拓扑量子态与拓扑电子材料

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Acknowledgement:

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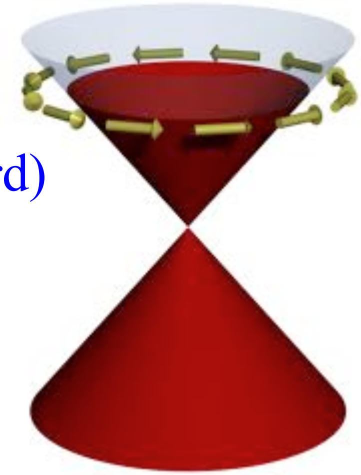


Contents

一、简介：对称性，拓扑量子态

二、拓扑不变量：

三、拓扑量子态（动量空间）：

（1）Chern Insulators

（2）Z_2 Topological Insulators

（3）Topological Semimetals

（4）Topological Superconductors

四、拓扑电子材料：

Bi_2Se_3, Bi_2Te_3, Cr-Bi_2Te_3, $HgCr_2Se_4$, Na_3Bi, Cd_3As_2, etc.

一、简介：对称性

“对称性”是物理学研究的重要部分

1)，对称性：➔ 守恒量

例如，Lorentz不变性：时间平移 ➔ 能量守恒
空间平移 ➔ 动量守恒，
空间旋转 ➔ 角动量守恒

2)，对称性分类：丰富多彩

例如：局域与整体对称性，分立与连续对称性
Time-Rversal, Parity, Gauge, Particle—Hole, etc

3)，对称性破缺：➔ 物质状态改变

（1）直接对称性破缺：Hamiltonian对称性破缺
（2）自发对称性破缺：H没有破缺，但是波函数对称性破缺

一、简介：凝聚态物质 ➔ 准粒子（低能物理）

- **电子** ➔ 三个量子特征，电荷、自旋、轨道
- **准粒子** ➔ 集体激发，相干性
- **费米统计** ➔ 化学势、费米面
- **晶体** ➔ 能带理论，动量空间

多体、多自由度？
强关联？
宏观量子现象？

电子的三个量子自由度

电荷 | 自旋 自旋—轨道耦合 | 轨道

电荷	自旋	轨道
传统电子学	自旋电子学	轨道电子学
传统电子器件	GMR、TMR 自旋注入产生稀磁半导体 用于硬盘	氧化物CMR

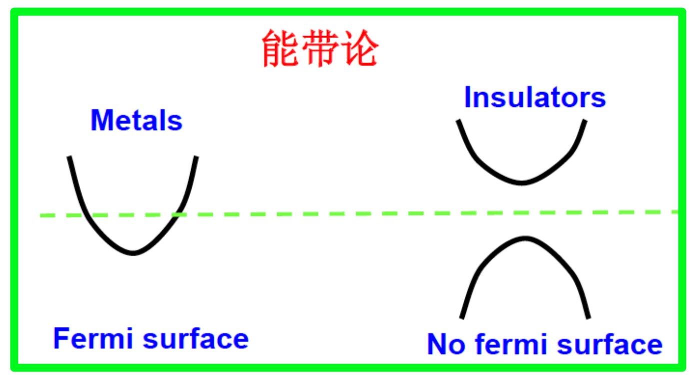
传统电子器件利用了电荷动力学，**但已达到瓶颈！**

拓扑电子学

丰富的有序态，新奇量子现象

自旋Hall、反常Hall效应，以及自旋与轨道输运特性等。

这三种自由度存在着耦合与竞争，会产生许多新奇的现象与特性。



一、简介：量子有序态

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

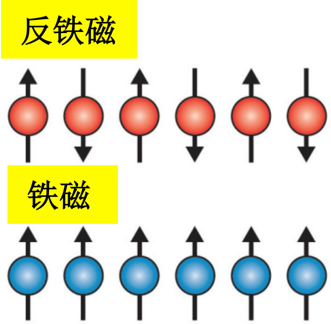
整体有序态：

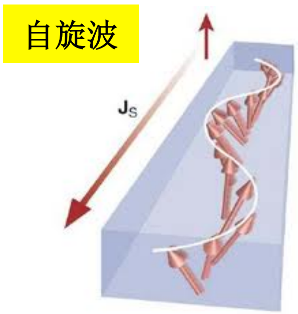
拓扑量子态
（量子物理与几何的完美结合）

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”

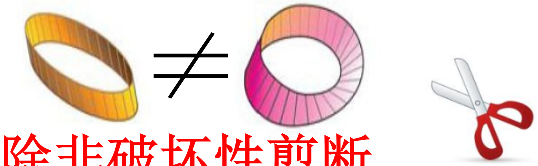
拓扑“1”

$\rho = \langle \Psi | \Psi \rangle$ VS. $|\Psi\rangle = e^{i\phi}|\psi\rangle$ Phase 非常重要

一、简介：拓扑量子态 ⟹ 新物态、新奇量子现象

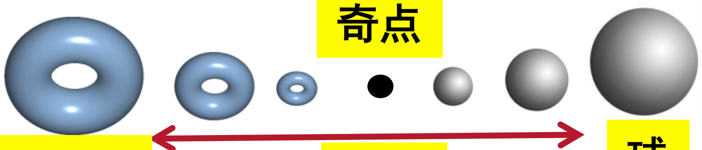
拓扑量子态的优点：对细节不敏感

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

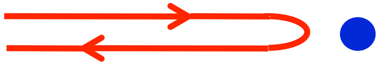
2. 与“奇点”密切相关，
   在边界上会有特殊量子态



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

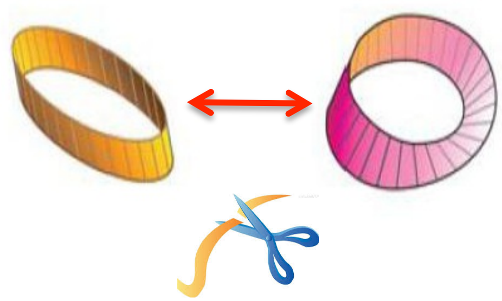
拓扑有序态

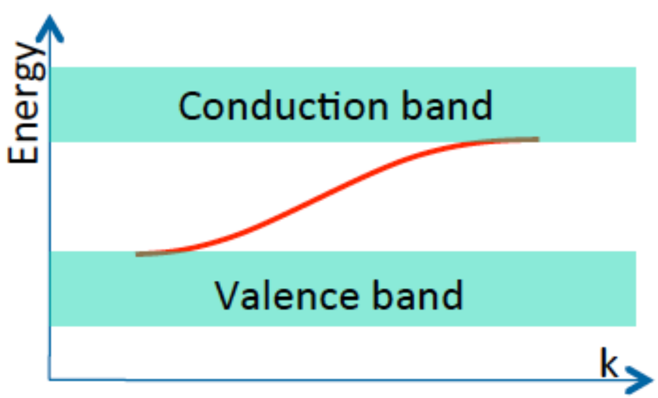
各行其道，永不混杂

遇到杂质，自动绕行

一、简介：拓扑态的边界效应

"twisted band"

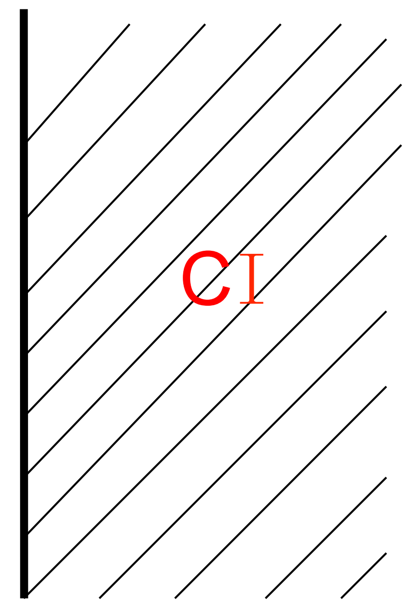




Boundary State

Boundary

Vaccum
Normal
insulator



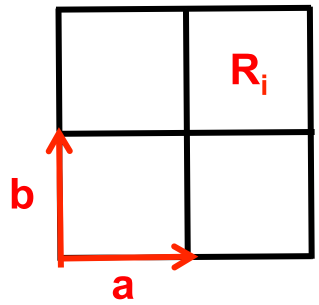
N=0 N=1

Cut:

No adiabatic connection between two sides

二、拓扑不变量：晶格平移不变性与动量空间

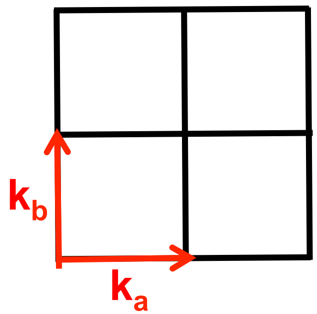
实空间：



$$H(\vec{r}) = H(\vec{r} + \vec{R}_i)$$

Bloch State： $\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r})$ $\quad H(\mathbf{r})\psi_{n\mathbf{k}}(\mathbf{r}) = \varepsilon_{n\mathbf{k}}\psi_{n\mathbf{k}}(\mathbf{r})$

倒空间（动量空间）：
（第一布里渊区）



$$H_{\mathbf{k}} = e^{-i\mathbf{k}\cdot\mathbf{r}} H e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$H_{\mathbf{k}}(\mathbf{r})u_{n\mathbf{k}}(\mathbf{r}) = \varepsilon_{n\mathbf{k}}u_{n\mathbf{k}}(\mathbf{r})$$

Gauge Freedom：

$$|u'_{n\mathbf{k}}\rangle = e^{i\phi(\mathbf{k})}|u_{n\mathbf{k}}\rangle$$

$$H_{\mathbf{k}}|u'_{n\mathbf{k}}\rangle = \varepsilon_{n\mathbf{k}}|u'_{n\mathbf{k}}\rangle$$

二、拓扑不变量：Berry connection & Curvature

K-space as the parameter space:

Connection: $\mathbf{A}_n(\mathbf{k}) = i\langle u_{n\mathbf{k}}|\nabla_{\mathbf{k}}|u_{n\mathbf{k}}\rangle$

Gauge dependent $\mathbf{A}'_n(\mathbf{k}) = i\langle u'_{n\mathbf{k}}|\nabla_{\mathbf{k}}|u'_{n\mathbf{k}}\rangle = \mathbf{A}_n(\mathbf{k}) - \nabla_{\mathbf{k}}\phi(\mathbf{k})$

Curvature: $\mathbf{\Omega}_n(\mathbf{k}) = \nabla_{\mathbf{k}} \times \mathbf{A}_n(\mathbf{k}) = i\langle \nabla_{\mathbf{k}} u_{n\mathbf{k}}| \times |\nabla_{\mathbf{k}} u_{n\mathbf{k}}\rangle$

Gauge invariant $\mathbf{\Omega}_n(\mathbf{k}) = \nabla_{\mathbf{k}} \times \mathbf{A}'_n(\mathbf{k}) = \nabla_{\mathbf{k}} \times \mathbf{A}_n(\mathbf{k})$

Symmetry: $\mathbf{\Omega}_n(\mathbf{k}) = \mathbf{\Omega}_n(-\mathbf{k})$ for inversion symmetry

$\mathbf{\Omega}_n(\mathbf{k}) = -\mathbf{\Omega}_n(-\mathbf{k})$ for time reversal symmetry

$\mathbf{\Omega}_n(\mathbf{k}) \equiv 0$ For systems with both T and I

二、拓扑不变量：Gauge Field

Gauge covariant position operator: $\hat{x}_\mu = i\partial_{k_\mu} - A_\mu(k)$

Commutation relation: $[\hat{x}_\mu, \hat{x}_\nu] = -i\mathcal{F}_{\mu\nu}$

$$\mathcal{F}_{\mu\nu} = \partial_{k_\mu} A_\nu - \partial_{k_\nu} A_\mu$$

Curvature can be written in anti-symmetric tensor form:

$$\epsilon_{\mu\nu\xi}\Omega_{n,\xi} = \mathcal{F}_{n,\mu\nu} = \frac{\partial}{\partial k_\mu} A_{n,\nu}(\mathbf{k}) - \frac{\partial}{\partial k_\nu} A_{n,\mu}(\mathbf{k})$$
$$= i\left[\langle \frac{\partial u_{n\mathbf{k}}}{\partial k_\mu} | \frac{\partial u_{n\mathbf{k}}}{\partial k_\nu} \rangle - \langle \frac{\partial u_{n\mathbf{k}}}{\partial k_\nu} | \frac{\partial u_{n\mathbf{k}}}{\partial k_\mu} \rangle\right]$$

$\epsilon_{\mu\nu\xi}$ **is the Levi-Civita antirsymmetirc tensor, and**

$$\Omega_{n,z} = \mathcal{F}_{n,xy}$$

二、拓扑不变量：Magnetic Field in K-space

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

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

can be viewed as magnetic field in k-space

[Sundaram & Niu, et.al, PRB (1999); Jungwirth & Niu, et.al, PRL (2002);

Fang, Nagaosa, Tokura, 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 $\vec{A}(\vec{k}) = \langle \psi \vert\, i\frac{\partial}{\partial \vec{k}} \vert \psi \rangle$	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:

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

Anomalous velocity

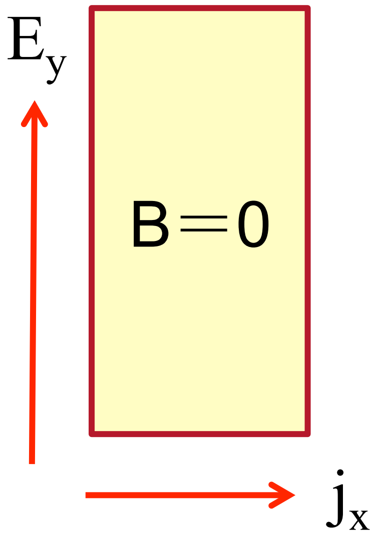
$$\hbar\dot{\mathbf{k}} = -e\mathbf{E}(\mathbf{r}) - e\dot{\mathbf{r}} \times \mathbf{B}(\mathbf{r})$$

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

$\Downarrow$

Anomalous Hall Effect

二、拓扑不变量：可观测量，Hall Conductivity



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

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

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

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

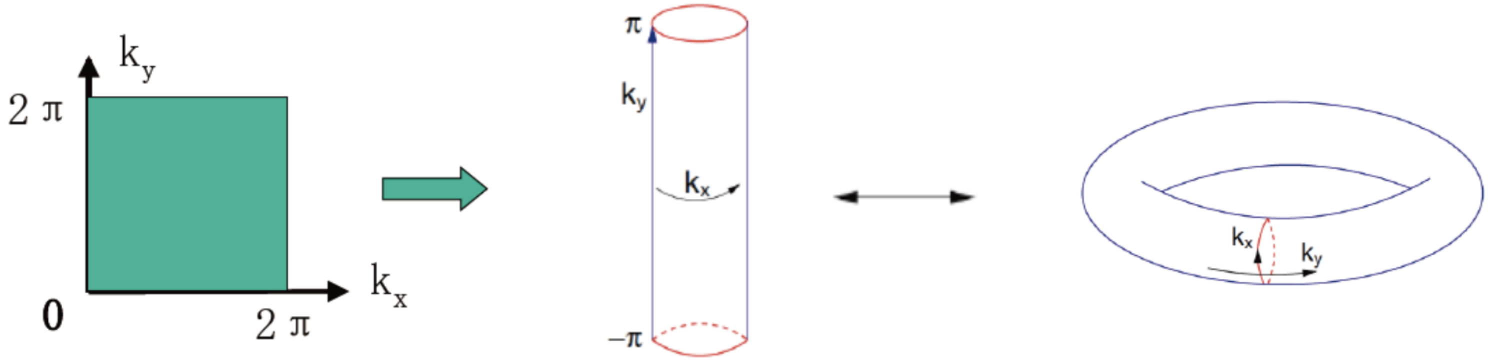
$$\sigma_{xy} = -\frac{e^2}{\hbar}\sum_n \int_{BZ} \frac{d^2\mathbf{k}}{(2\pi)^2} f_n(\mathbf{k}) \Omega_{n,z}(\mathbf{k})$$

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

二、拓扑不变量：Chern Number

Chern theorem: $$\int_{\mathcal{S}} \mathbf{\Omega}(\mathbf{k}) \cdot d\mathcal{S} = 2\pi Z$$ Z=interger Chern number

2D Brillouin Zone:

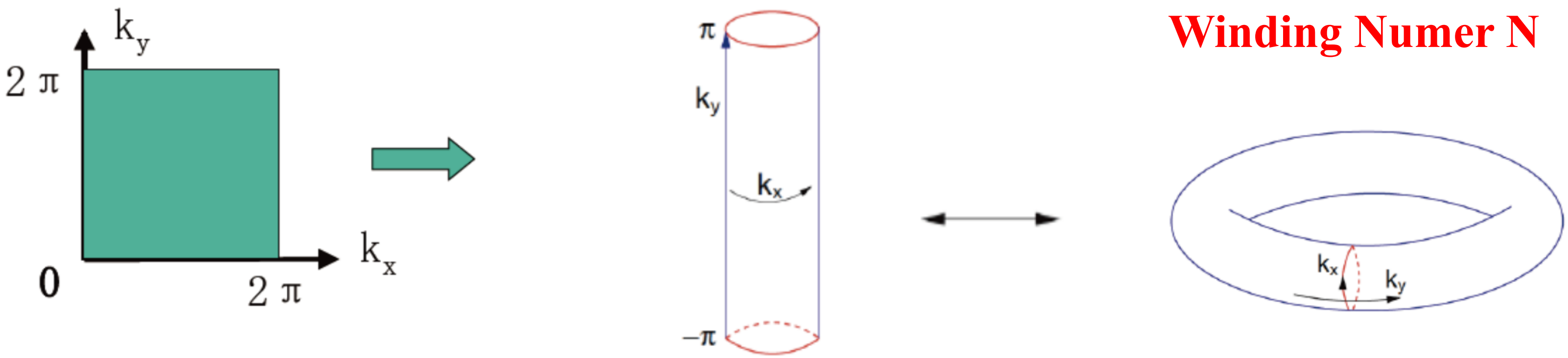


Quantization:

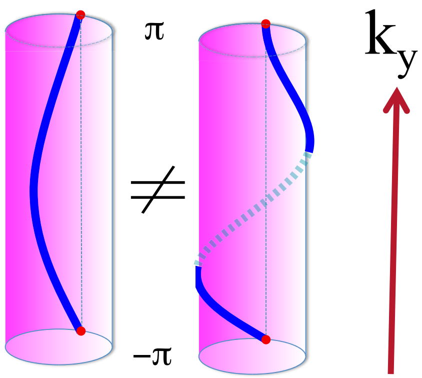
$$\int_{BZ} d^2\mathbf{k}\Omega_z(\mathbf{k}) = \int_{\mathcal{S}} \mathbf{\Omega}(\mathbf{k}) \cdot d\mathcal{S}$$

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

二、拓扑不变量: Chern Number as Wannier Center



$$
\begin{aligned}
2\pi Z &= -\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} dk_x dk_y (\partial_{k_x} A_y - \partial_{k_y} A_x) \\
&= \int_{-\pi}^{\pi} dk_y \partial_{k_y} \left(\int_{-\pi}^{\pi} dk_x A_x(k_x, k_y)\right) \\
&= \int_{-\pi}^{\pi} d\theta(k_y).
\end{aligned}
$$

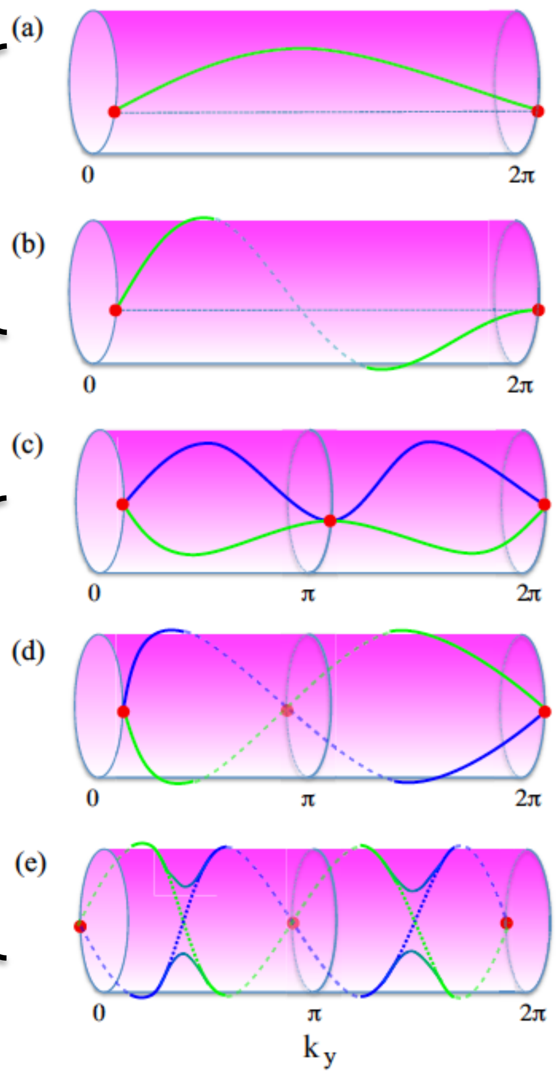


Berry Phase: $P_n(k_y) = \dfrac{\theta_n(k_y)}{2\pi} = \dfrac{1}{2\pi}\displaystyle\int_{-\pi}^{\pi} dk_x A_{n,x}(k_x, k_y)$

Wannier Center: $\overline{x}(k_y) = \langle nR_{x=0}, k_y|\hat{x}|nR_{x=0}, k_y\rangle = i\dfrac{1}{(2\pi)}\displaystyle\int_{-\pi}^{\pi} dk_x \langle u_{n\mathbf{k}}|\nabla_{k_x}|u_{n\mathbf{k}}\rangle = P_n(k_y)$

二、拓扑不变量：T-symmetry and Z_2 Invariant

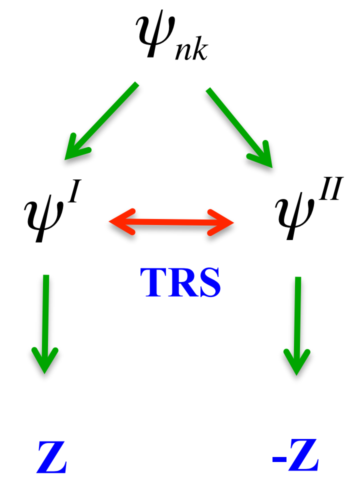
No T



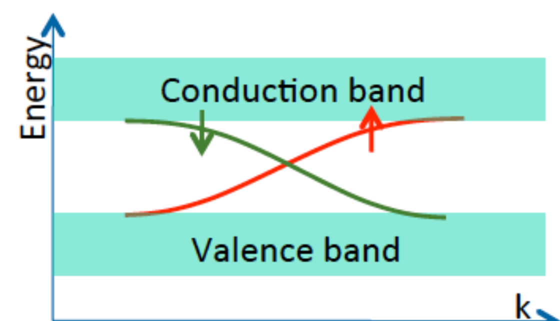
Chern Instulator

With T

Z_2 TI



Invariant: Z_2=Z mod 2



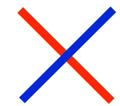
Ref: (1) Hasan & Kane, RMP (2010).
(2) Qi & Zhang, RMP (2011).

Z_2 TI can be extended to 3D!

二、拓扑不变量：Magnetic Monopole and Weyl node

Any 2x2 Hamiltonian: $H(\vec{k}) = \vec{f}(\vec{k})\cdot\vec{\sigma} = f_x(k)\sigma_x + f(k)_y\sigma_y + f(k)_z\sigma_z$

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



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:

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

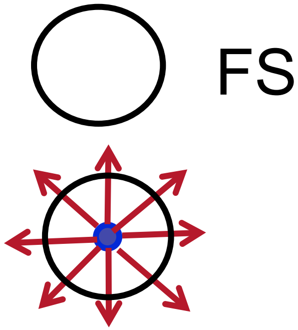
$$\frac{1}{2\pi}\oint_S \vec{\Omega}(k)\cdot dS(k) = Q$$

Q=magnetic Charge

Fang, Science (2003).

二、拓扑不变量：Topological Invariant for 3D Metals

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 metal

if E_f at node (k=0) ➔ topological semimetal

Volovik, JETP (2002).
X. L. Qi, et.al., PRB (2010).
Z. J. Wang, et.al., PRB (2012)

Notes:

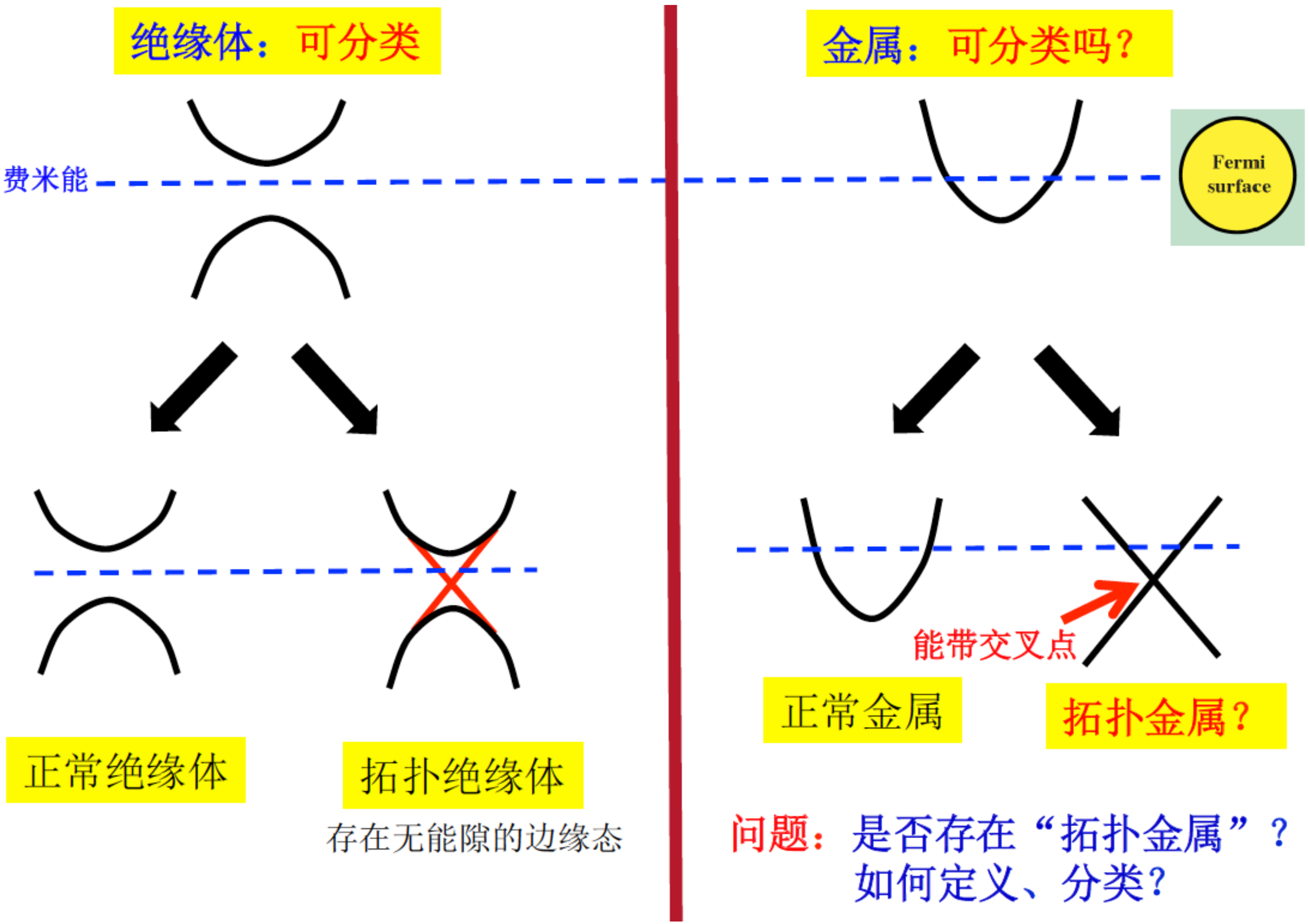
(1) |Q| can be more than 1

(2) +Q & -Q monopoles have to appear in pair in lattice, but may separate in K.

(3) +Q & -Q monopoles can annihilate.

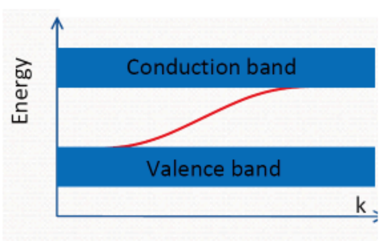
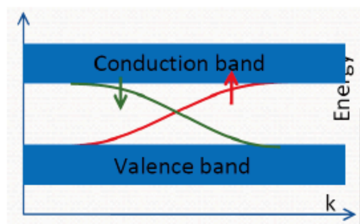
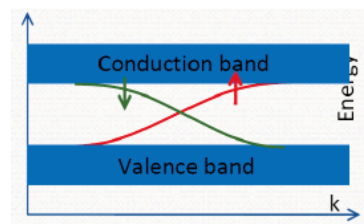
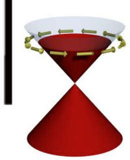
(4) Defined only for 3D k-space

三、拓扑量子态：Momentum Space



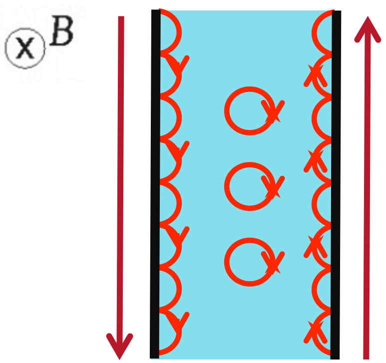
问题：是否存在“拓扑金属”？如何定义、分类？

三、拓扑量子态：丰富的拓扑电子态

2D		3D	
T-broken	T-invariant	T-invariant	T-Broken
QHE QAHE	QSHE	Kondo Topo. Band Insu. Anderson Mott …	Semi-metal
			
Edge States TKNN Chern number, Z	Z2	 Surface States Z2	Weyl points (in bulk)
量子霍尔效应	量子自旋霍尔效应 2D拓扑绝缘体	3D拓扑绝缘体	拓扑金属
$Z \neq 0$	$Z_2 \neq 0$	$Z_2 \neq 0$	$C_{FS} \neq 0$

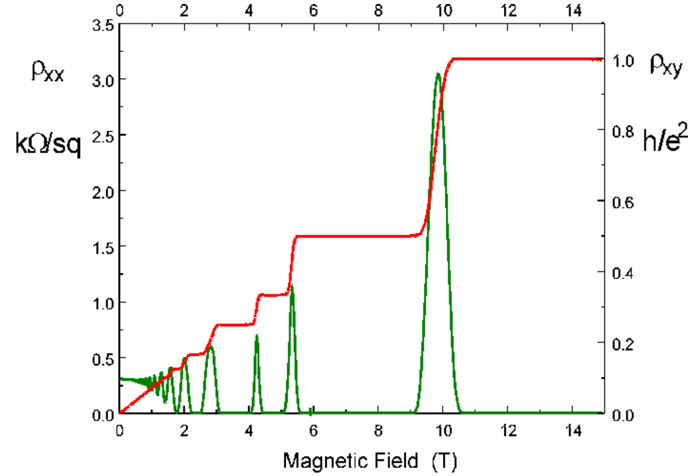
三、拓扑量子态：Integer Quantum Hall Effect

典型的宏观量子现象！



2DEG

Dissipationless edge
有电流，没有电压



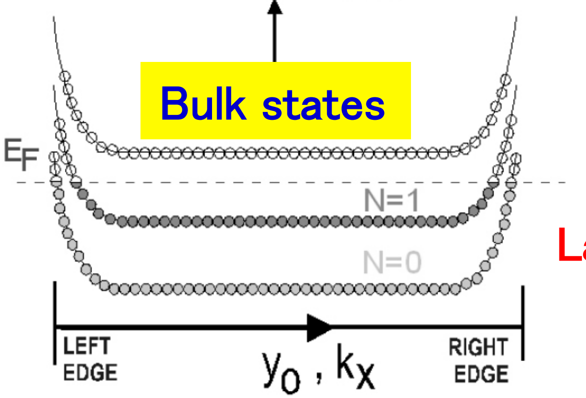
Quantization

K. Von Klitzing, et.al., PRL(1980)

Edge states

Edge states

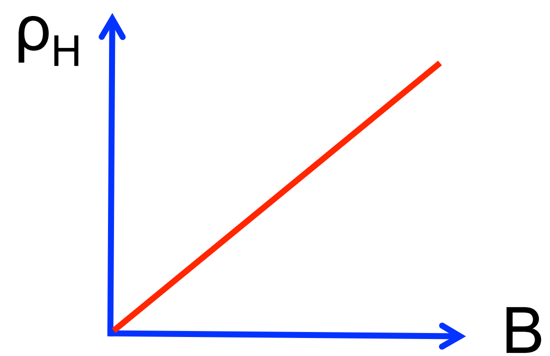
Bulk states



Landau Levels

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

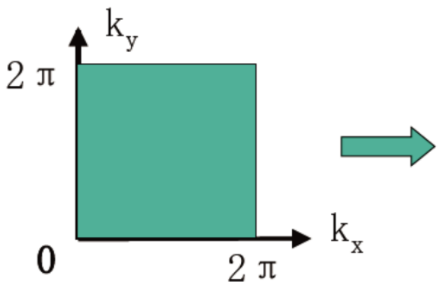
Quantum Hall Effect



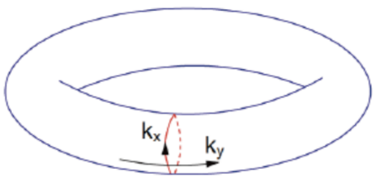
Hall Effect $\rho_{\mathrm{Hall}} = \mathrm{R_0 B}$

三、拓扑量子态：IQHE

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



Winding Numer N



$$\sigma_{xy} = -\frac{e^2}{2\pi h}\int_{BZ} \Omega_z(k) d^2k = -n\frac{e^2}{h}$$

n=Chern number

TKNN, PRL (1982): $$n = \sum_{bands} \frac{i}{2\pi}\int d^2k \left(\left\langle \frac{\partial u}{\partial k_1} \middle| \frac{\partial u}{\partial k_2} \right\rangle - \left\langle \frac{\partial u}{\partial k_2} \middle| \frac{\partial u}{\partial k_1} \right\rangle \right)$$

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

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

Realization: Fang &Dai, Science 2010 (Theory); Xue, Science 2013 (Exp.)

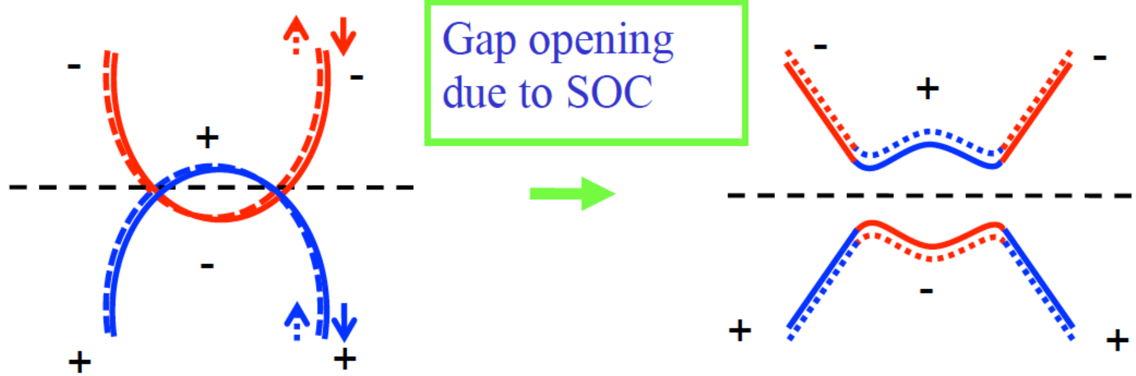
(Cr-doped (BiSb)Te_3 thin film)

四、拓扑电子材料：Band Inversion Mechanism

Guidelines:

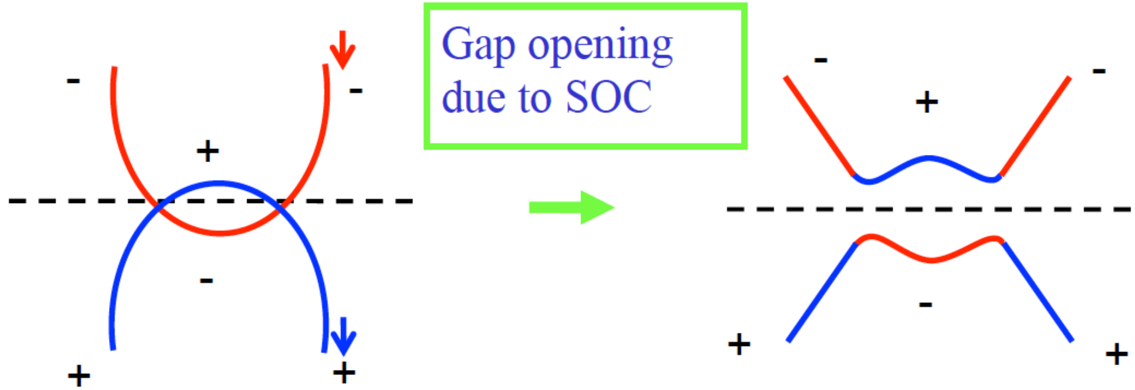
1. Semiconductor with inverted band structure
2. Strong SOC

Z_2 Topological Insulators:



$$H_{\text{eff}}(k_x, k_y) = \begin{pmatrix} H(k) & 0 \\ 0 & H^*(-k) \end{pmatrix}$$

2D Chern Insulators:



$$H_{eff}(\mathbf{k}) = \begin{bmatrix} E_+(\mathbf{k}) & M(\mathbf{k})^* \\ M(\mathbf{k}) & E_-(\mathbf{k}) \end{bmatrix}$$

$$E_\pm(\mathbf{k}) = \mp m \pm \mathbf{k}^2$$

$$M(\mathbf{k}) = (k_x \pm i k_y)^n$$

$$Z = n$$

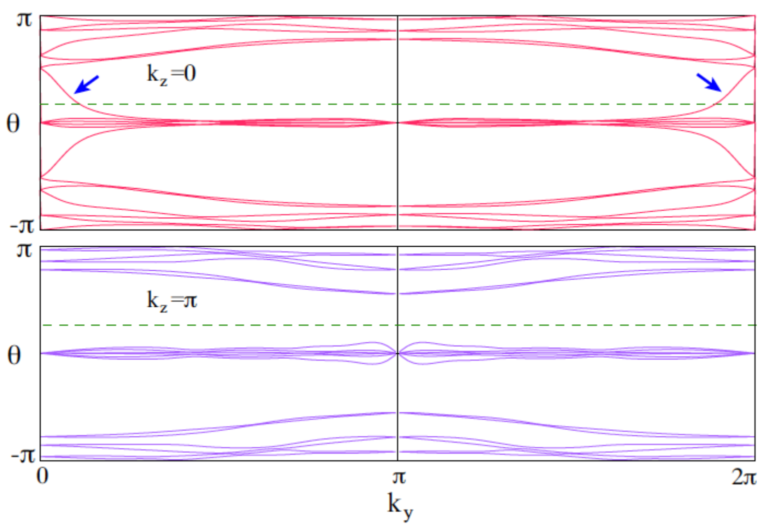
四、拓扑电子材料：First-principles Calculations

Matrix element: $$\mathbf{v}_{m,n}(\mathbf{k}) = \langle \psi_{m\mathbf{k}} | \mathbf{v} | \psi_{n\mathbf{k}} \rangle = \frac{1}{\hbar} \langle u_{m\mathbf{k}} | \nabla_{\mathbf{k}} \mathbf{H}(\mathbf{k}) | u_{n\mathbf{k}} \rangle$$

Berry phase: $$\gamma(\mathbf{k}_\perp) = \mathbf{Im}\left[\ln\det \prod_{j=1}^{J-1} \langle u_{n,(\mathbf{k}_\perp,k_j)} | u_{m,(\mathbf{k}_\perp,k_{j+1})} \rangle \right]$$

or Wilson Loop method to avoid the gauge-fix condition

Winding number: $$P_n(k_y) = \frac{\theta_n(k_y)}{2\pi} = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk_x A_{n,x}(k_x, k_y)$$



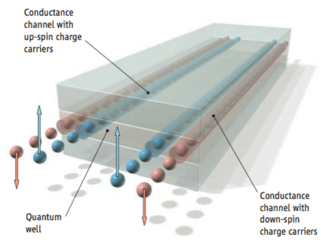
Bi_2Se_3

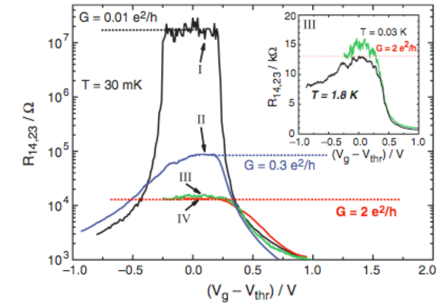
四、拓扑电子材料：重要进展

2D TI (QSH Insulator): HgTe Quantum Well

Theory: Bernevig, Science (2006),

Exp: Konig, Science (2007).



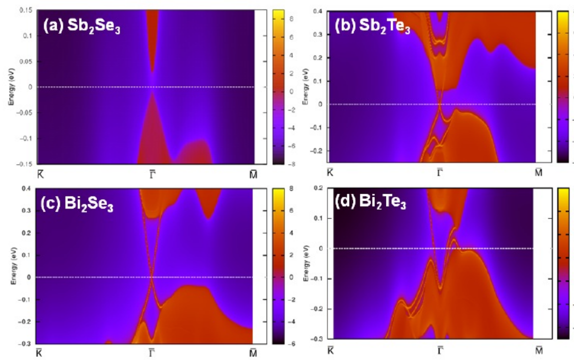


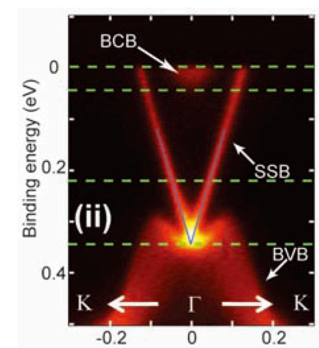
3D TI: Bi_2Se_3, Bi_2Te_3, Sb_2Te_3

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

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

Y. L. Chen, Science (2009).

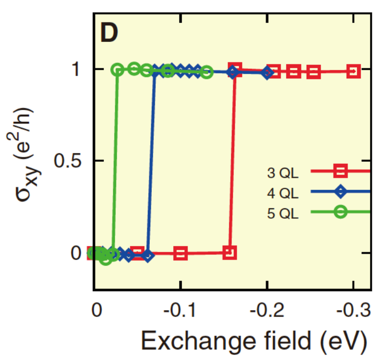


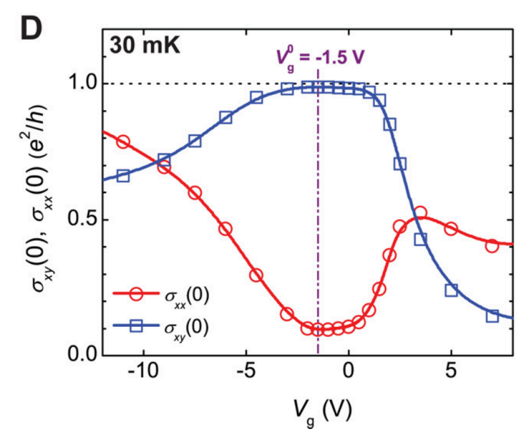


QAHE Insulator: Cr-doped Bi_2Te_3

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

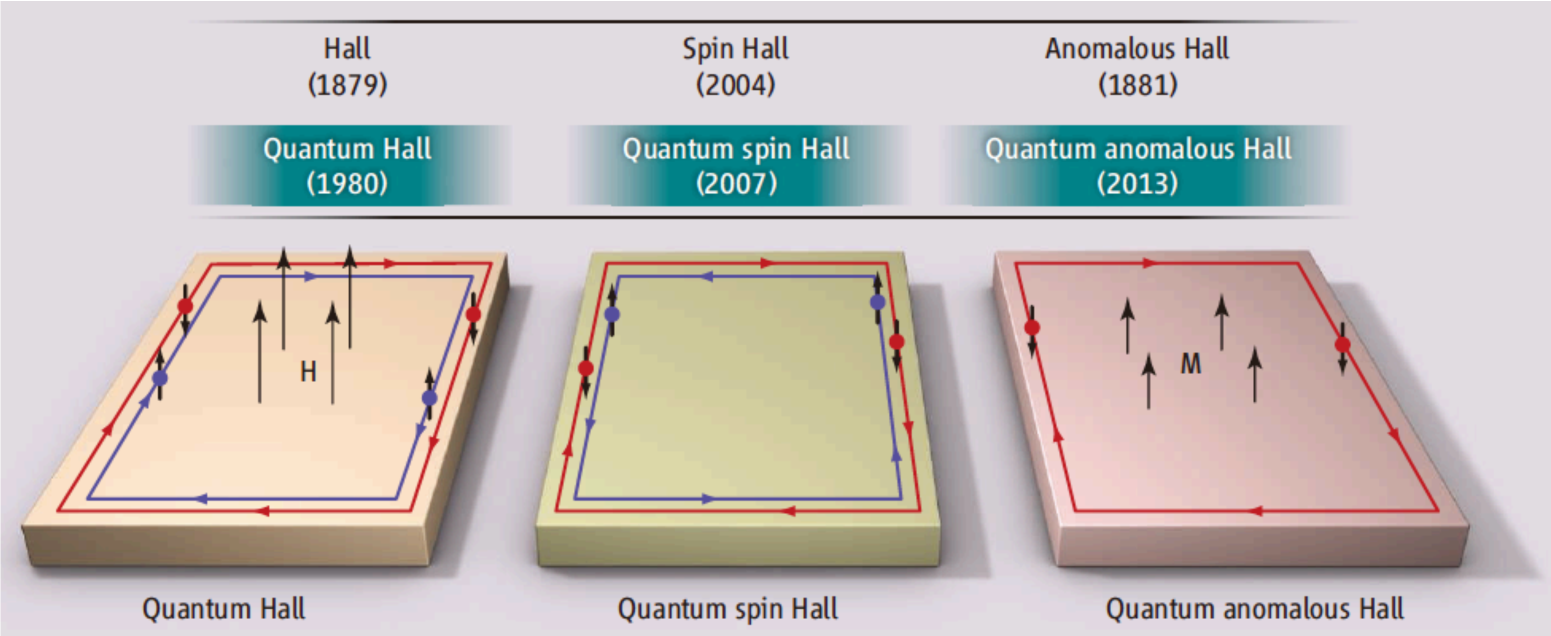
Exp: C. Z. Chang, Science (2013).





四、拓扑电子材料：Quantum Hall Trio

The Complete Quantum Hall Trio
Seongshik Oh
Science **340**, 153 (2013);
DOI: 10.1126/science.1237215



HgTe

Bi_2Te_3, Bi_2Se_3
with Cr-doping

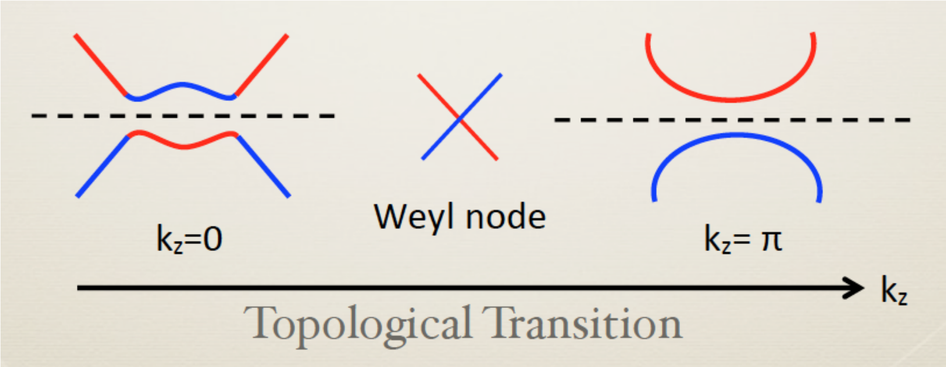
四、拓扑电子材料：拓扑Weyl半金属

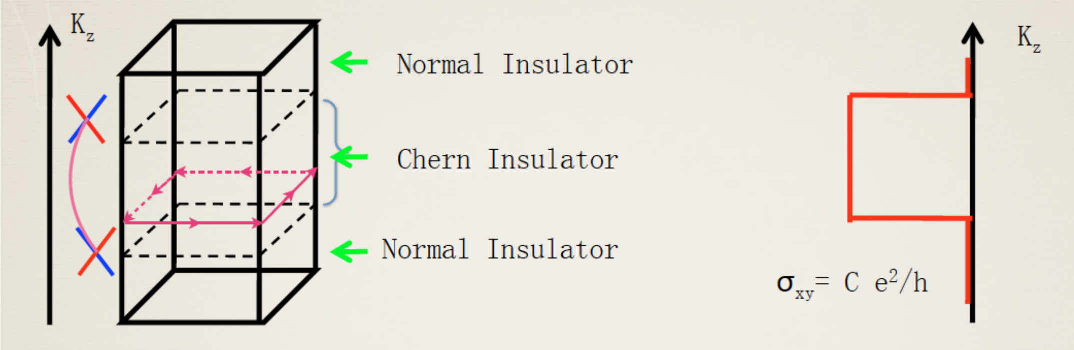
Considering 2D sheet (fixed k_z=m).

Topological phase transition as function of k_z.

$$H(\vec{k}) = \begin{bmatrix} m & k_x - ik_y \\ k_x + ik_y & -m \end{bmatrix}$$

m<0, Chern I $\Rightarrow$ m>0, NI





3D Weyl semimetal:

(1) Spin-Momentum Lock in 3D
(2) Fermi arcs on side surface,
(3) Magnetic monopoles in bulk,
(4) QAHE in Quantum-well structure
(5) ABJ anomaly, and etc.
(Negative MR for E//B)

X. G. Wan, et.al. PRB (2011).
A. A. Burkov, et.al, PRL (2011);PRB (2011)
G. Xu, et.al., PRL (2011).

四、拓扑电子材料：拓扑Dirac Semimetal

If both T and I symmetry are present:

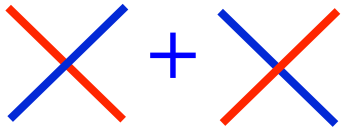
+Q & -Q Weyl nodes have to overlap in K-space

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

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.

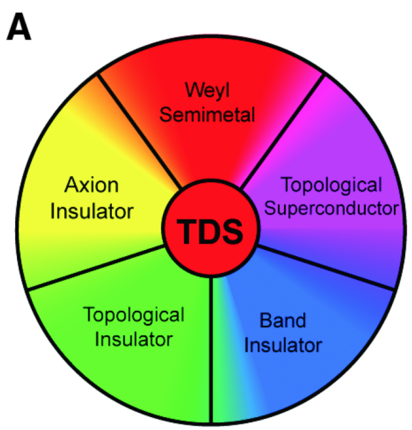
3D Dirac semimetal:

(1) Pseudo fermi arcs on surface

(2) Giant diamagnetism: χ(ε)≈log(1/ε)

(3) Linear Quantum magneto-resistance.

(4) QSHE in its quantum-well structure



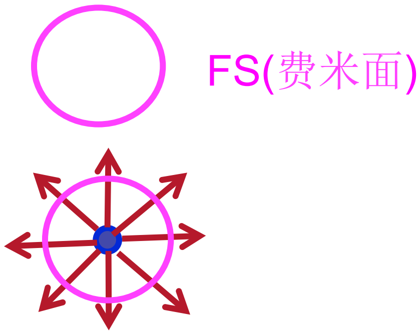
Critical Point

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

四、拓扑电子材料：拓扑半金属

◆ **拓扑金属的定义：PRB 85, 195320（2012）**

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



$C_{FS}=0$，一般金属

$C_{FS}\neq 0$，拓扑金属

如果费米面正好在能带交叉点➔拓扑半金属

◆ **拓扑半金属材料：**

（1）$HgCr_2Se_4$：PRL 107, 186806（2011）

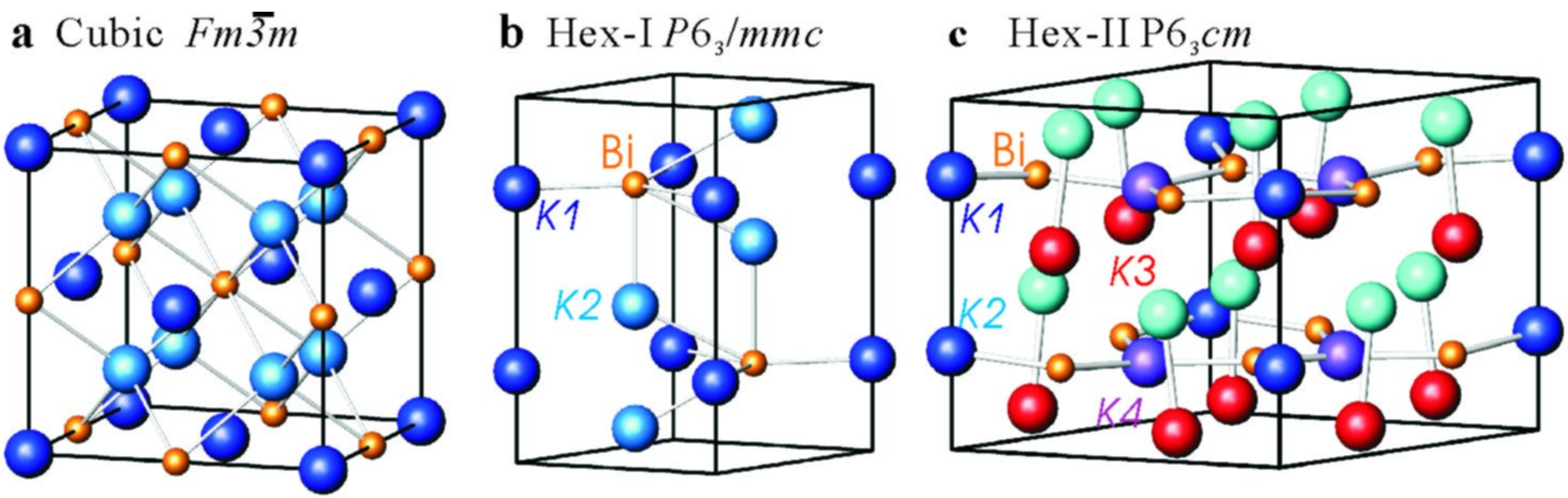
（2）Na_3Bi：PRB 85, 195320（2012）

（3）Cd_3As_2：PRB 88, 125427（2013）

拓扑半金属具有与普通金属不同的新奇物性：磁阻、抗磁性、拓扑超导等

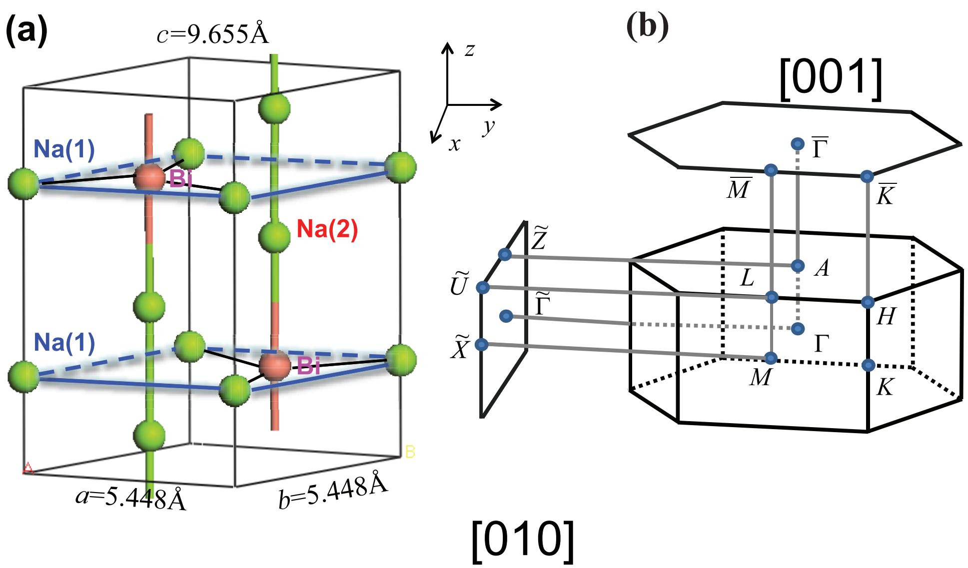
四、拓扑电子材料：拓扑半金属

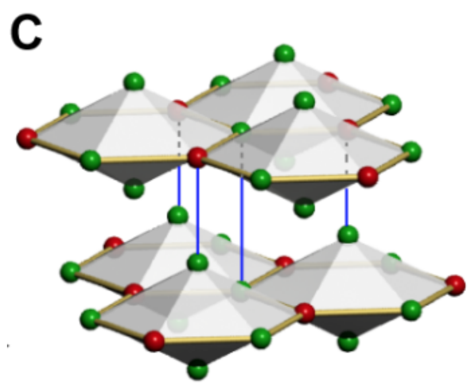
Crystal Structure of A_3Bi



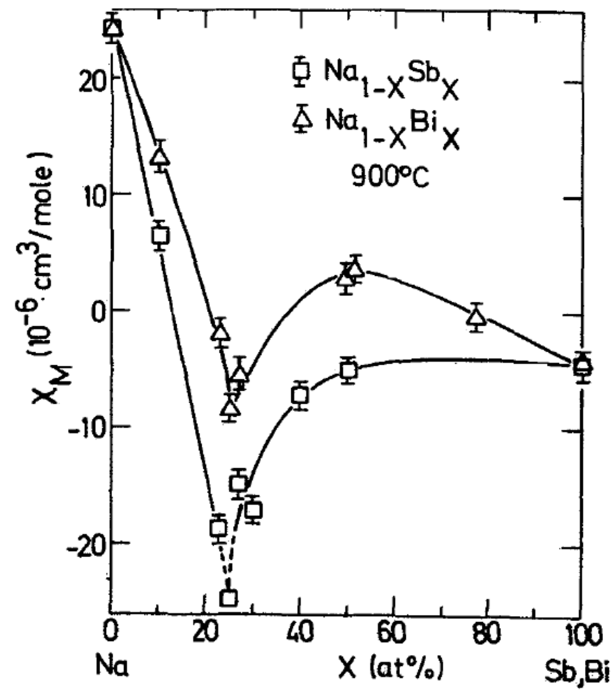
	Li_3Bi	K_3Bi	Na_3Bi	Rb_3Bi	Cs_3Bi
Cubic	O	O	O	O	O
Hex-I		O	O	O	
Hex-II		O			

Basic properties of Na_3Bi





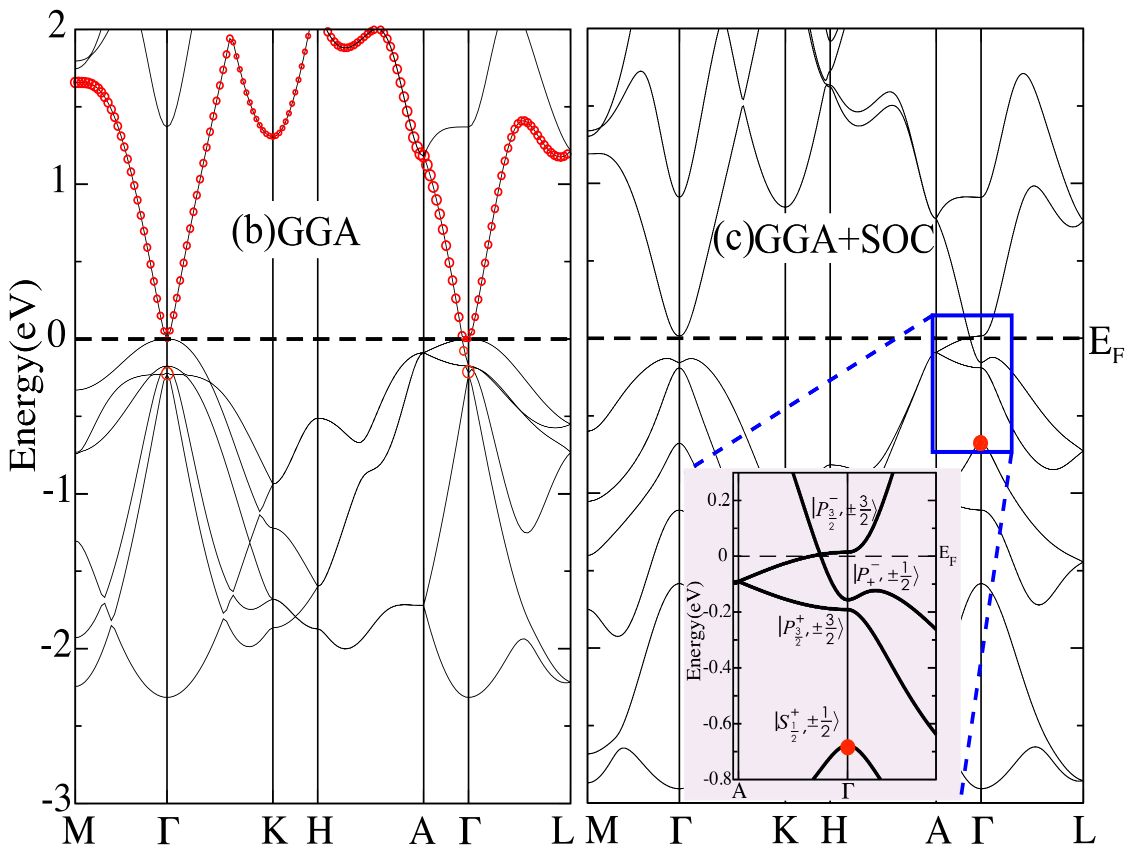
Space group: $P6_3/mmc$
(1) C6 around z;
(2) C2 around y;
(3) Inversion symmetry.



Diamagnetism
K. Hackstein,
J. de. Phys. (1980)

四、拓扑电子材料：拓扑半金属

Band inversion in Na_3Bi



(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 $(0,0,\pm k_z^c)$

(Complete splitting of p at Γ , different with HgTe and etc. $|p_{3/2}, 3/2\rangle$ is the highest state.)

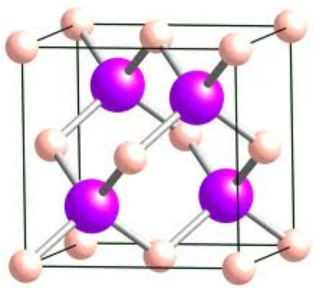
$$H_\Gamma(\mathbf{k}) = \epsilon_0(\mathbf{k}) + \begin{pmatrix} M(\mathbf{k}) & \boxed{Ak_+} & 0 & B^*(\mathbf{k}) \\ Ak_- & -M(\mathbf{k}) & B^*(\mathbf{k}) & 0 \\ 0 & B(\mathbf{k}) & M(\mathbf{k}) & -Ak_- \\ B(\mathbf{k}) & 0 & -Ak_+ & -M(\mathbf{k}) \end{pmatrix}$$

$$B(\mathbf{k}) = B_3 k_z^c k_+^2$$

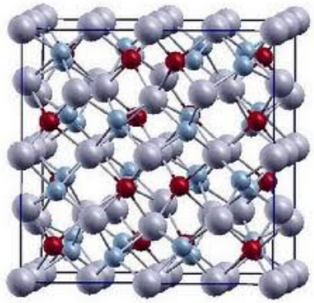
Z. J. Wang, et.al, PRB (2012)

四、拓扑电子材料：拓扑半金属

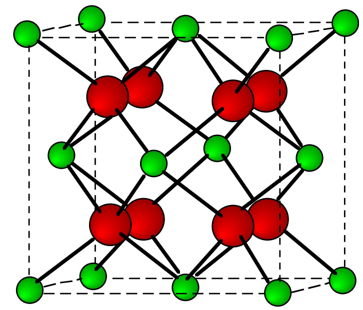
Strcture of Cd_3As_2, Zn_3P_2, Zn_3As_2, Cd_3P_2



Adding Cd



Cd Vacancy

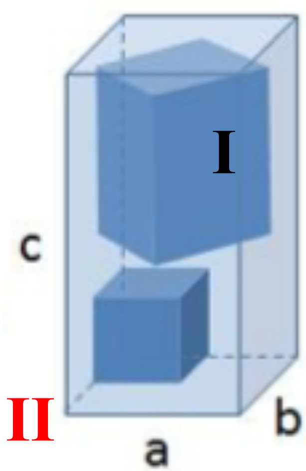


Zinc Blende

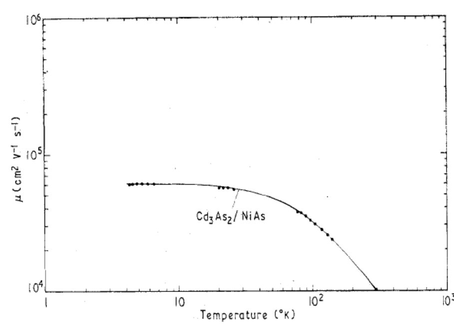
Anti-fluorite

Two Structures

Structure I:
D_{4h} ($P4_2/nmc$)
40 atoms per cell
With inversion

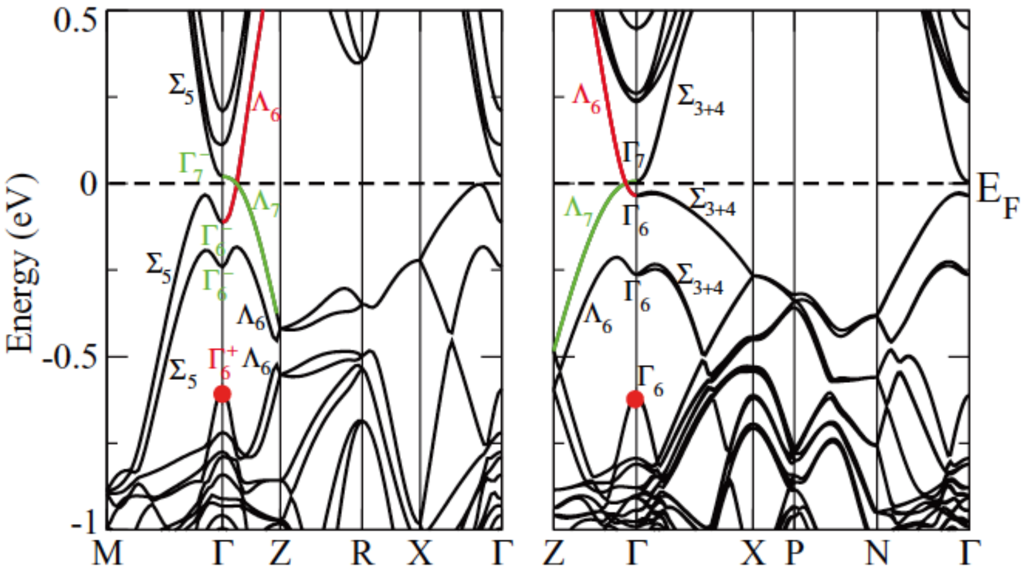


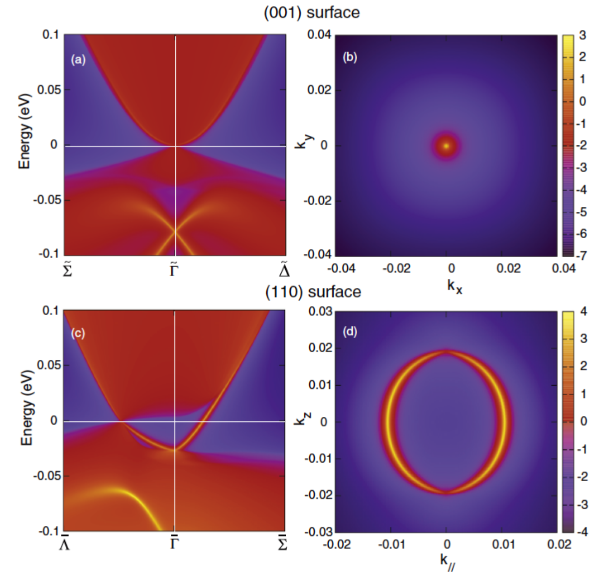
Structure II:
C_{4v} ($I4_1cd$)
80 atoms per cell
No inversion
(most stable phase)

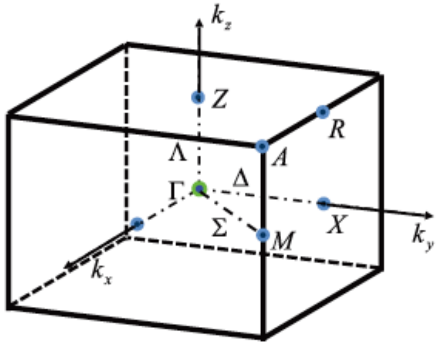


Cd_3As_2, Mobility up to 10^5
C. T. Elliott, J. Phys. D (1969).

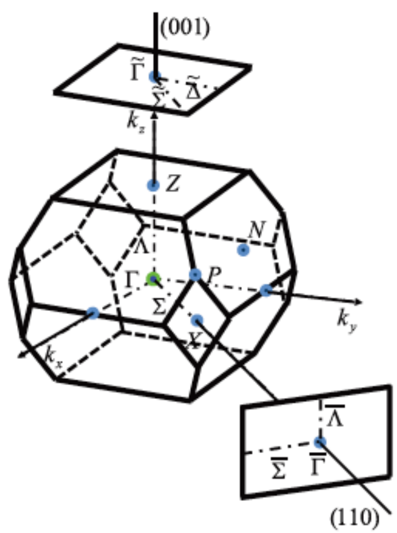
四、拓扑电子材料：拓扑半金属



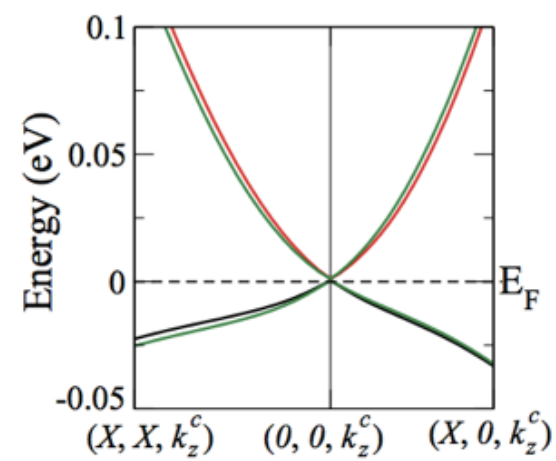




(a) structure I



(b) structure II



(1) Protected by C4

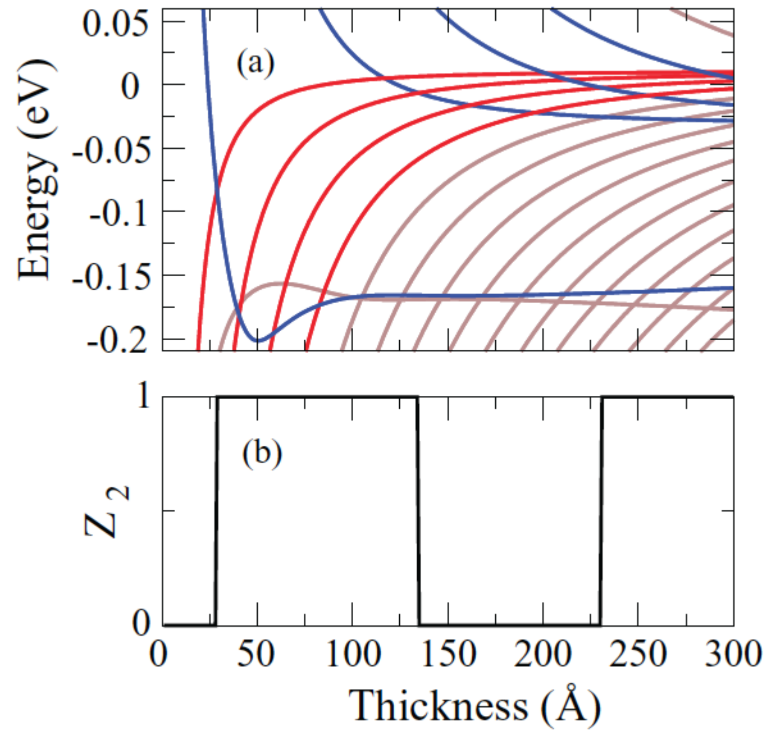
(2) Band-Splitting

Z. J. Wang, et.al, PRB (2013)

四、拓扑电子材料：拓扑半金属

$$|S^{+}_{\frac{1}{2}}, \tfrac{1}{2}\rangle, \ |P^{-}_{\frac{3}{2}}, \tfrac{3}{2}\rangle, \ |S^{+}_{\frac{1}{2}}, -\tfrac{1}{2}\rangle, \ |P^{-}_{\frac{3}{2}}, -\tfrac{3}{2}\rangle$$

$$H_{\Gamma}(\vec{k}) = \epsilon_0(\vec{k}) + \begin{pmatrix} M(\vec{k}) & Ak_+ & Dk_- & B^*(\vec{k}) \\ Ak_- & -M(\vec{k}) & B^*(\vec{k}) & 0 \\ Dk_+ & B(\vec{k}) & M(\vec{k}) & -Ak_- \\ B(\vec{k}) & 0 & -Ak_+ & -M(\vec{k}) \end{pmatrix},$$



Similar to Na3Bi, but:

(1) B(k)≈0 by C_4 symmetry

(2) D≠0 for the structure II.

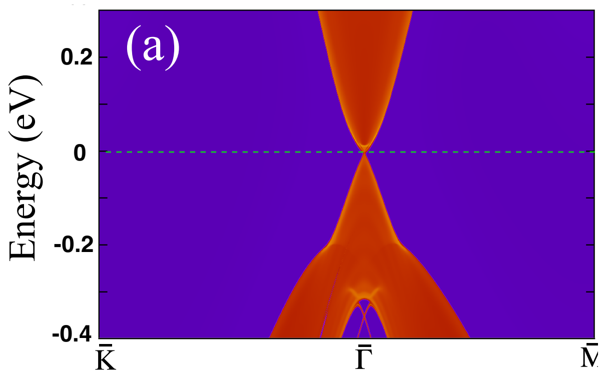
Large gap QSHE
gap ≈ 0.1eV

Z. J. Wang, et.al, PRB (2013)

Quantum MR?? B⊥E
Negative MR?? B//E

四、拓扑电子材料：拓扑半金属

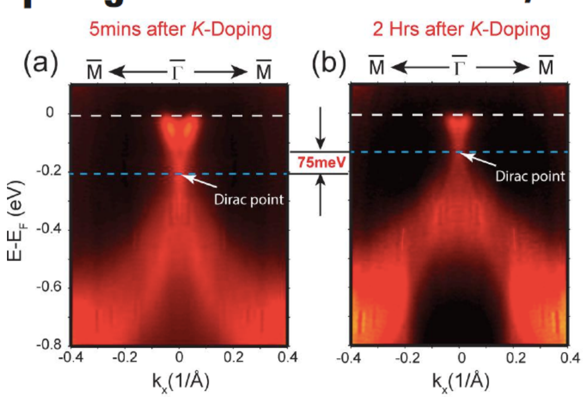
与实验合作



理论

Sciencexpress

Discovery of a Three-Dimensional Topological Dirac Semimetal, Na_3Bi



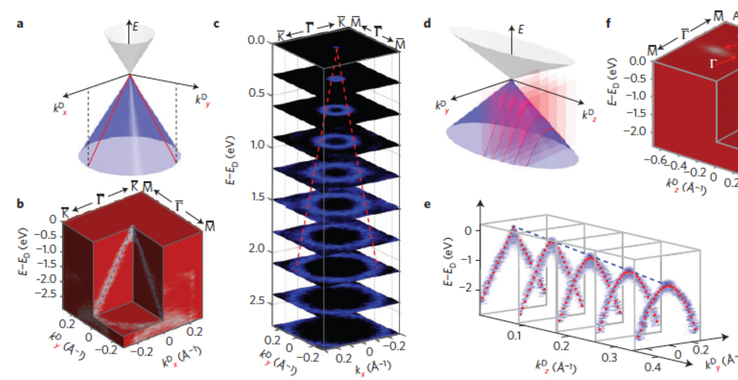
实验

Science 343, 6173 (2014)：Na_3Bi

nature materials | LETTERS

PUBLISHED ONLINE: 25 MAY 2014 | DOI: 10.1038/NMAT3990

A stable three-dimensional topological Dirac semimetal Cd_3As_2



Nature Materials, 3990 (2014)：Cd_3As_2

观测到了三维Dirac锥

首次发现拓扑半金属态

—— 三维版本的石墨烯

Summary:

动量（参数）空间 → Berry Curvature → Gauge field

→ 拓扑不变量 → 拓扑量子态 → 拓扑电子材料

拓扑电子态家族（future）：

	无时间反演	有时间反演	材料	强关联
拓扑绝缘体	O✔	O✔	O✔	O✔
拓扑金属	O✔?	✔	✔	?
拓扑超导	?	?	?	?