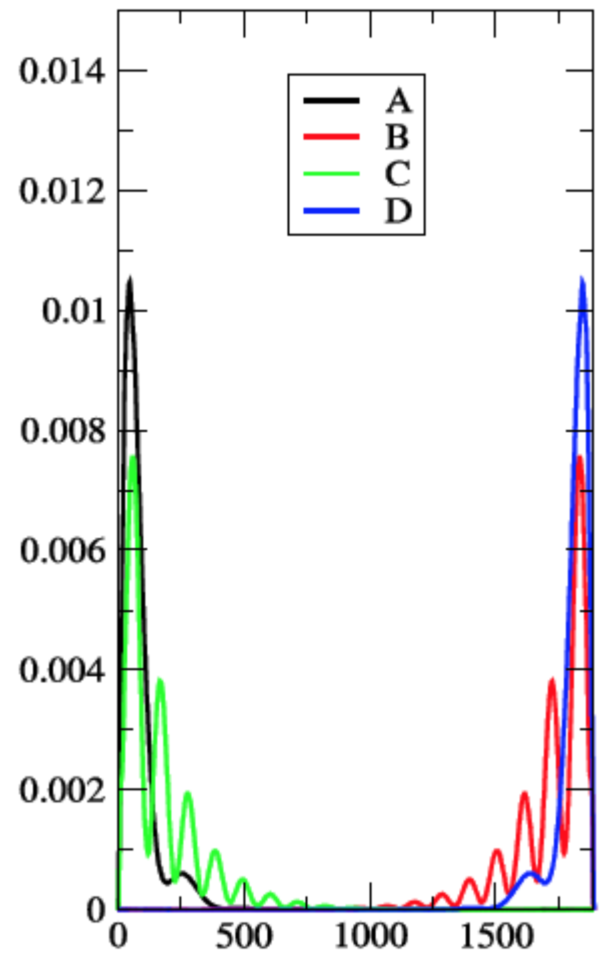
Edge state in k_z=0.06π plane



Band of bulk



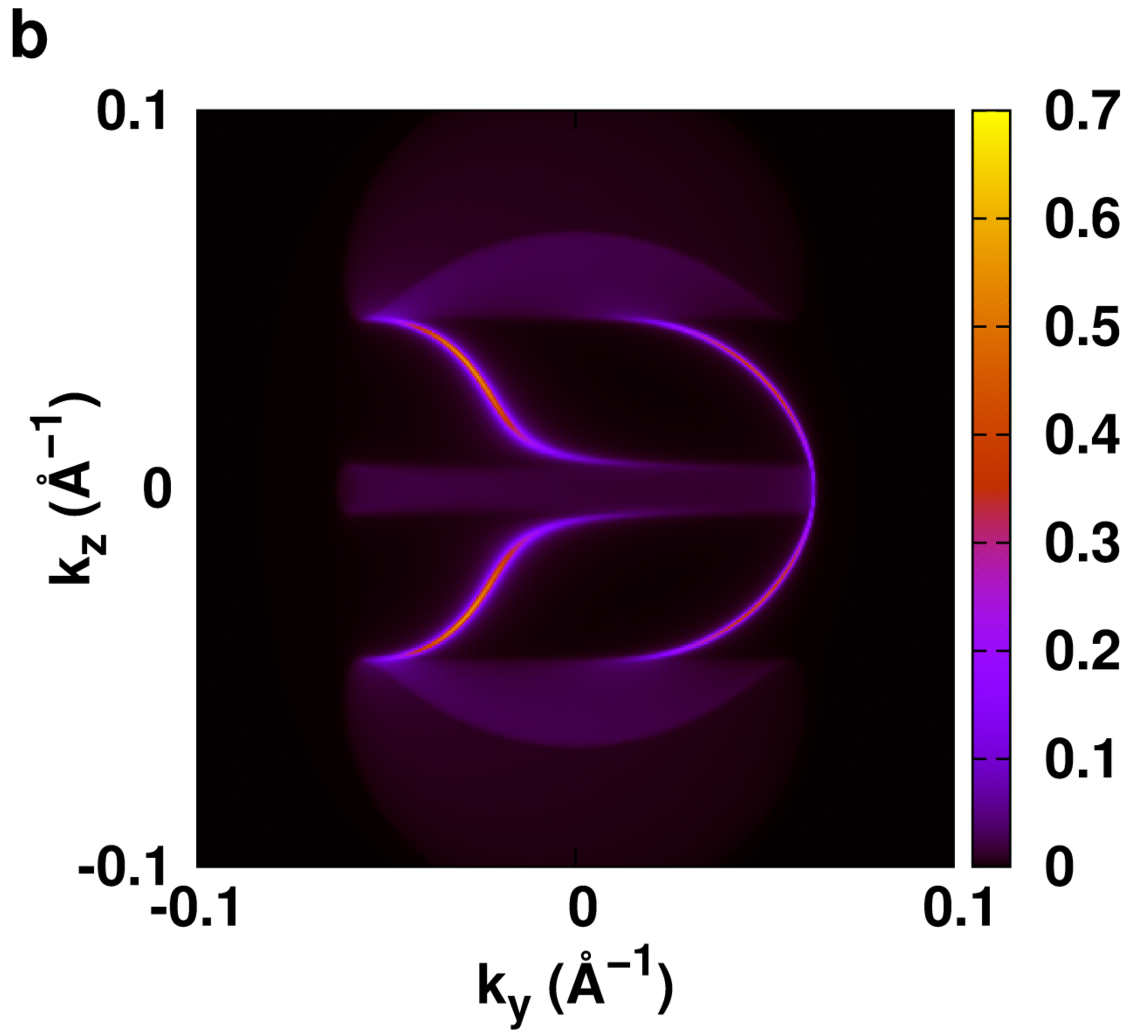
Edge state



Distribution along x

Edge states and fermi arcs on surface

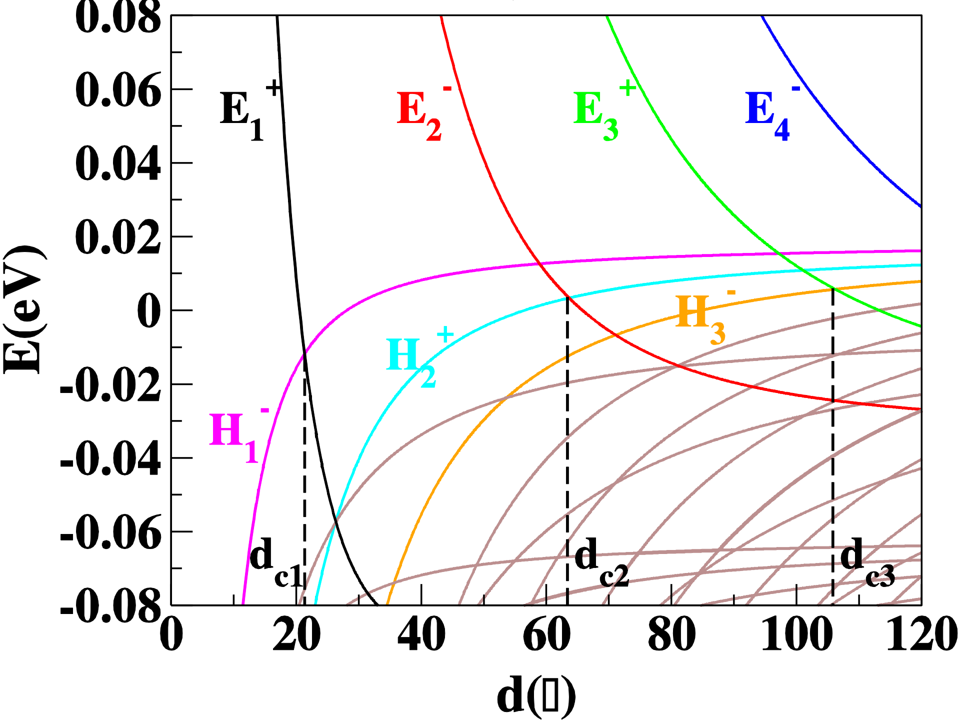
Fermi arcs for the (k_y, k_z) side surface

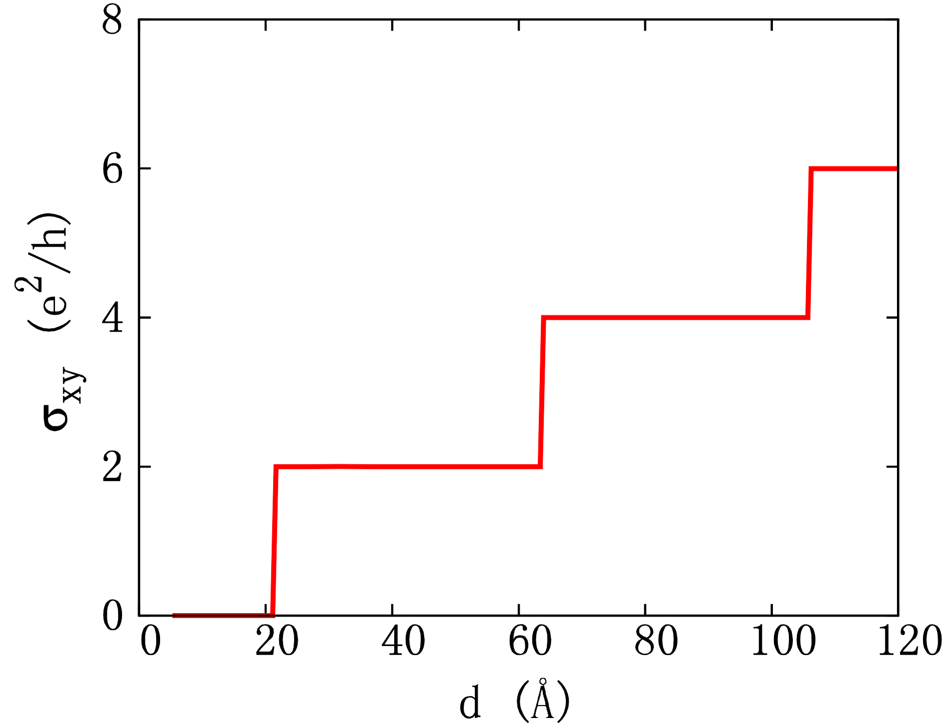


Fang & Dai, et.al, PRL（2011）

QAHE in the quantum well structure

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





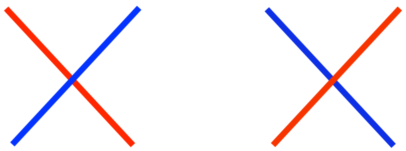
Energy gap at Γ vs. d

Hall conductance vs. d

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

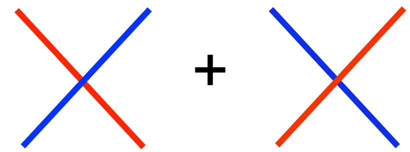
4. Topological Dirac Semimetal:

Weyl Semi-metal



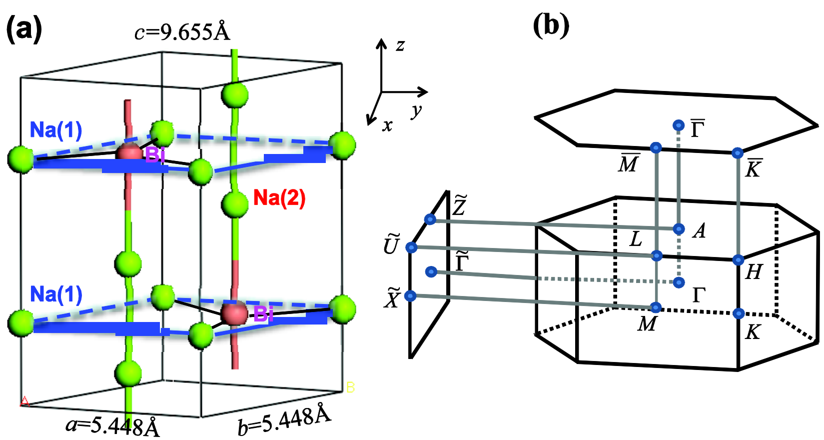
Separated in K
2x2 Hamiltonian
No T or I symm

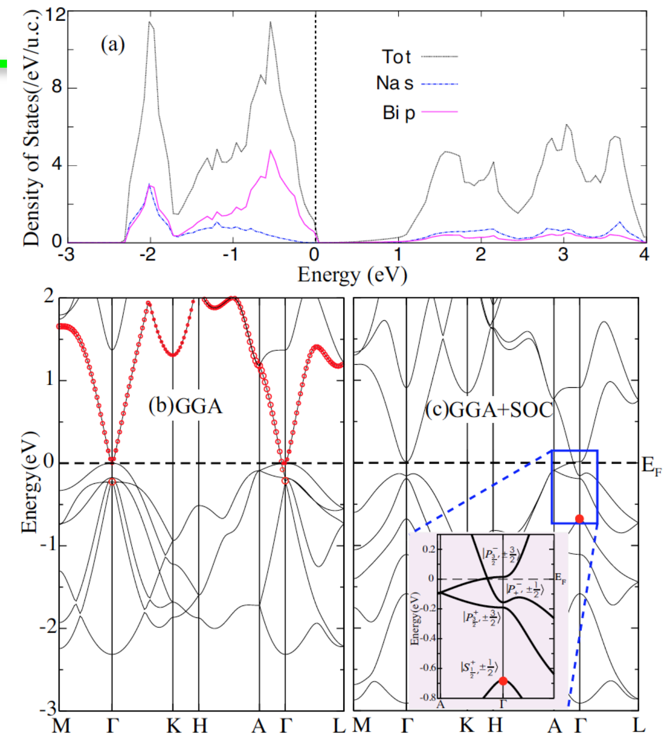
Dirac Semi-metal



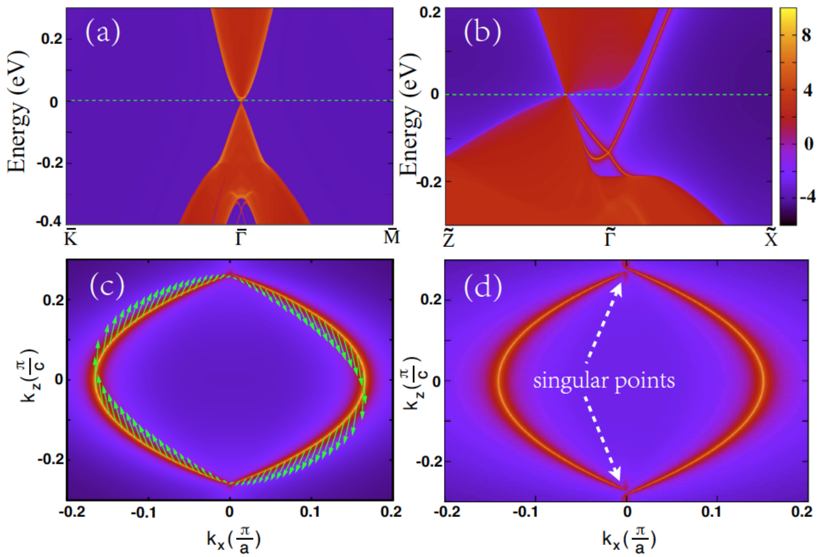
Overlapped in K
4x4 Hamiltonian
Protected by crystal Symm

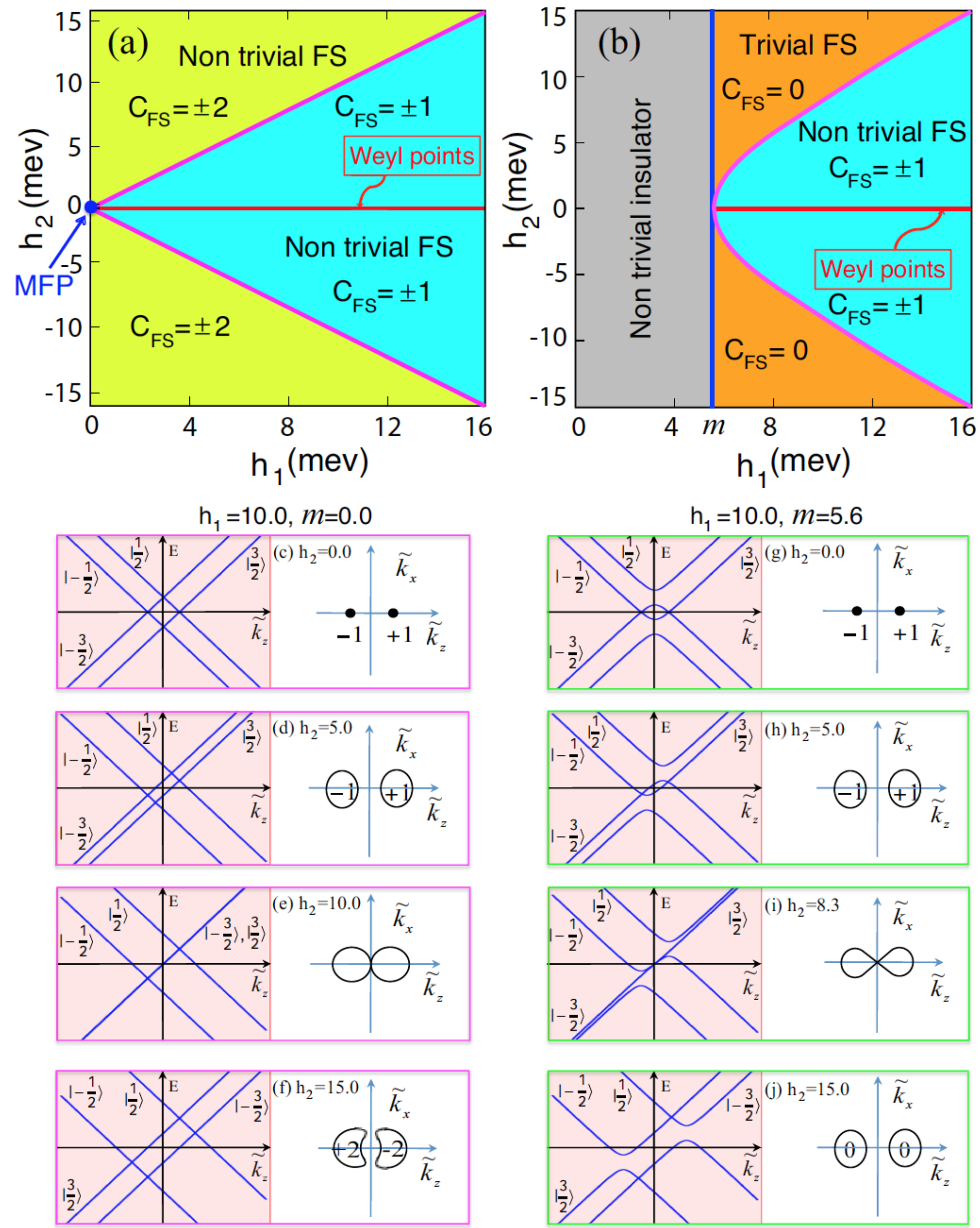
Na_3Bi, K_3Bi, Rb_3Bi





4. Topological Dirac Semimetal:





Marginal Fermi points in Na_3Bi, K_3Bi, Rb_3Bi

Arxiv.org: 1202.5636 (2012)

谢　　谢！