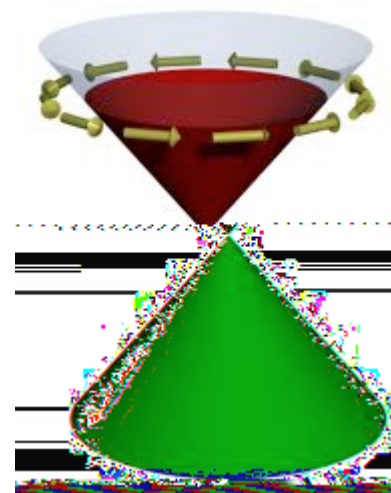
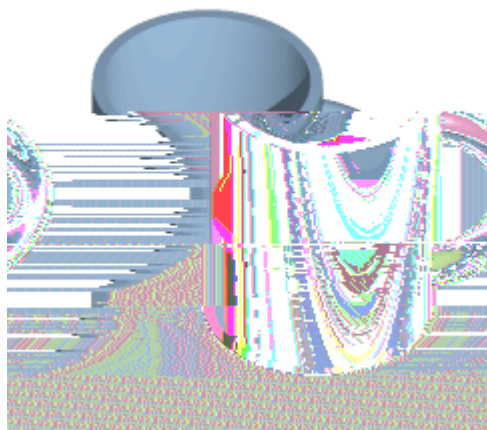
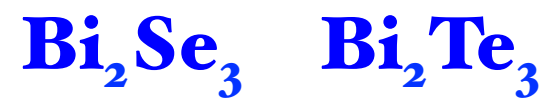


拓扑绝缘体与拓扑半金属





有序态是凝聚态物理研究的基本内涵之一

例如： 有序态、 有序态、 导态

局域有序态

称性破缺 致有序
(朗道 称性破缺理)

1.物 可以用局域序参量描写

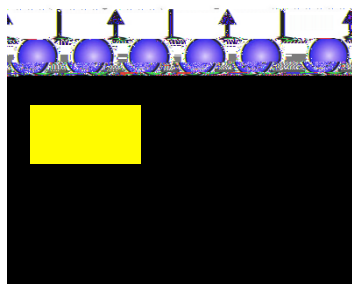
如： 磁 的磁化 度 $M(r)$

2.相 伴随着 称性破缺

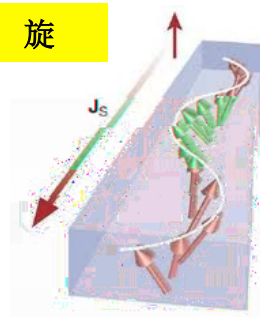
如： $M(r)$ 的出 破坏了

旋 称性

反



旋



宏观有序态

拓扑有序态

(子 与几何 完 合)

1. 具有拓扑性 “ 子态”

2. 不 局域序参 描写,
全局拓扑不变 描写

3. 变 并不伴 对 性

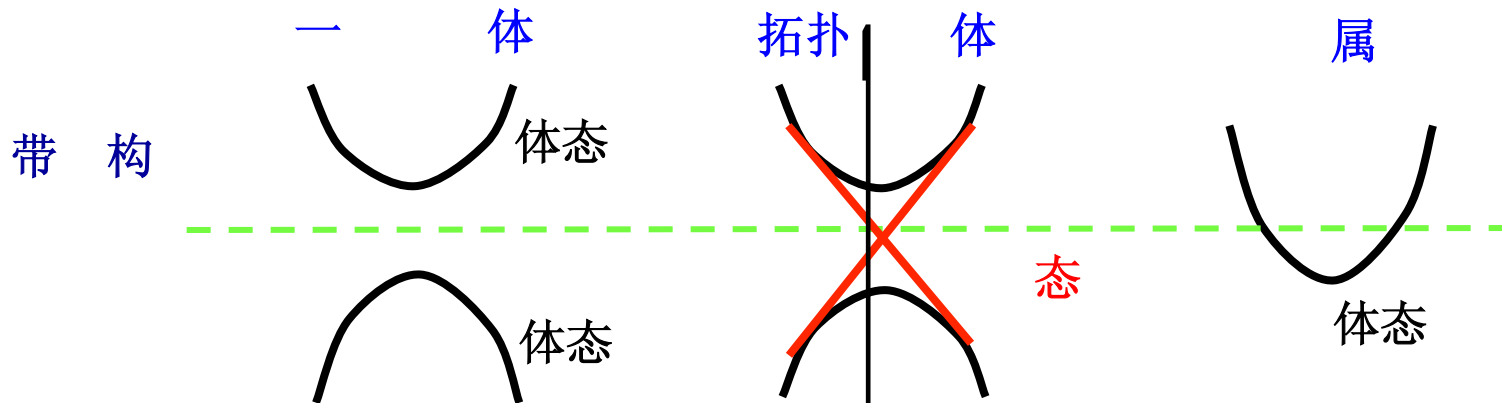


拓扑 “0”



拓扑 “1”

拓扑绝缘体 — 全新 拓扑有序态：受时 反 性保护
对 + 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 材料： L. Molenkamp, Science (2007)
2. 三 材料： 方忠 , Na e Ph . (2009)
(Bi_2Te_3 , Bi_2Se_3 , Sb_2Te_3)

与一

态区别：

无 如何切样品， 态总是存在

1. 介: Why edge states?

Band i



Bo nda

Vacc m
No mal
in la o

TI



C ing Band Ring

Defined by the $\mathbb{Z}_2$ invariant
(or parity of the number of occupied states)

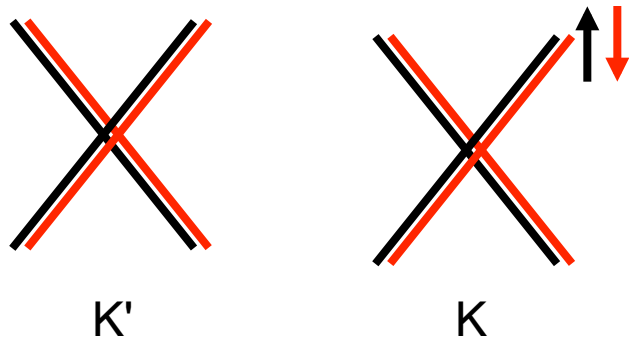
Ref:

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

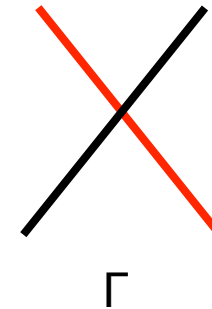


1. 介: Surface state vs Graphene

G aphenes



S face a e of TI



- (1) p do- pin
- (2) Klien Pa ado
- (3) linea n E,
- linea σ E,
- linea m E
- (4) Locali a ion?
- (5) Uni e al σ ?
- (6)

- (1) 1/4 of G aphenes,
- pin pli ing,
- T-in a ian
- (2) 2DEG i ho ma
- (3) Klien Pa ado
- (4) linea n E,
- linea σ E,
- linea m E
- (5) QHE? Locali a ion?
- (6) M I i-fe oic?

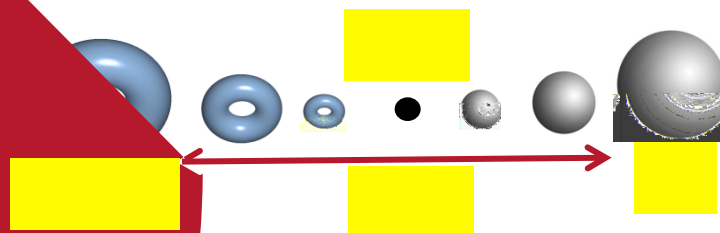
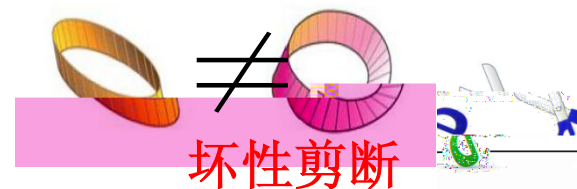
1.



拓扑有序 子态 优 :

1. “0” 与 “1” 严格区分,
无微扰 , 不怕干扰、噪声

2. 与 “奇 ” 密切 关,
在 上会有 子态



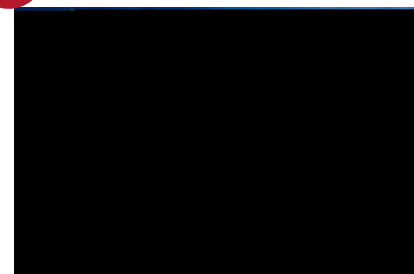
信息 公 : 极低 、 极低
普 态



杂, 杂乱无



到杂 , 会 散射



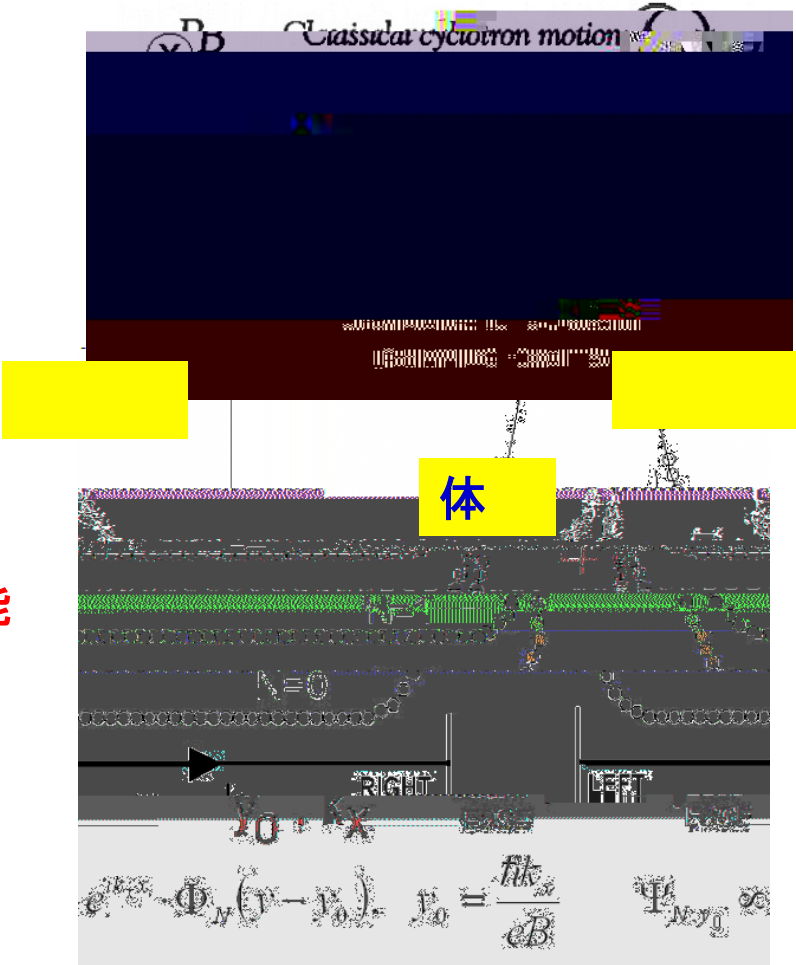
各 其 , 不 杂



到杂 , 动

中
界

朗道能



1. Very Stable
2. No backscattering
(Edge state can not localize)

- 1.
- 2.
- 3.
- 4.

量子Hall效应

性:

1 基础科学发展 全新 概念、 、效应

1. 新奇 子效应
2. 基本 常数 定

2 下一代电子技术 新性

数

1. 准 子器件: 无 “ 想导 ”
2. “ ” 与 “ ” 交叉 控, 巨大响应
3. 器件: 效应、 性光学
4. 拓扑催化
5. 核 料 : 、 导

3 国际发展的趋势 是当前国 发展 前

1. 已投入巨
2. 日本 在启动

1. 介: Family of TIs?

2D

3D

T-broken

T-invariant

T-invariant

T-Broken

QHE

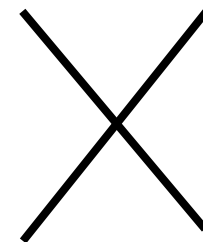
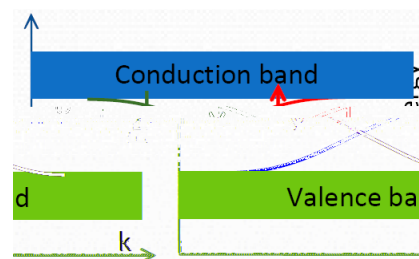
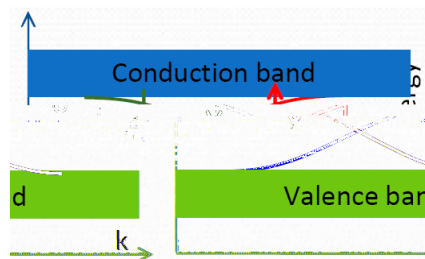
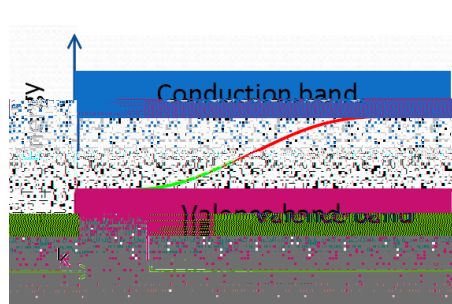
QAHE

QSHE

Topological Band Insulator

Kondo
Anderson
Mott

Semi-metal



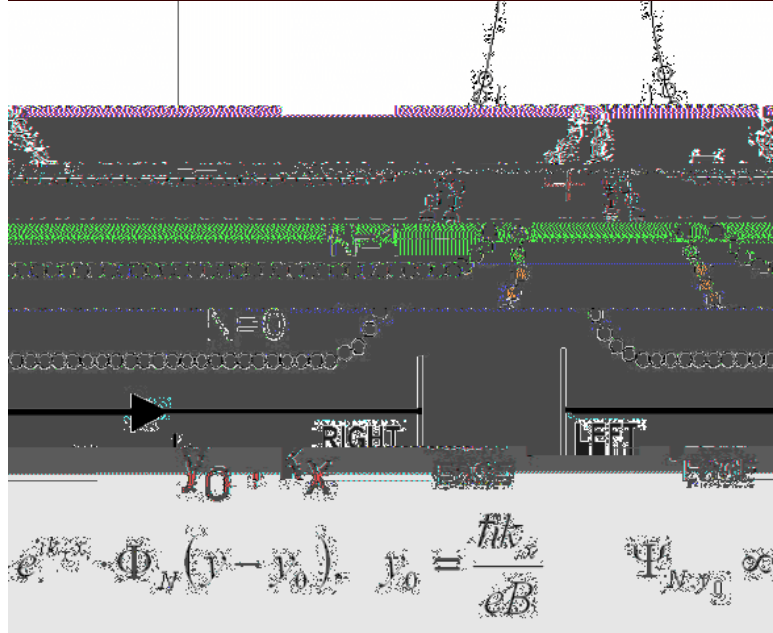
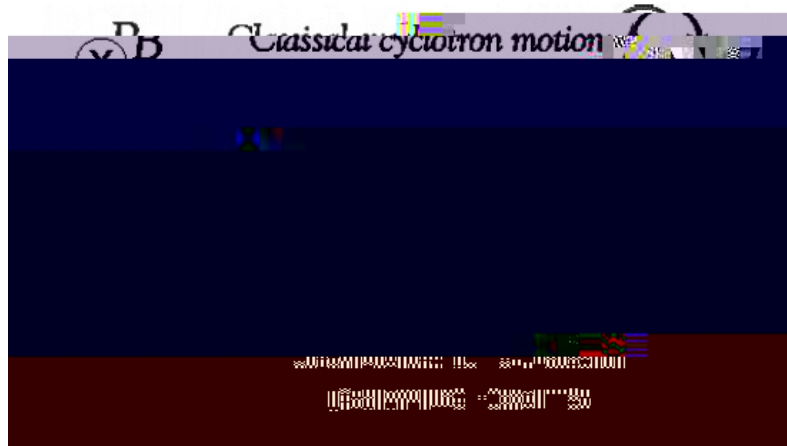
Edge States
TKNN
Chern number

Z_2

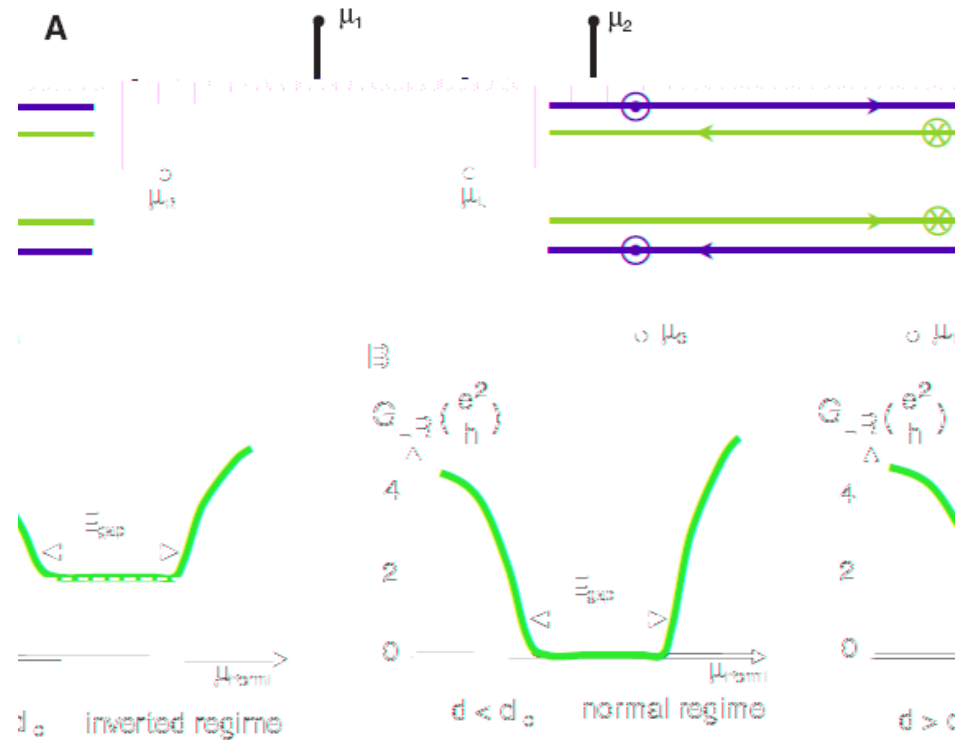
Surface States

Femi points
(in bulk)

2. 拓扑体: T-broken vs T-Invariant



QHE

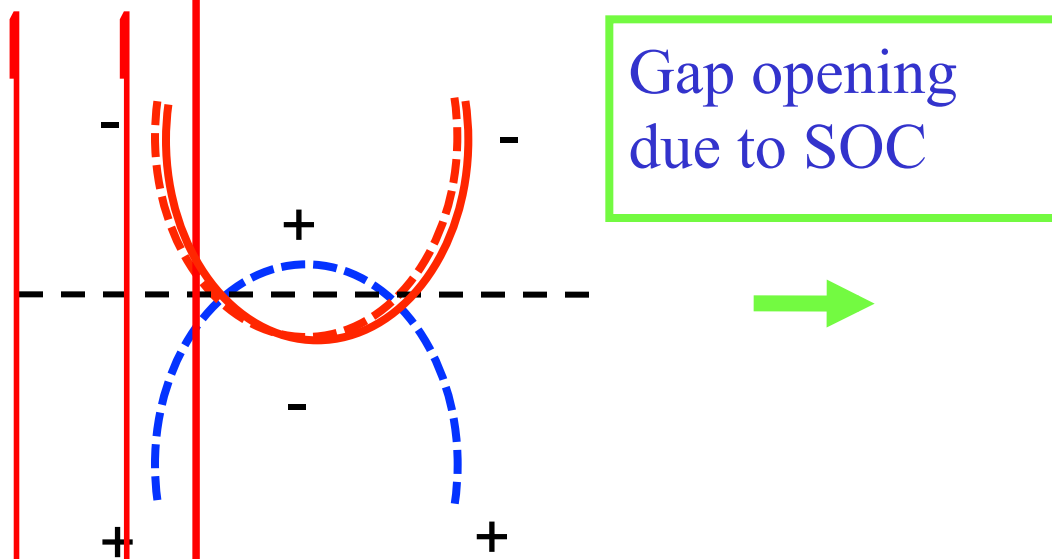


QSHE in HgTe/CdTe
(S. C. Zhang, SCIENCE 2006)

2. 拓扑材料: Materials.

Guidelines:

1. Semiconductor with inverted band structure
2. Strong SOC



困: Real material for 3D TI?

inverted band



2. 拓扑 体: Bi_2Te_3 , Bi_2Se_3 , Sb_2Te_3

Predictions for Bi_2Te_3 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 thermoelectric materials.

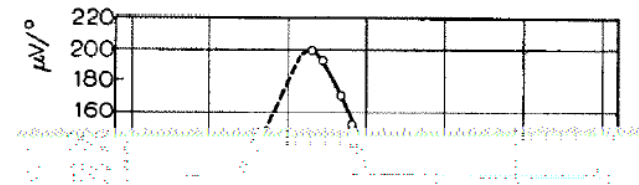
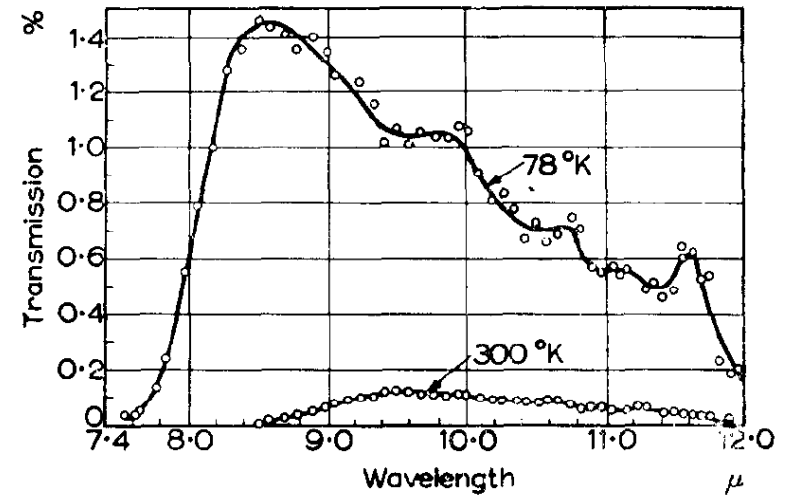
$ZT \sim 1$ at room T

4. Easy to be synthesized

5. Whole Family:

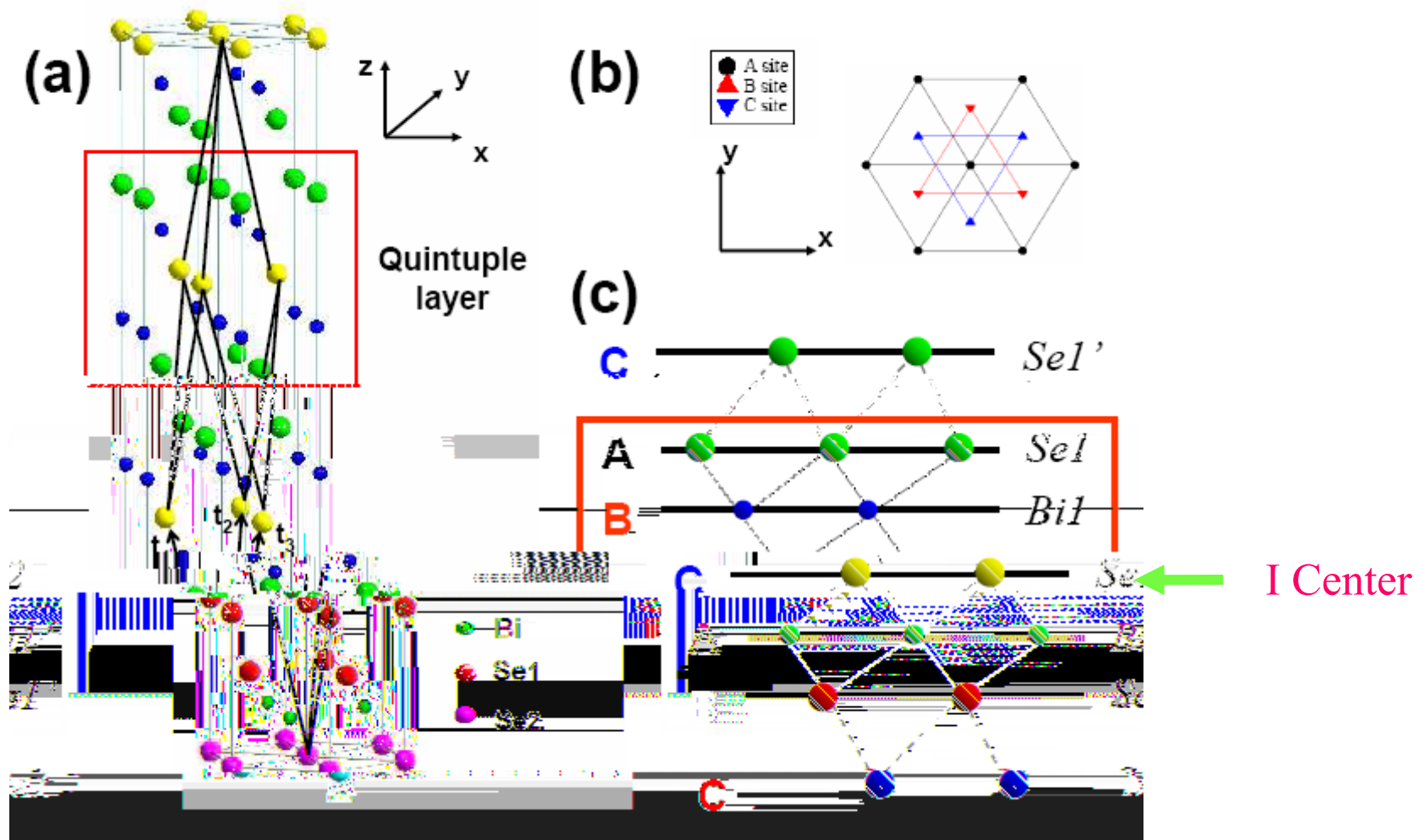
Bi_2Te_3 , Sb_2Te_3

Bi_2Se_3 , Sb_2Se_3

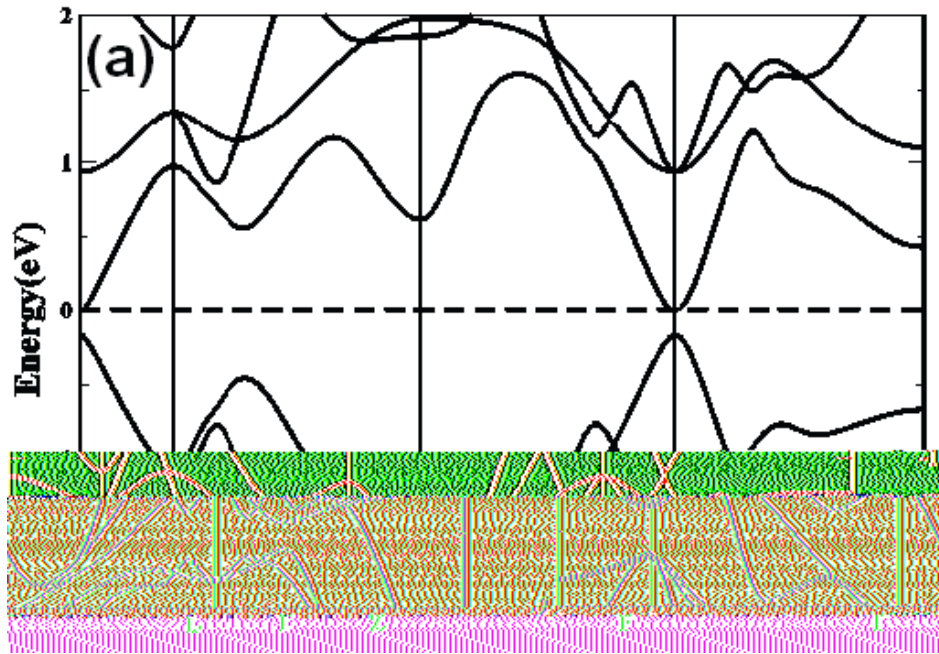


2. 拓扑 体: Bi_2Te_3 , Bi_2Se_3 , Sb_2Te_3

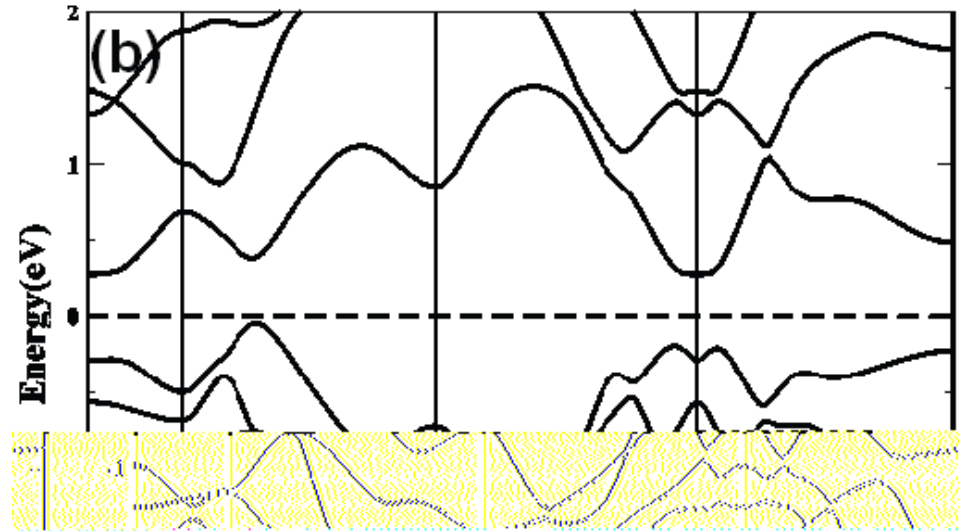
Crystal Structure $D_{3d}^5 (R\bar{3}m)$



Band Structure Bi₂Se₃

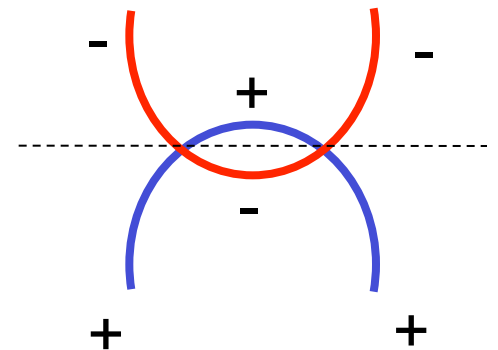


Without SOC

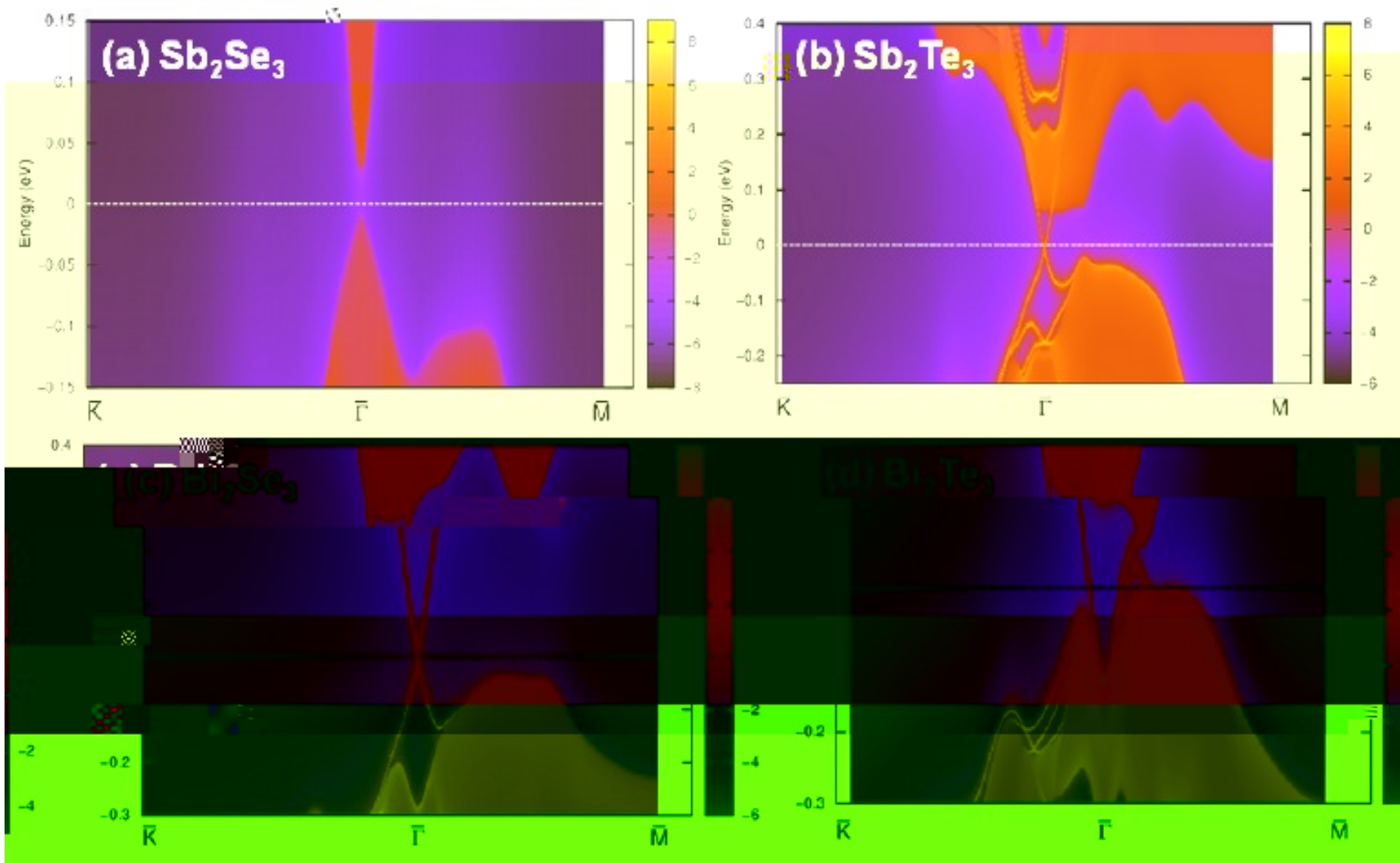


With SOC

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



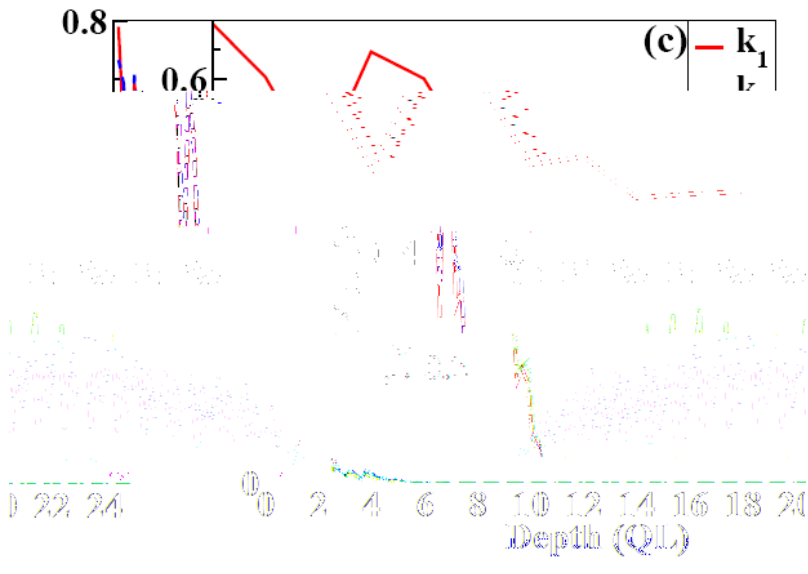
ab-initio Surface States:
 Bi_2Se_3 has the bigger Gap around 0.3eV



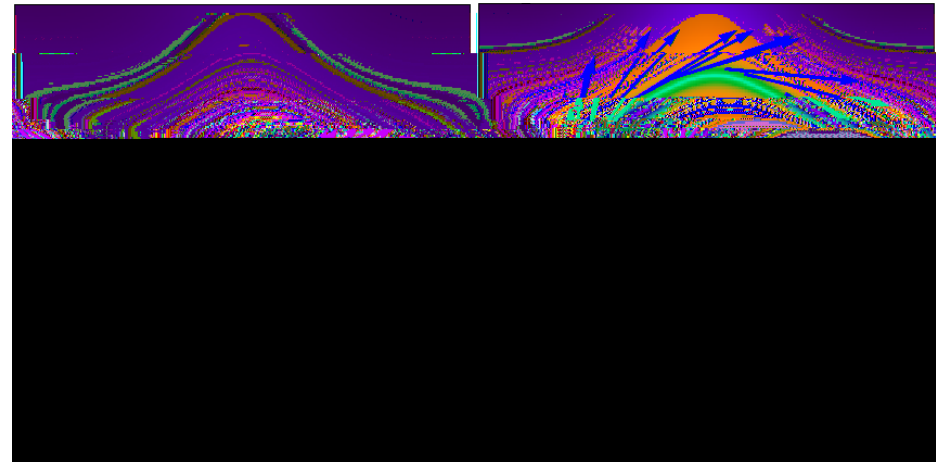
H. J. Zhang, et.al., Nature Phys. (2009)

2. Materials: Bi_2Te_3 , Bi_2Se_3 , Sb_2Te_3

Penetration Depth
of Surface state, 2nm



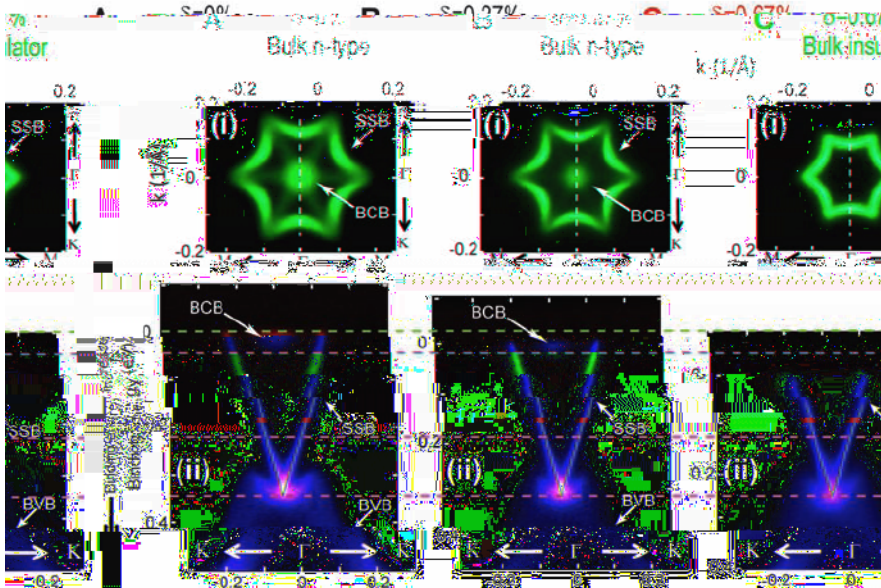
Chiral Spin texture



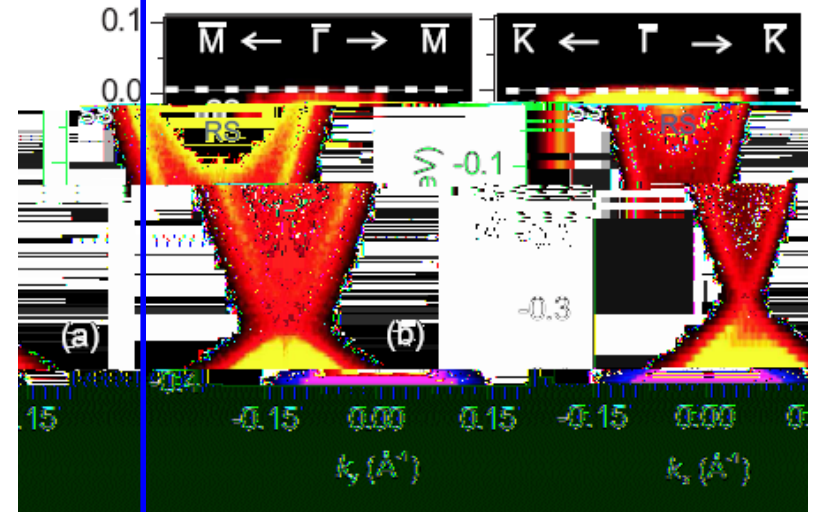
W. Zhang, et.al., New J. Phys, 12, 065013 (2010)

2. I Materials: Exp. evidence

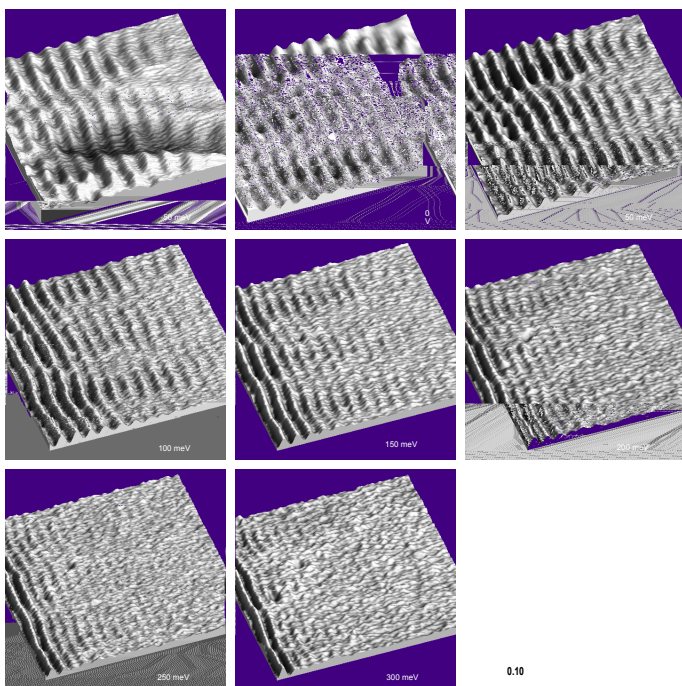
ARPES



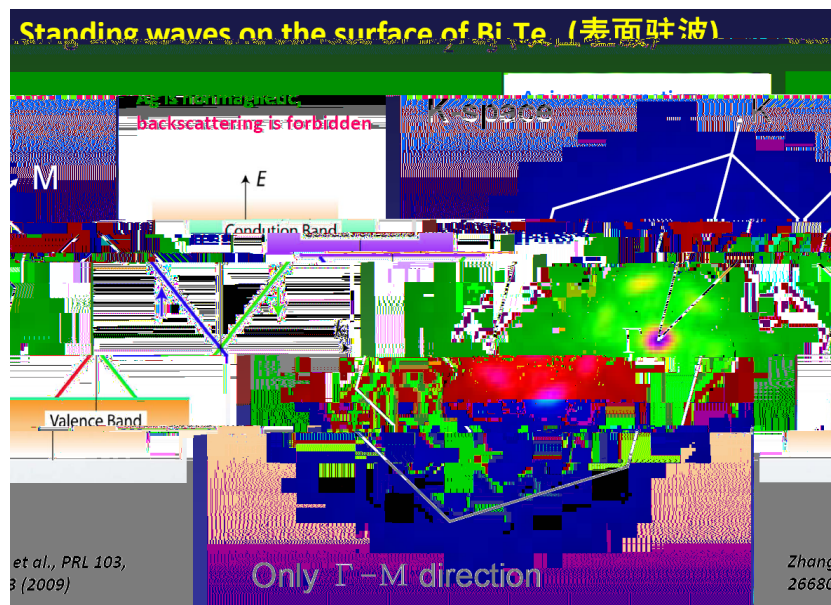
Y. L. Chen, et al.
SCIENCE (2009)
 Bi_2Te_3



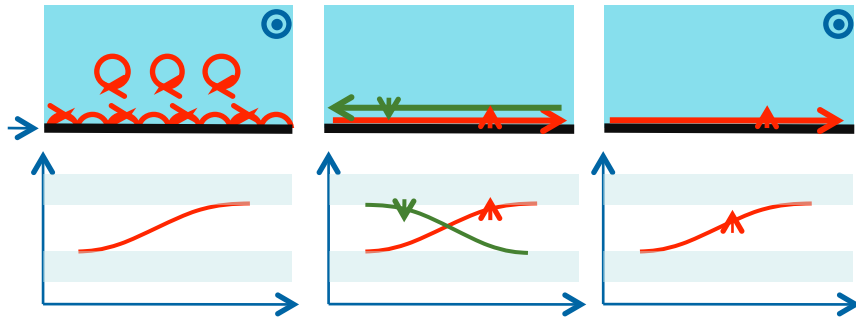
Y. Xia, et al.
Nature Physics (2009)
 Bi_2Se_3



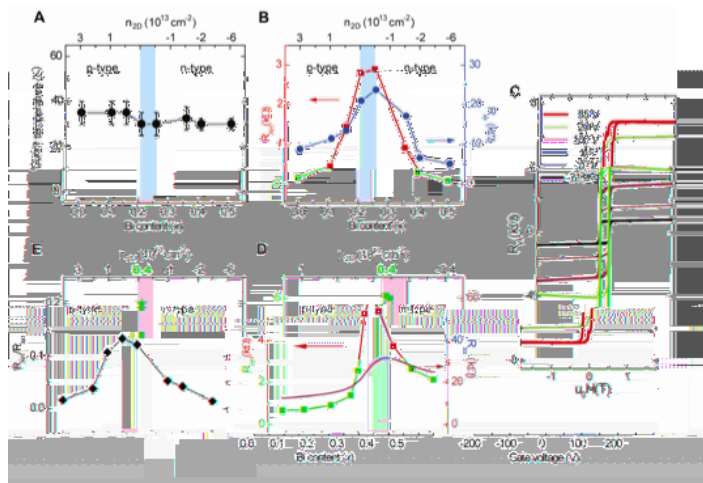
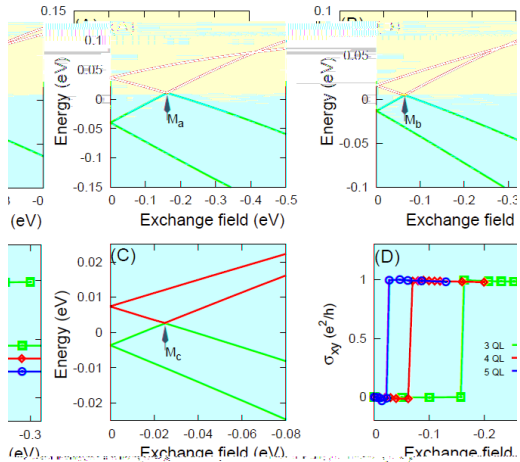
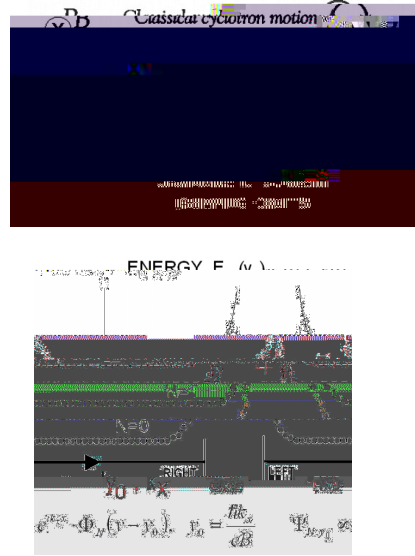
0.10



拓扑体----子化反常Hall效应



Bi₂Se₃ film doped with Cr or Fe



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

已得初实实:
何柯, 旭村, 其坤 ,
Cr-Bi₂Te₃-Sb₂Te₃ film,
arxiv: 1108.4754(2011).

子反常Hall效应
方忠、戴希 , SCIENCE(2010)
子Hall效应
无外加场实子Hall效应!

2. TI Materials: Ag_2Te

Crystal Structure:

$T > 417 \text{ K}$,

$\alpha\text{-Ag}_2\text{Te}$,

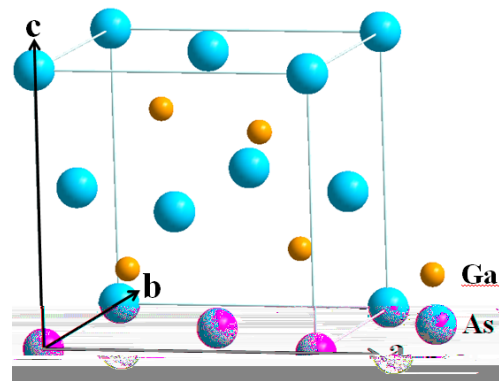
anti-fluorite ($\text{Fm}\bar{3}\text{m}$)

$T < 417 \text{ K}$,

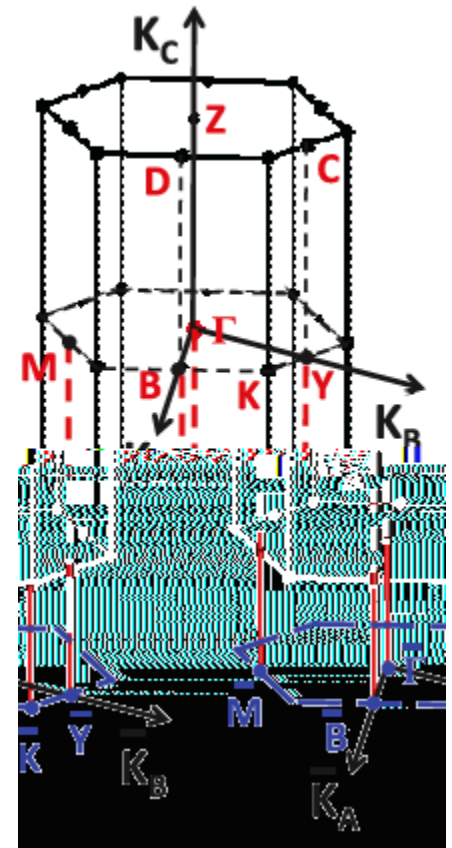
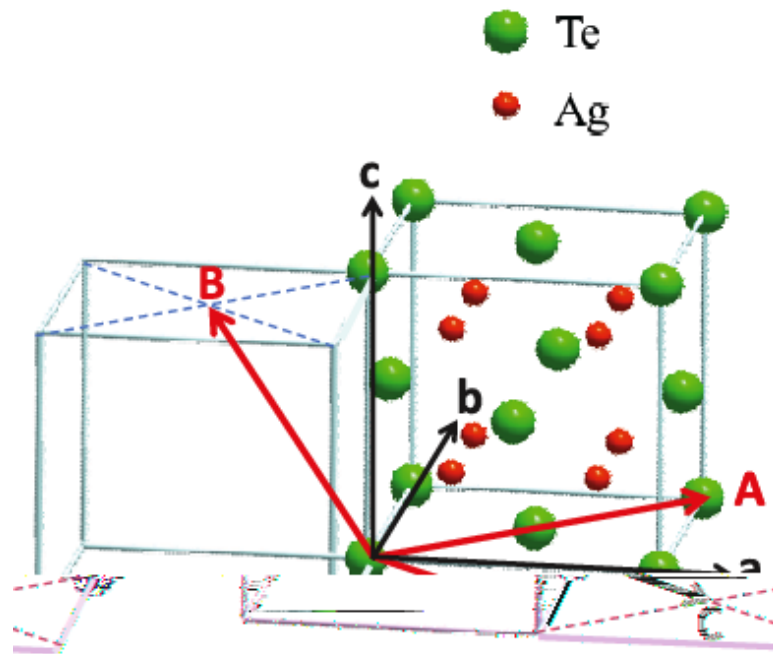
$\beta\text{-Ag}_2\text{Te}$,

distorted ($\text{P}2_1/\text{c}$)

Cubic: a, b, c

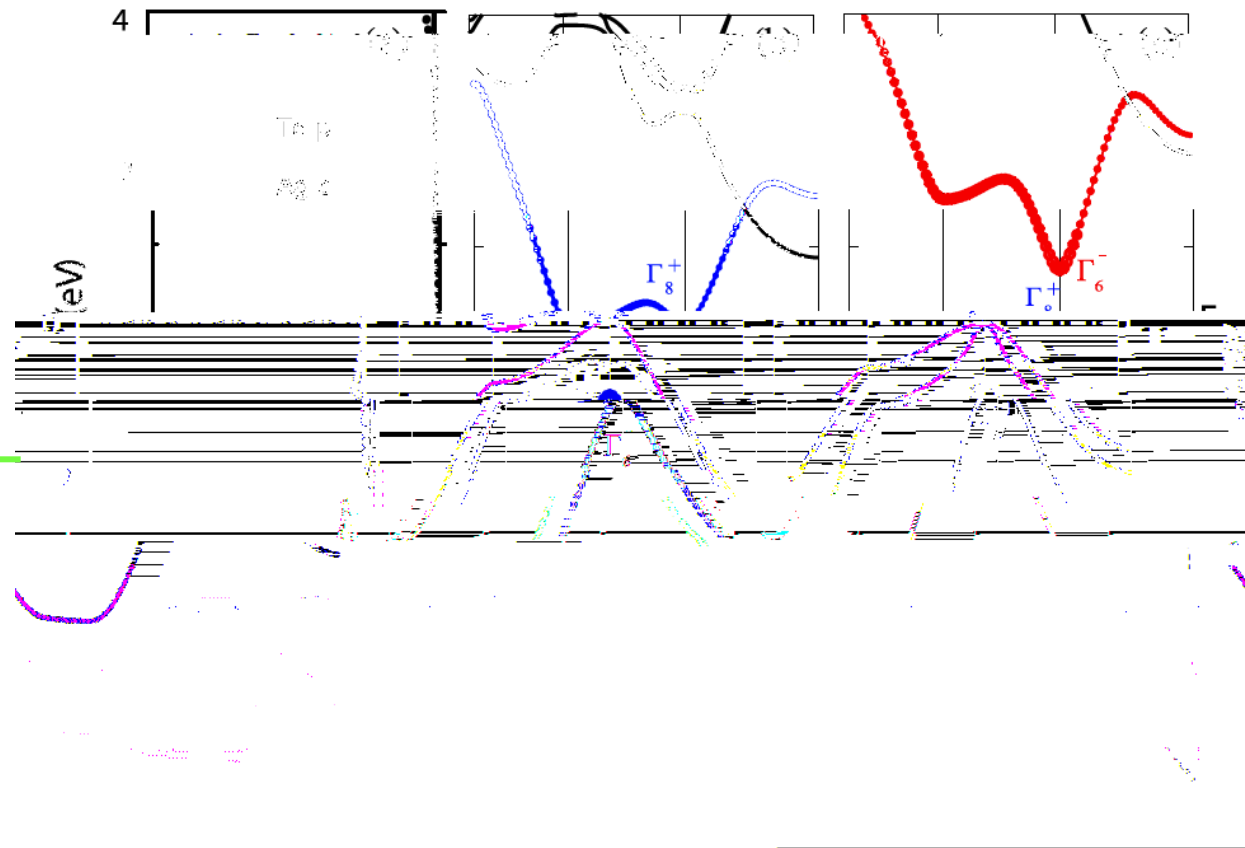
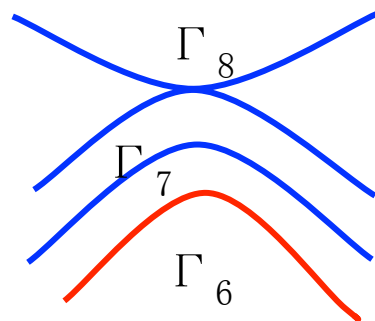
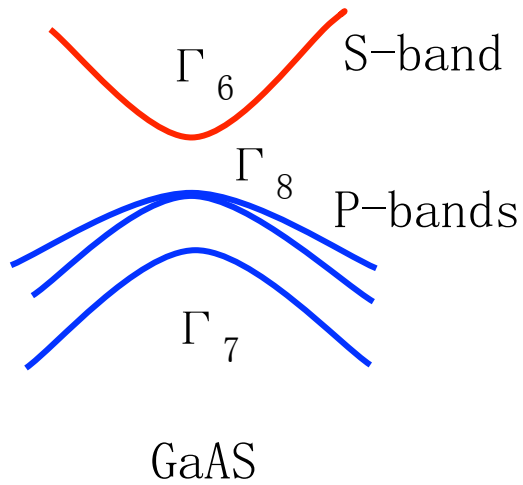


GaAs



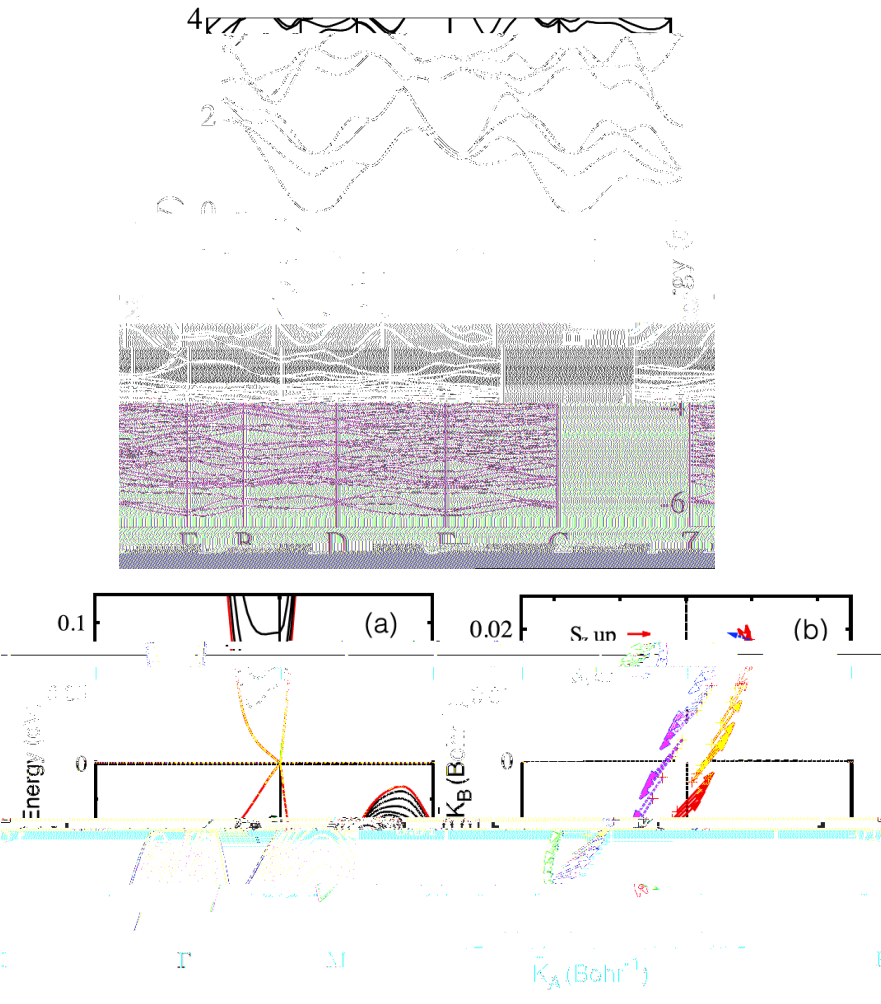
2. TI Materials: Ag_2Te

Inverted Band Structure of $\alpha\text{-Ag}_2\text{Te}$ Similar to HgTe

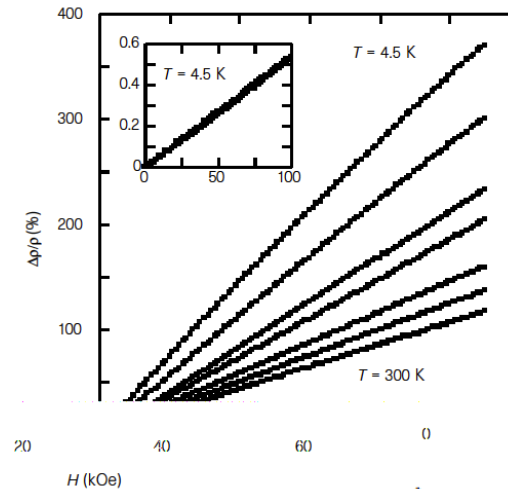


2. TI Materials: Ag_2Te

β - Ag_2Te , gap=80meV



Quantum Magneto-resistance in $\text{Ag}_{2+\delta}\text{Te}$



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:

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

Linear Dispersion is Important!
Landau Level Spacing. $\propto \sqrt{B}$

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

3.

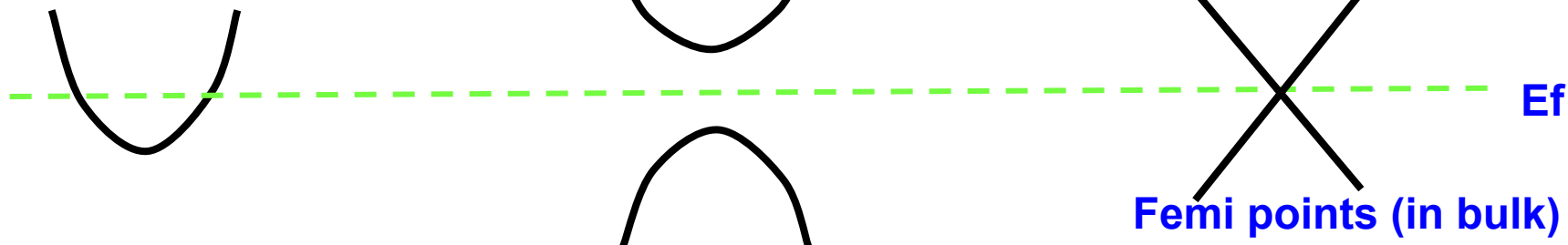
Moment in Space Topology

Three distinct stable classes in 3D:

Metals

Insulators

Semi-metal



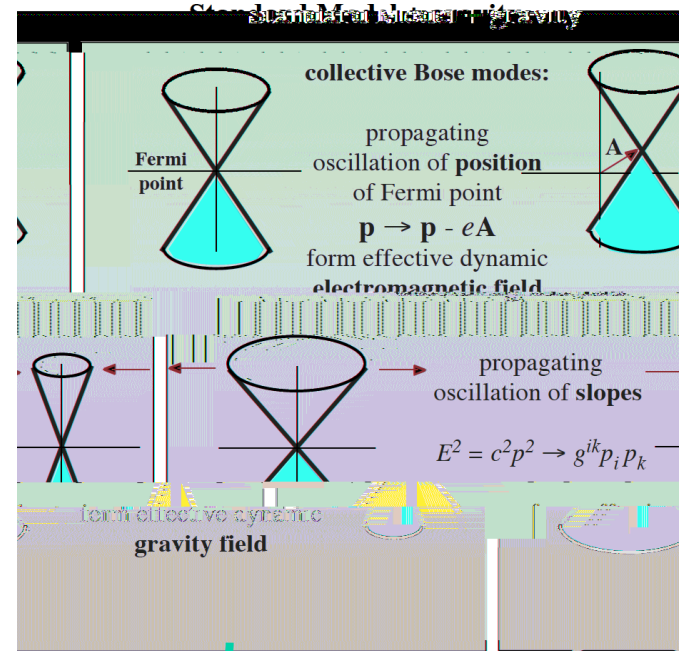
Fermi surface

No fermi surface

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

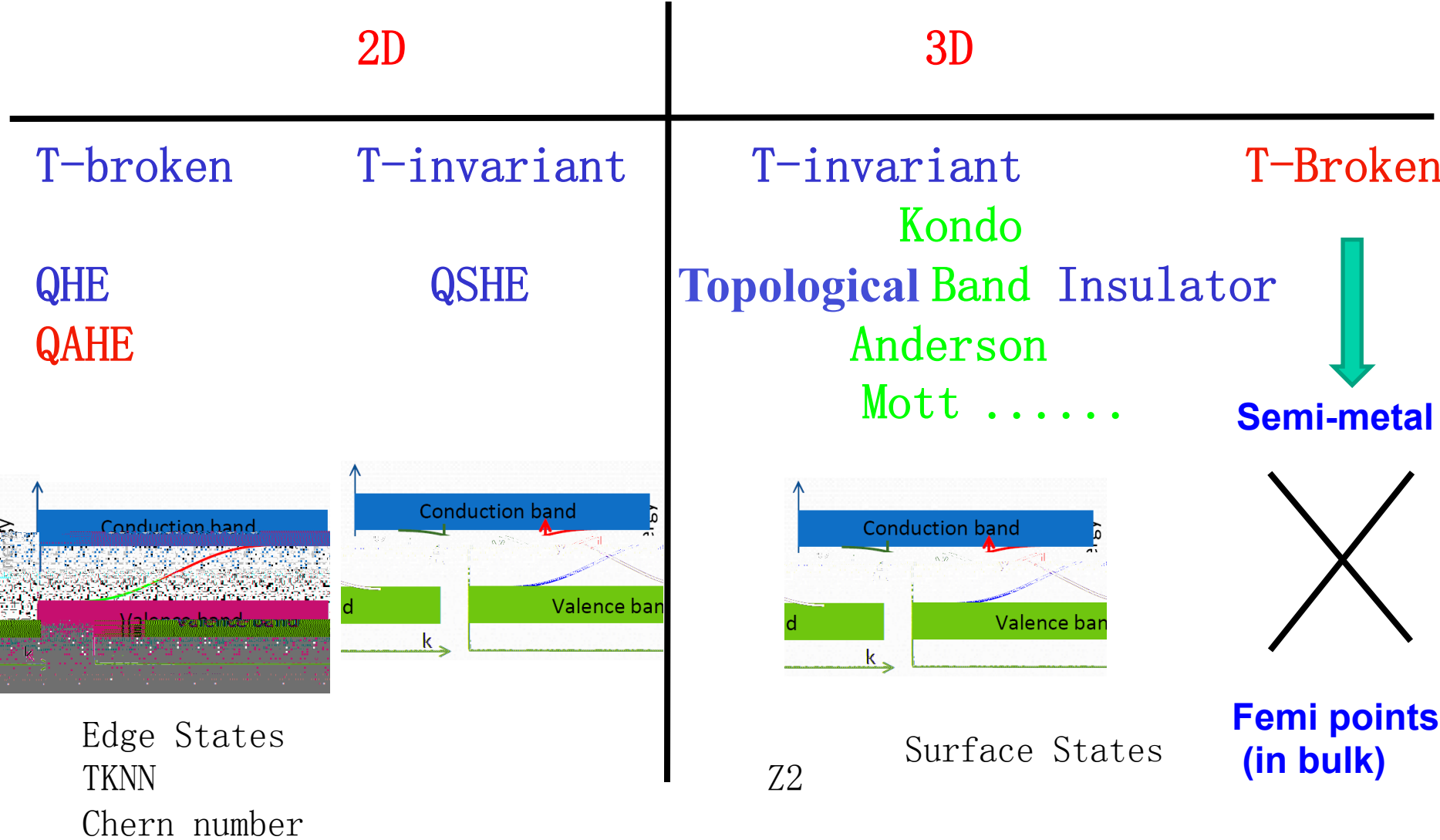


Normal Insulators
+
Topological Insulators
(Weyl points at Boundary)



Our Subjects

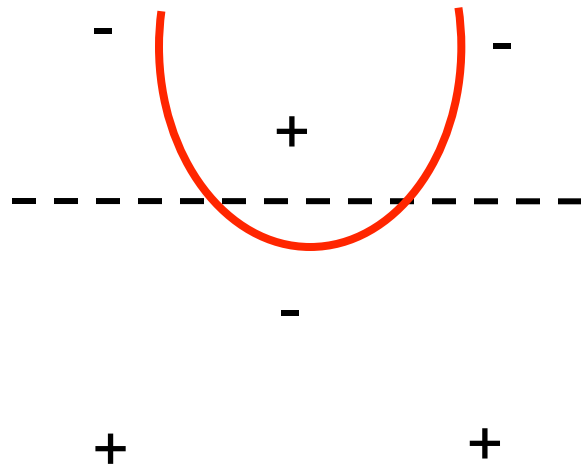
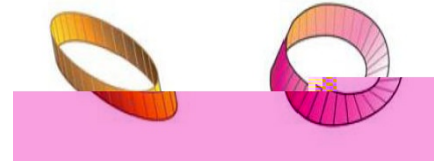
3. 拓扑半 属: Family of TIs?



3. S

: From 2D to 3D without TRS?

2D Chern Insulators:



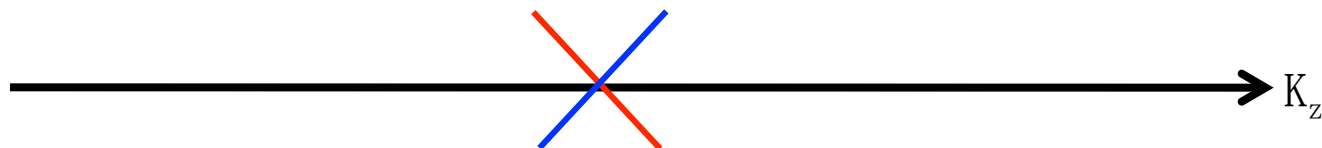
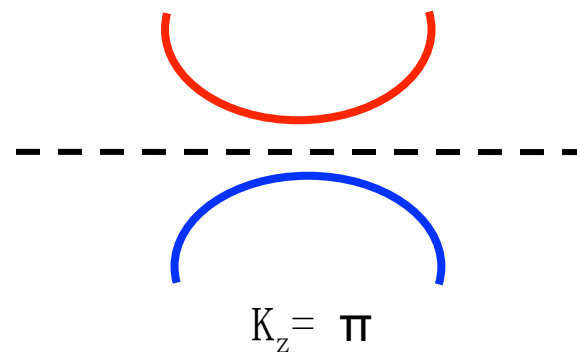
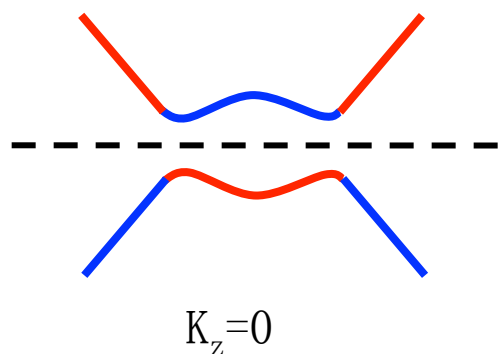
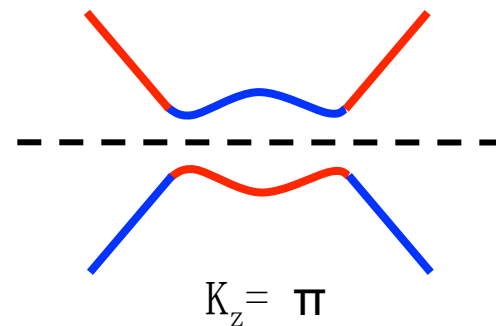
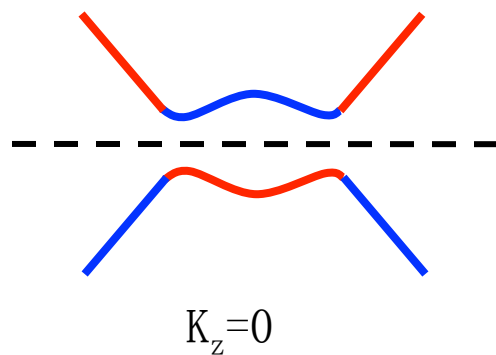
Gap opening
due to SOC



3. S

: Chern Insulators and semi-metal?

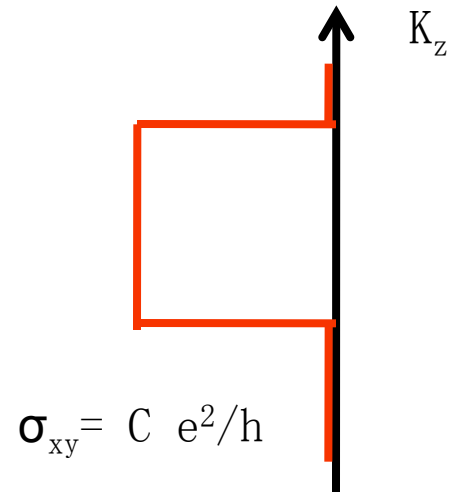
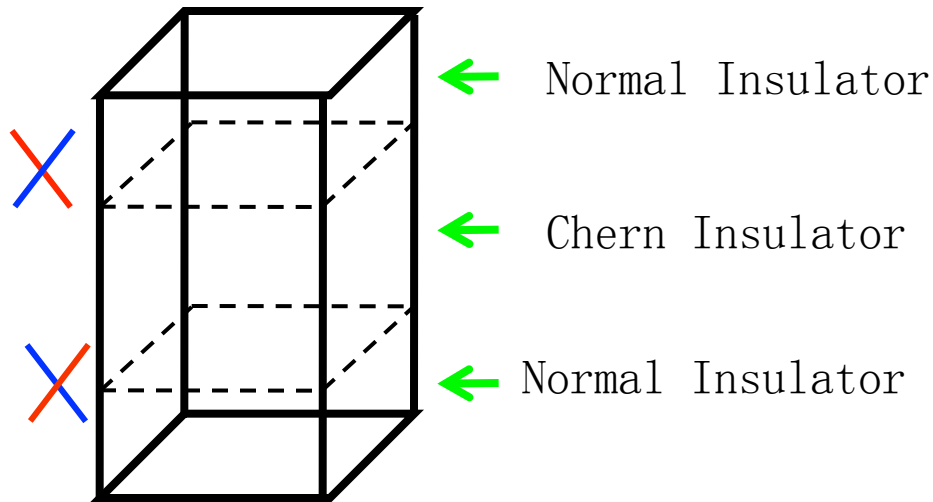
Weak Chern Insulators:



Topological Phase Transition

3. S

: Chern semi-metal?



2x2 Hamiltonian in Bulk (not 4x4):

$$H(\vec{k}) = \epsilon_{\pm}(\vec{k}) + \vec{p}(\vec{k}) \cdot \vec{\sigma}$$

$$\vec{p}(\vec{k}) = \vec{p}(\vec{k}) + \vec{p}(\vec{k}) + \dots$$

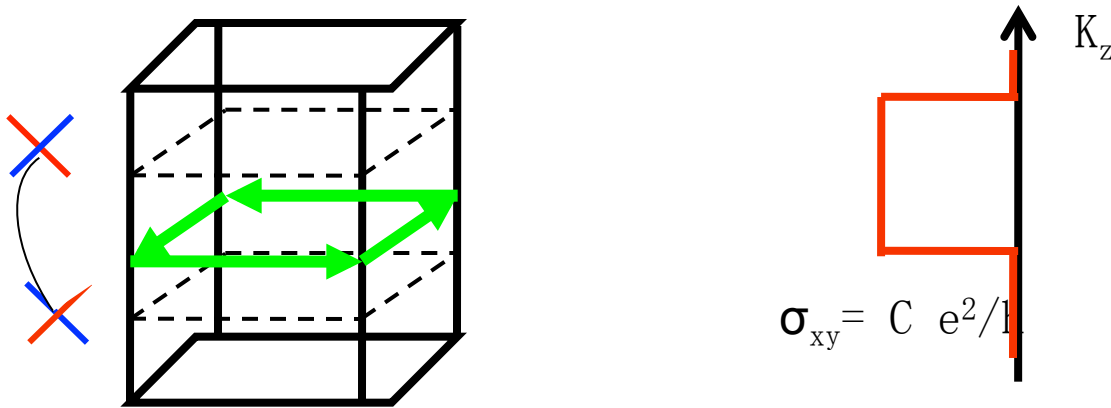
3. $\mathbf{S}$: Chern semi-metal?

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

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

$$\vec{\Omega} = \pm \frac{\vec{f}}{|\vec{f}|^3} \quad \text{around} \quad |\vec{f}|=0 \quad (\text{See, Z. Fang, Science (2003)})$$

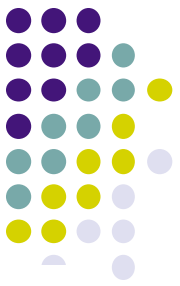
(3) Fermi arcs on the side surface.



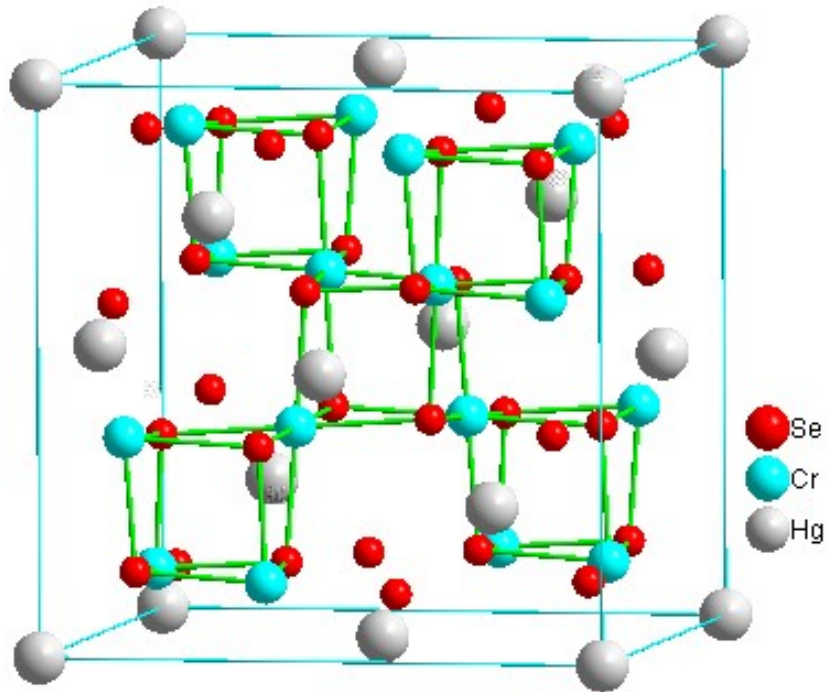
(See, X. G. Wan & Savaraso, PRB (2011), on AF Pyrochlore iridates)

(4) QAHE in quantum well structure.

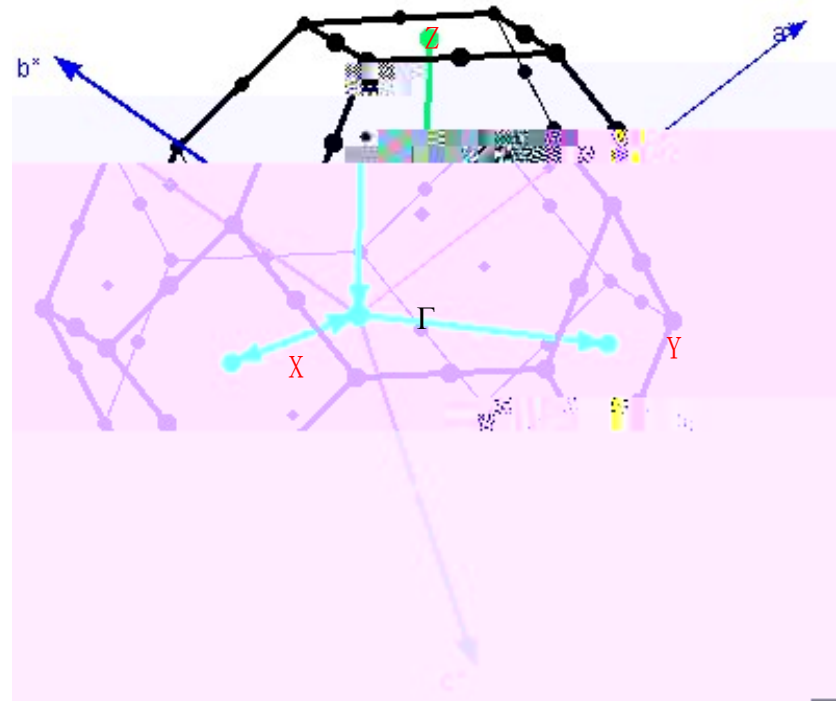
Crystal structure of HgCr_2Se_4



Crystal structure



BZ



HgX sublattice is zinc-blende

Two HgX sublattice are connected by Inversion, like Diamond.

Space group $Fd\bar{3}m$ (point group O_h).

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

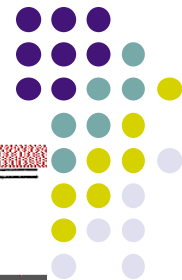


TABLE II. Magnetic and crystallographic properties of ferromagnetic spinels.

Composition	Lattice parameter a , Å	a , Å	Magnetic moment (4.2°K) μ_B /molecule	Curie temp T_c , °K	Curie-Weiss θ , °K	Curie constant C_M	θ
Fe_3O_4	8.44	8.44	4.1	858	190	0.75	190
Mn_3O_4	8.44	8.44	4.1	43	190	0.75	190
Co_3O_4	8.44	8.44	4.1	125	190	0.75	190
Ni_3O_4	8.44	8.44	4.1	253	190	0.75	190
Cu_3O_4	8.44	8.44	4.1	230	190	0.75	190
Zn_3O_4	8.44	8.44	4.1	0	190	0.75	190
CdCr_2Se_4	8.44	8.44	4.1	0	190	0.75	190
HgCr_2Se_4	8.44	8.44	4.1	0	190	0.75	190

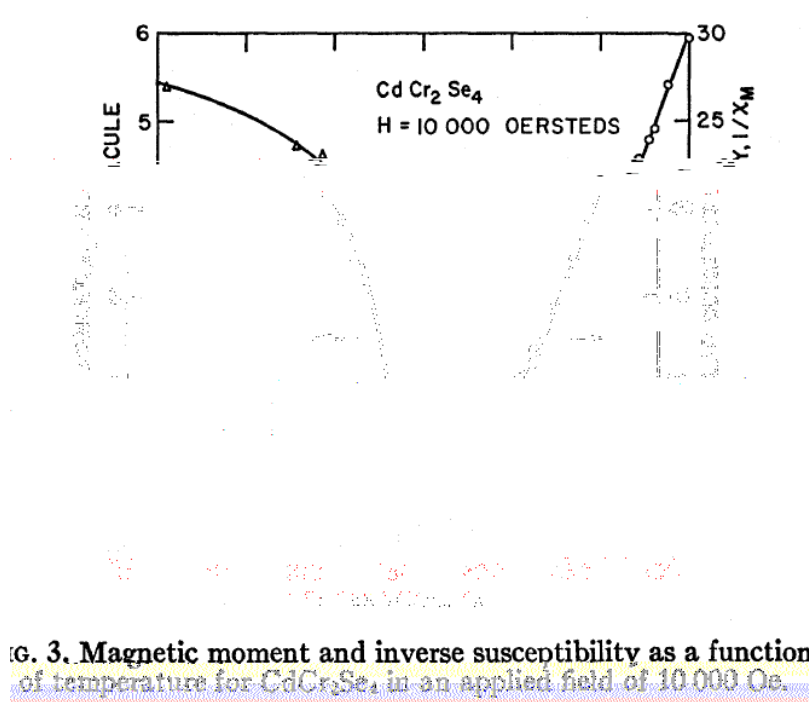
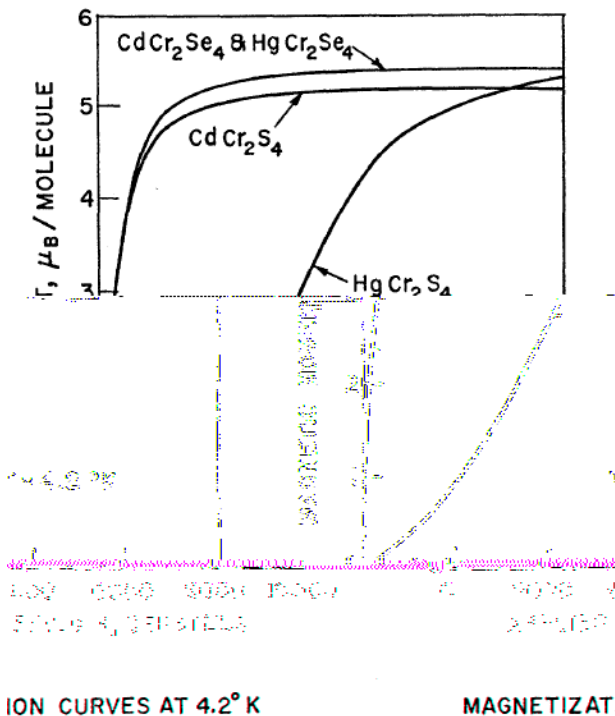
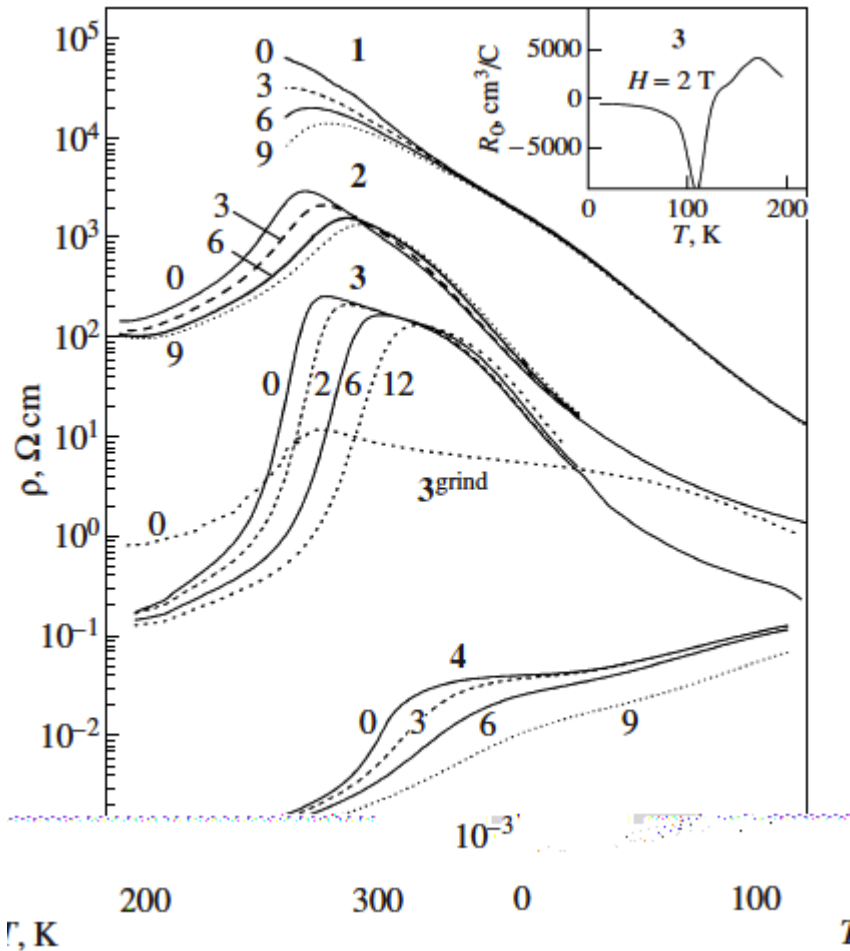


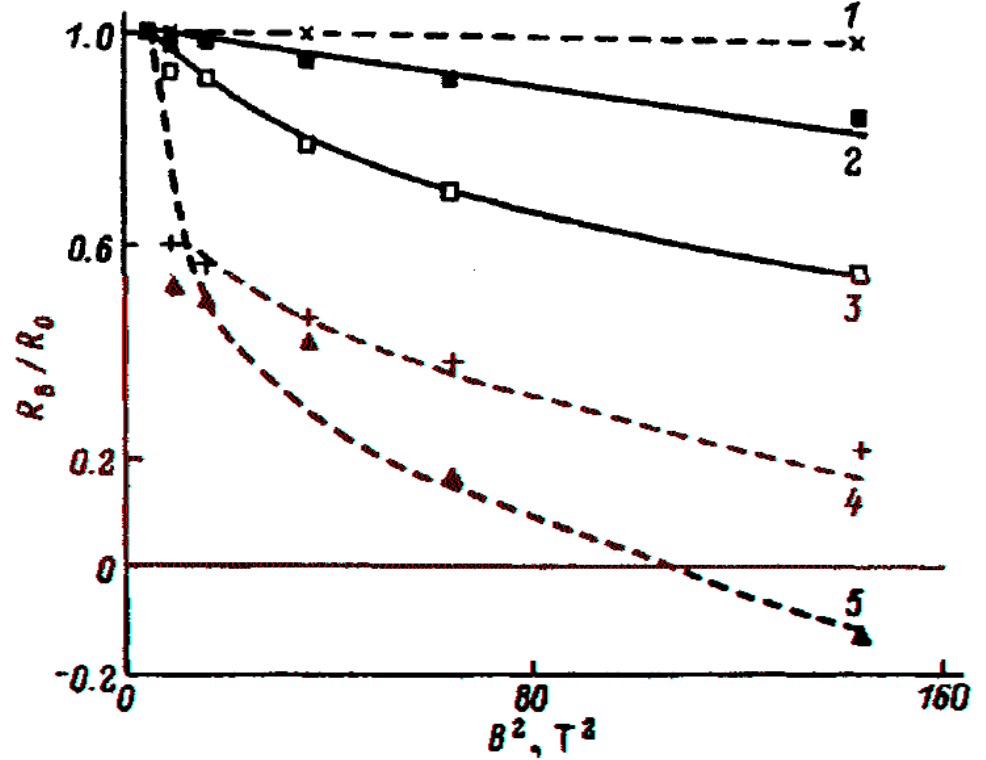
Fig. 3. Magnetic moment and inverse susceptibility as a function of temperature for CdCr₂Se₄ in an applied field of 10 000 Oe.

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



Metallic

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

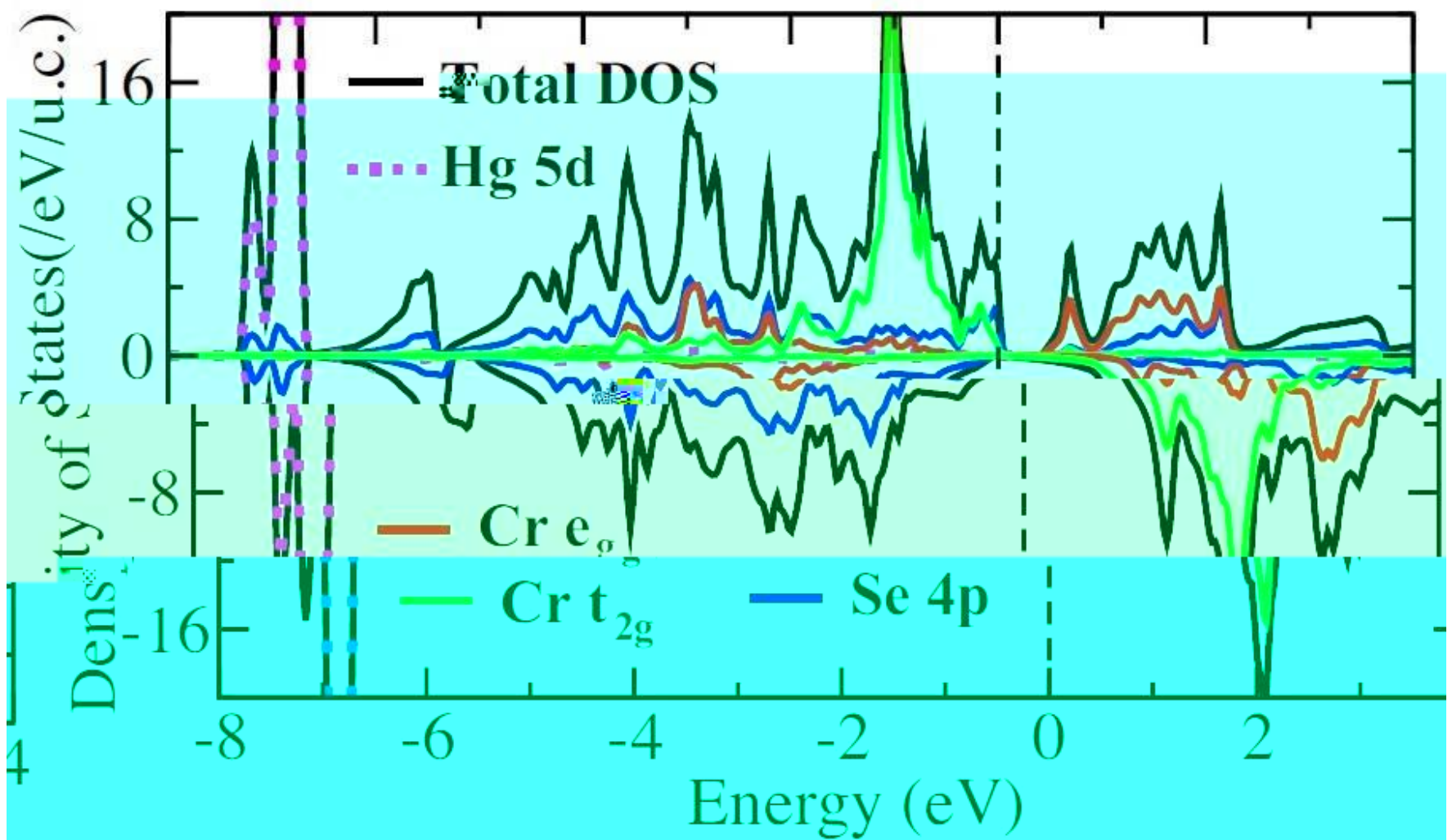
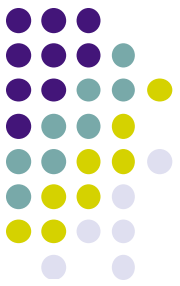


AHE

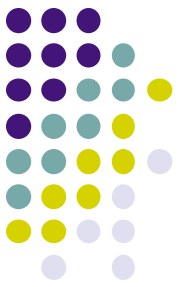
N. I. Solin, et.al,
Phys. Solid State (1996)

Electronic structure without SOC

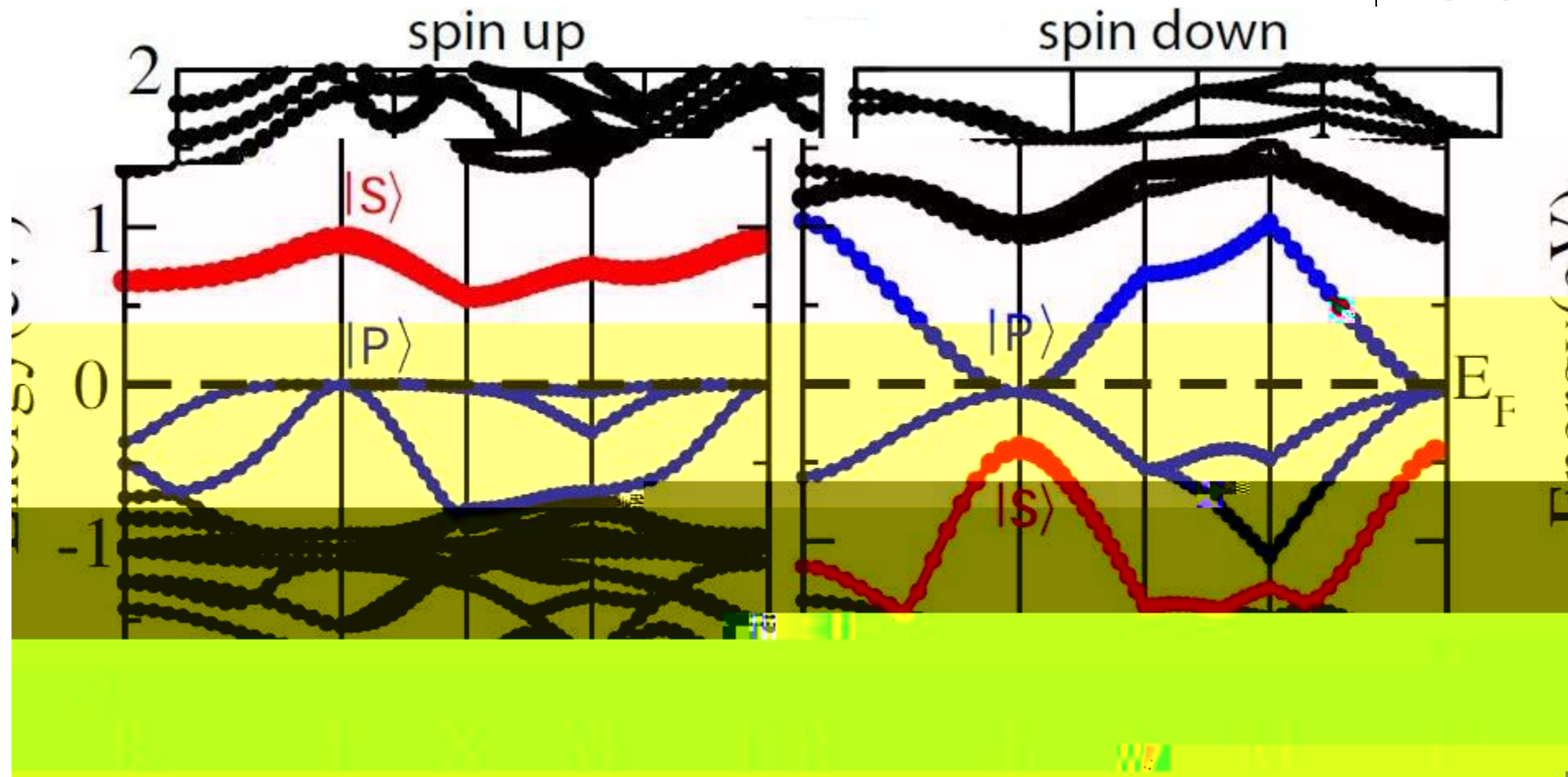
DOS



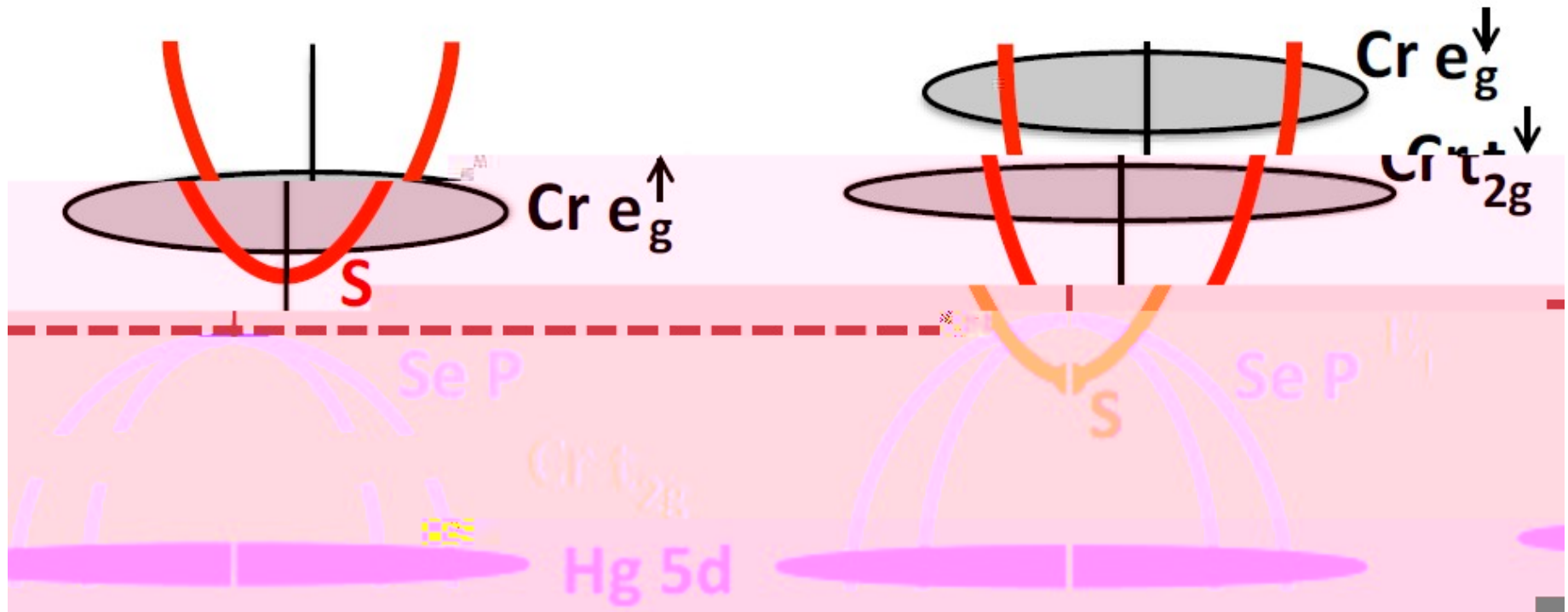
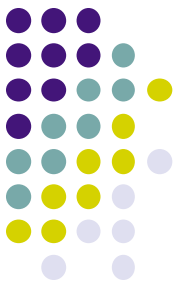
Electronic structure without SOC



Band

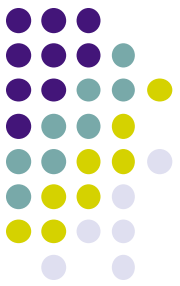
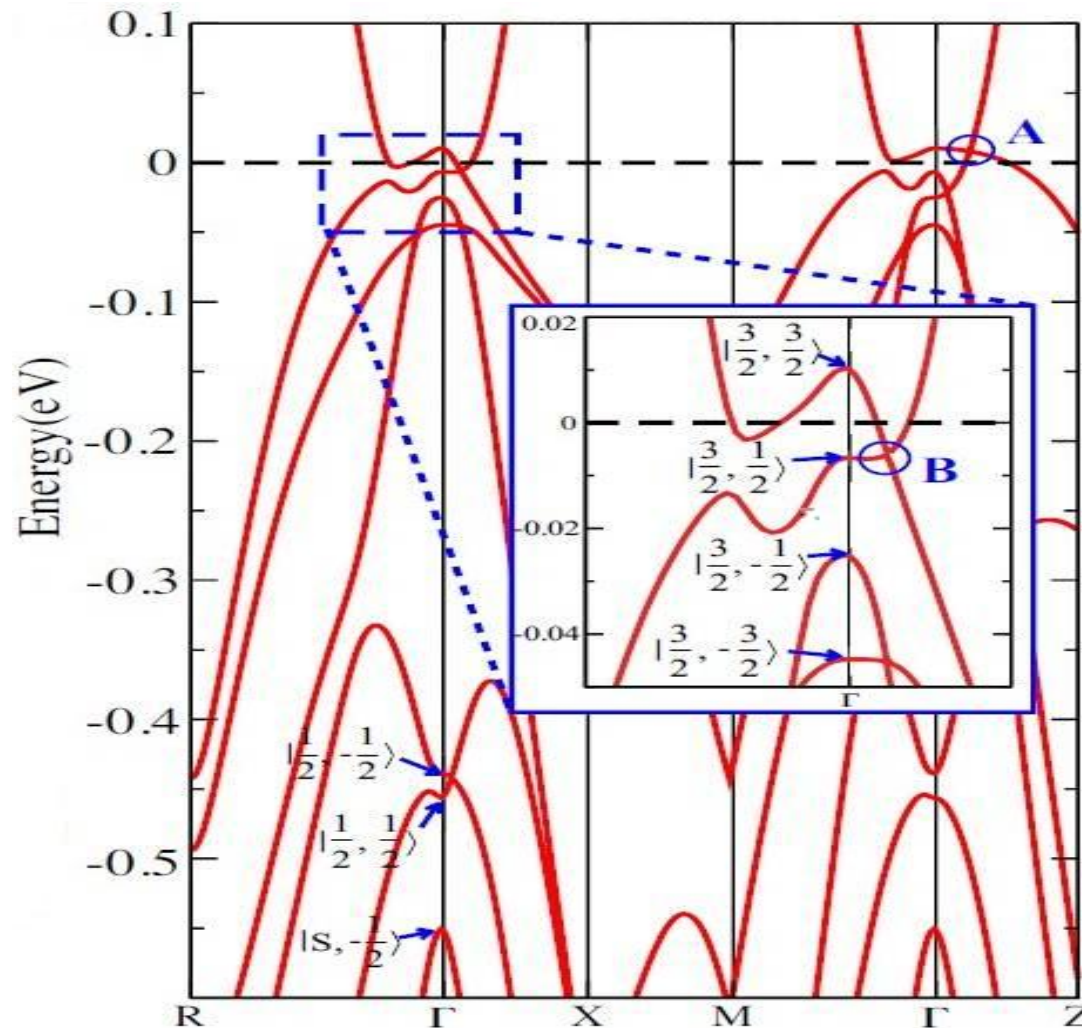


Schematic diagram for the band-inversion

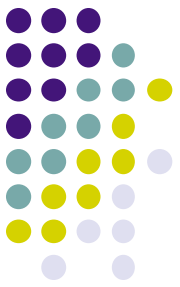


Electronic structure with SOC

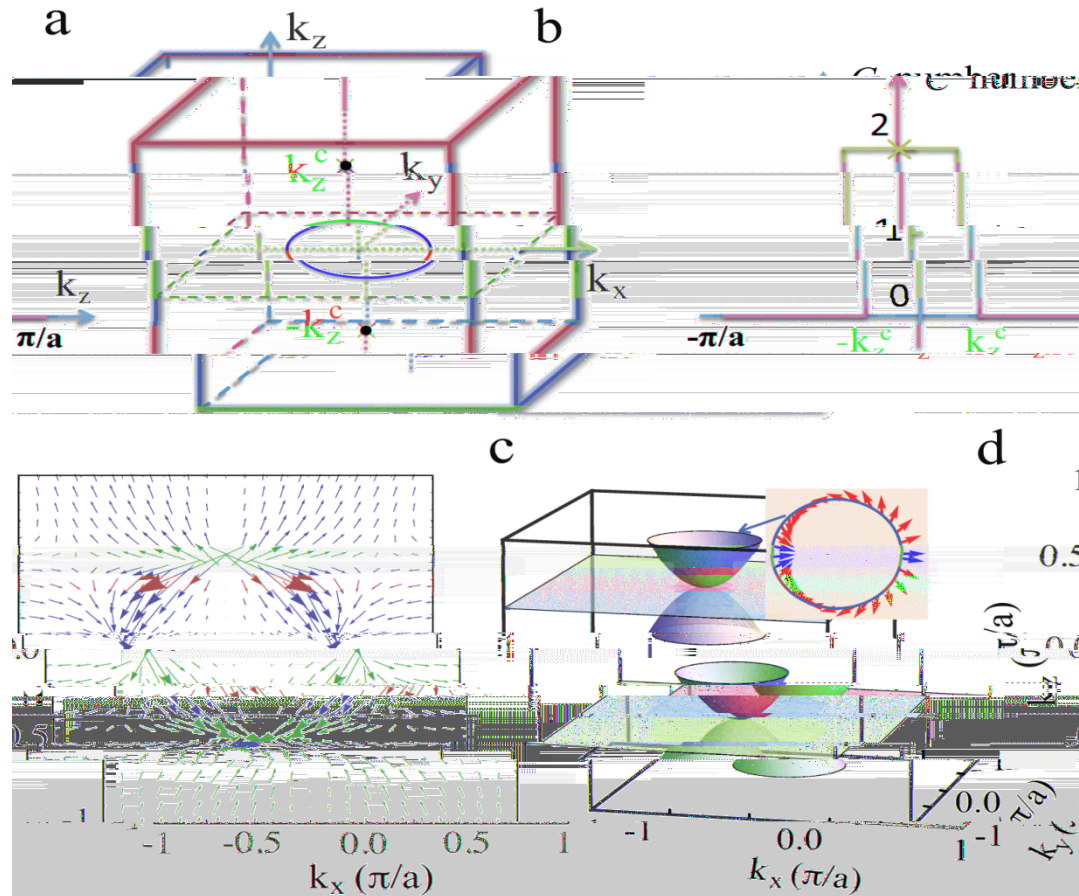
low energy band with SOC



Weyl fermions and magnetic monopoles



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



The in-plane band dispersions near the $k_z = \pm k_z^c$ 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: $|3/2, 3/2\rangle$, $|S, -1/2\rangle$ with band-inversion

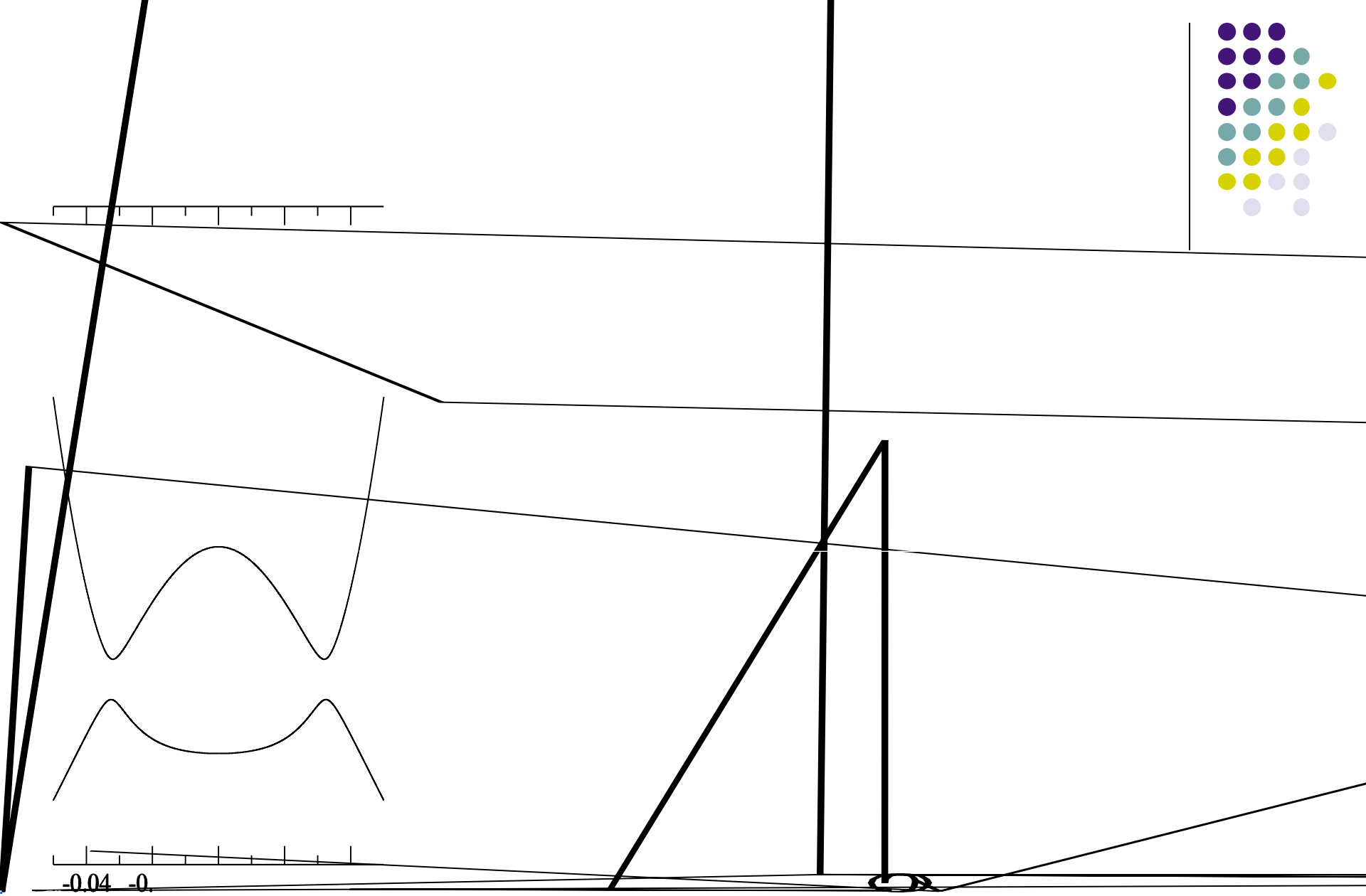
$$H_{eff} = \begin{bmatrix} M & Dk_{\pm}^2 \\ Dk_z^2 & M \end{bmatrix}$$

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.

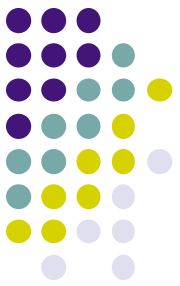
$$E(\mathbf{k}) = \pm \sqrt{M^2 + D^2 k_z^2 (k_x^2 + k_y^2)} \quad \text{two gapless solutions:}$$

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

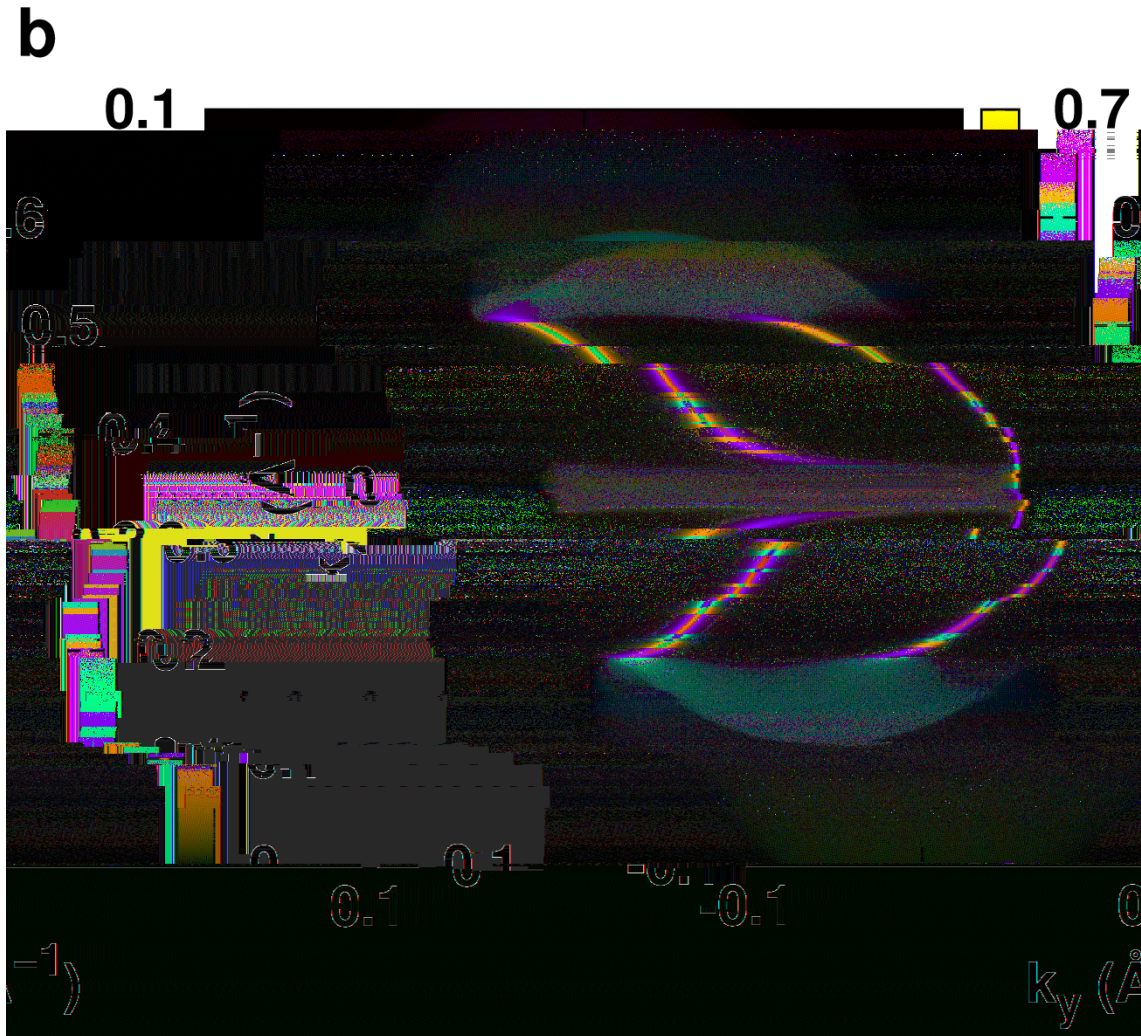
$$k_x^2 + k_y^2 = M_0 /$$



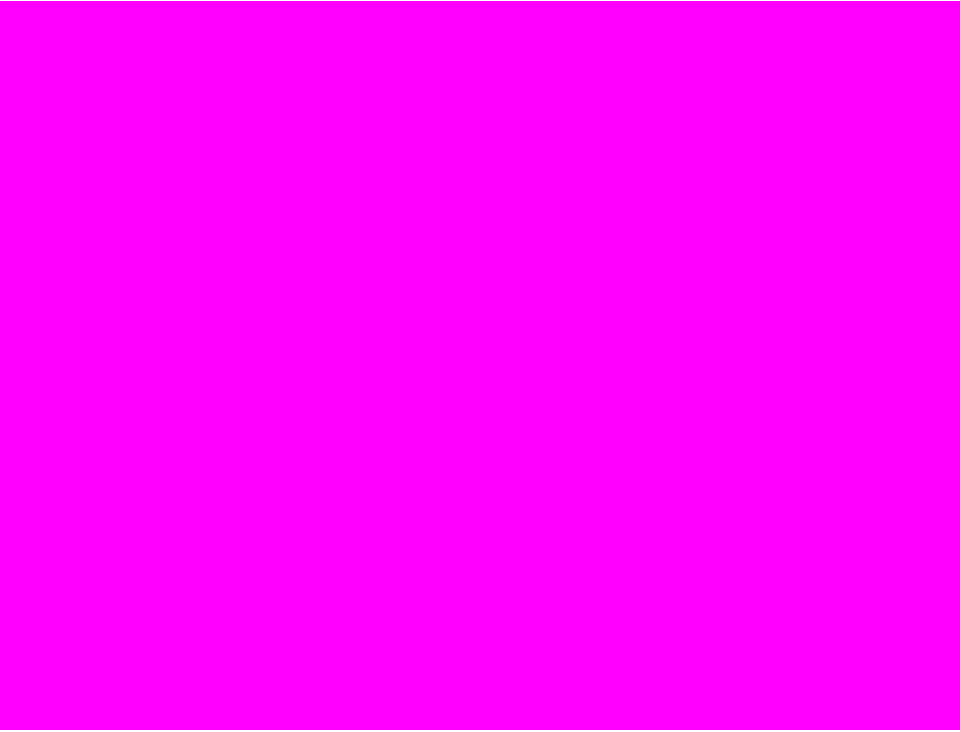
Edge states and fermi arcs on surface



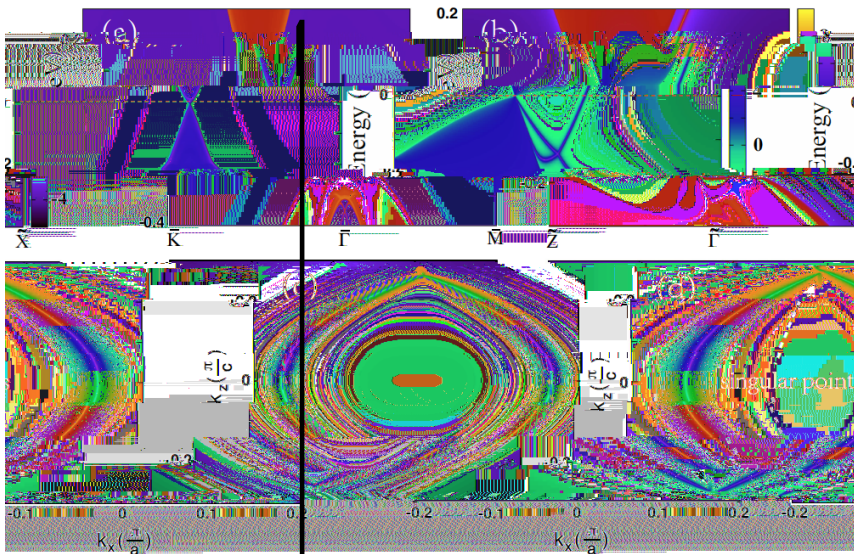
Fermi arcs for the (k_y , k_z) side surface



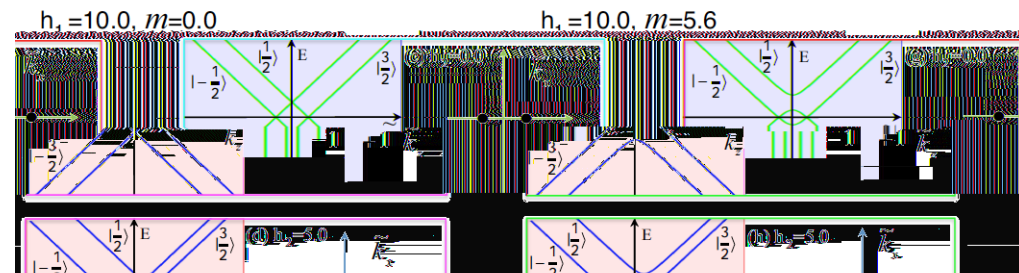
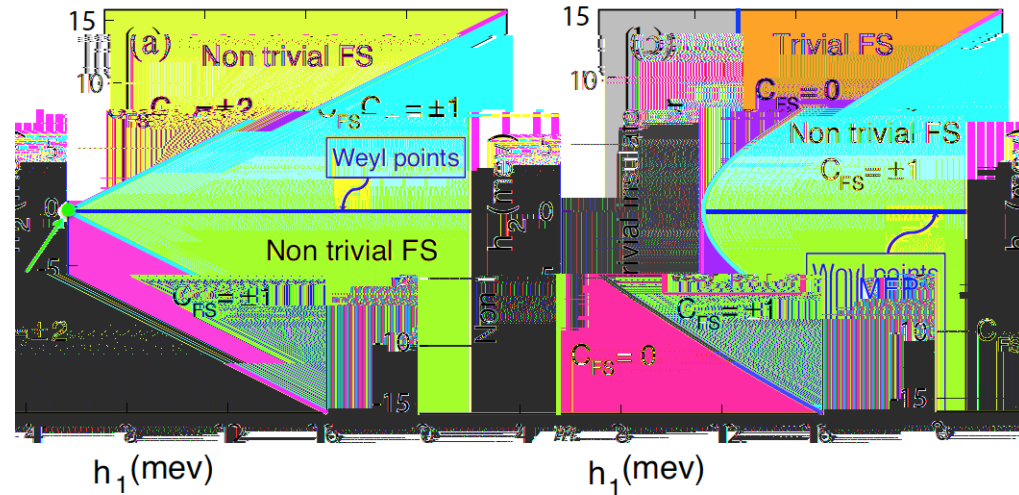
Fang & Dai, et.al, PRL (2011)



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Marginal Fermi point in
 $\text{Na}_3\text{Bi}, \text{K}_3\text{Bi}, \text{Rb}_3\text{Bi}$
 ArXiv: 1202.5636 (2012)



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