

Topological Materials



Outline

1. Introduction

Band theory

Topology in condensed matter physics

Basics properties: Robust, invariant number, gapless surface states

Comparing with Landau's approach

Density functional theory (DFT)

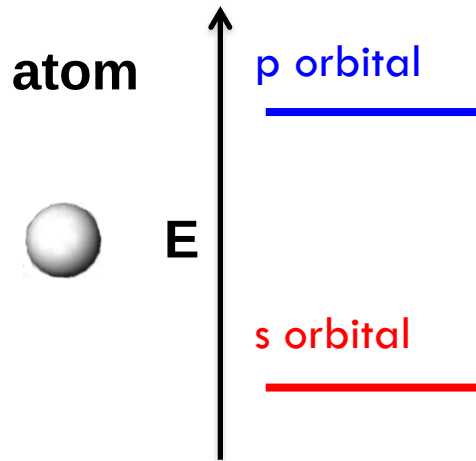
2. Topological insulator (quantum spin Hall insulator)

Strong topological insulator, weak topological insulator, topological crystalline insulator, topological Kondo insulator, quantum anomalous Hall effect...etc

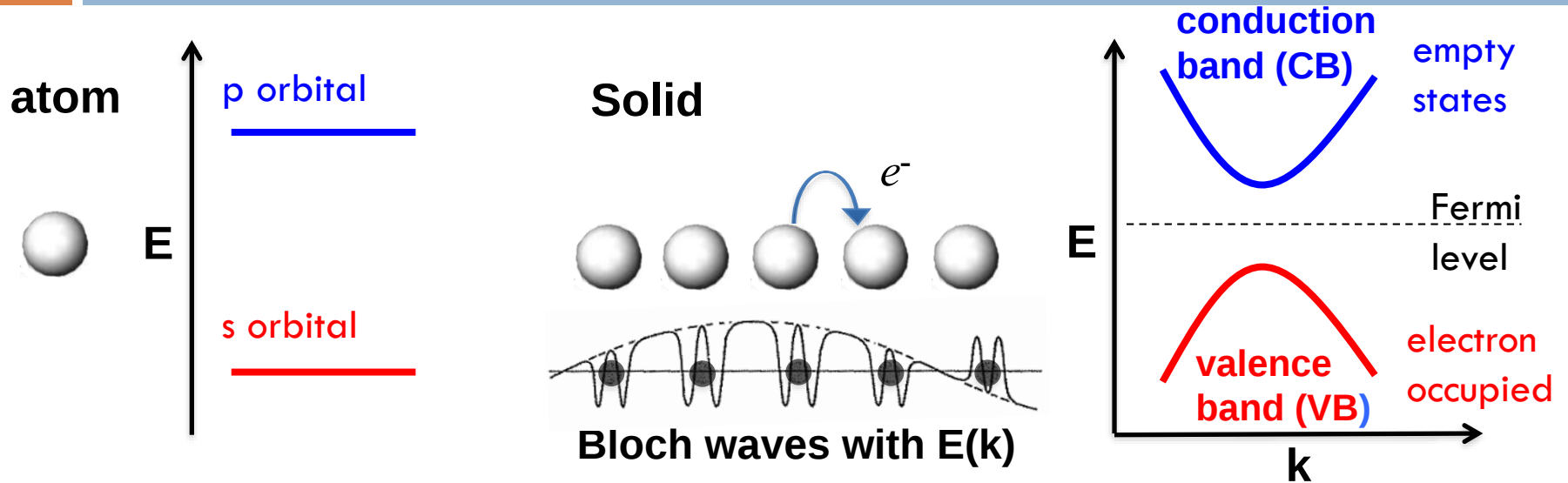
3. Topological semimetal

3D Dirac semimetal, Weyl semimetal, Nodal-line semimetal, topological superconductor, New Fermion

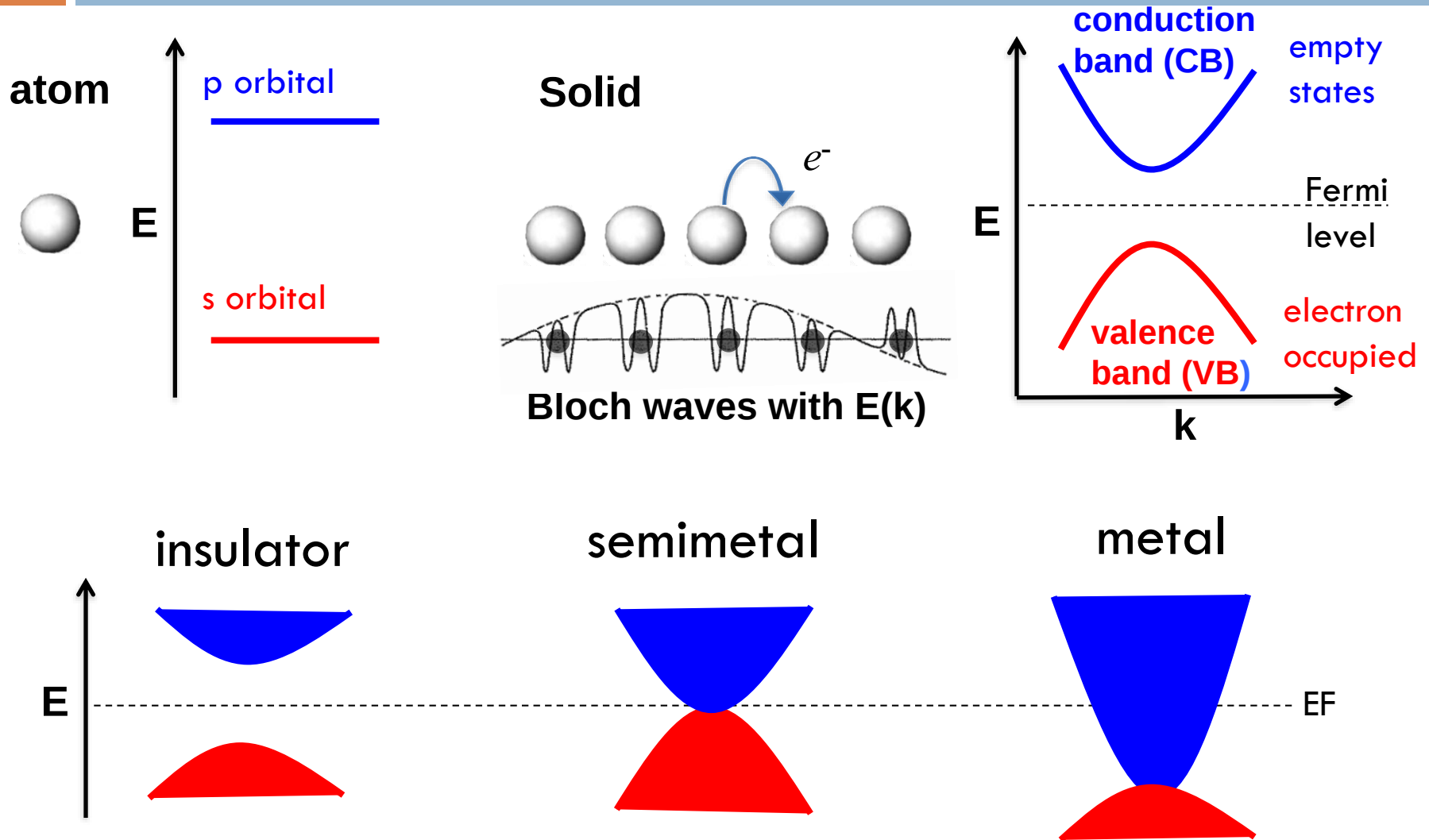
Condensed matter physics: band theory



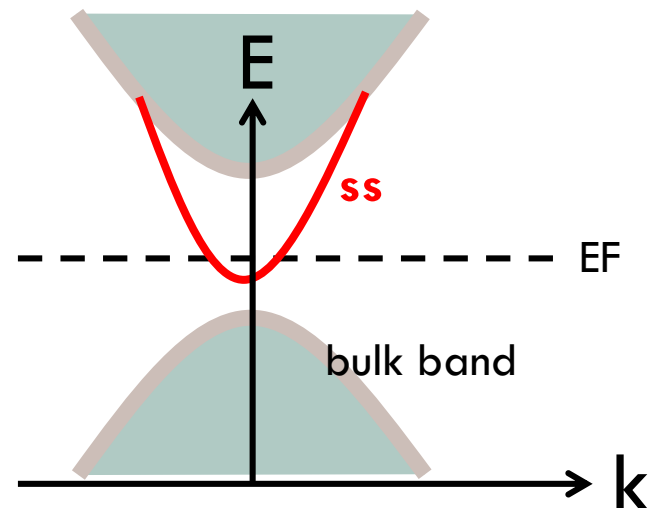
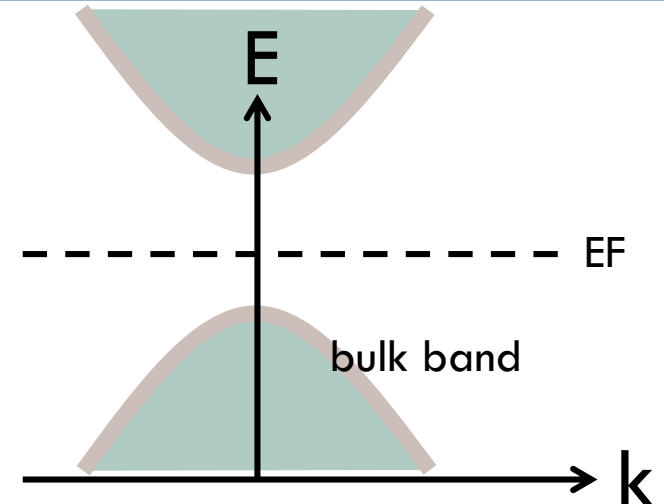
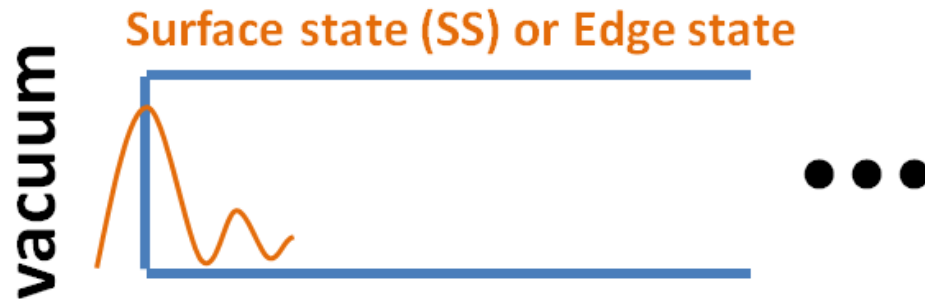
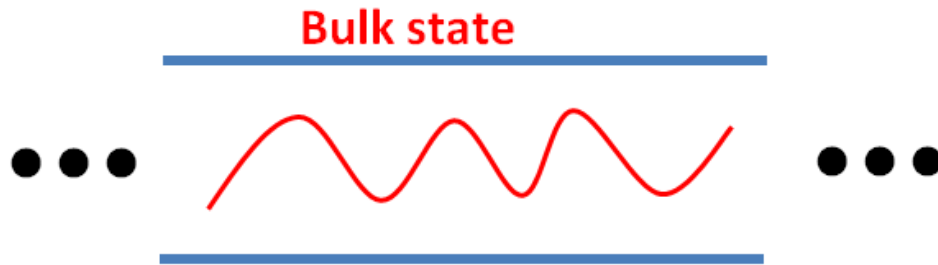
Condensed matter physics: band theory



Condensed matter physics: band theory



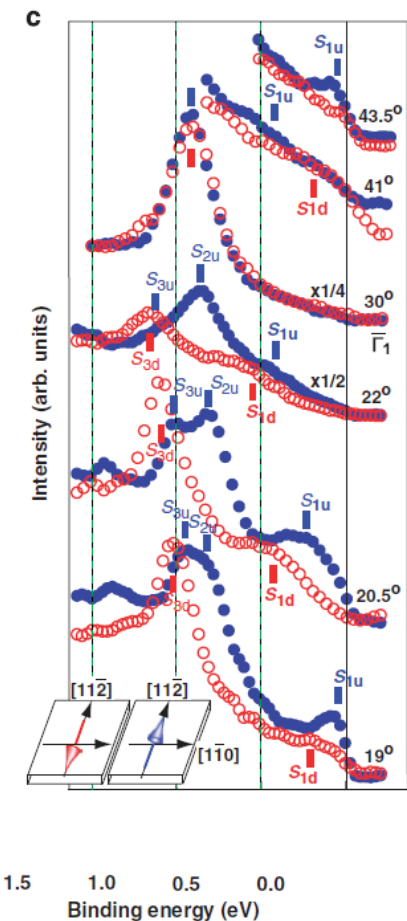
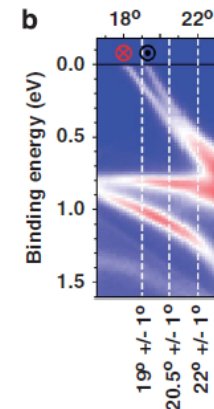
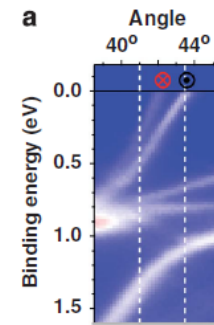
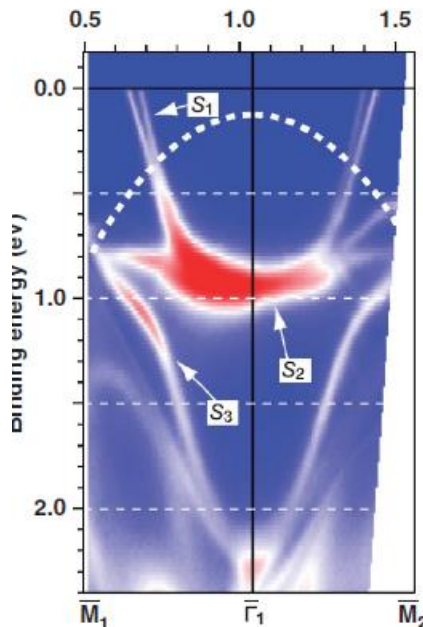
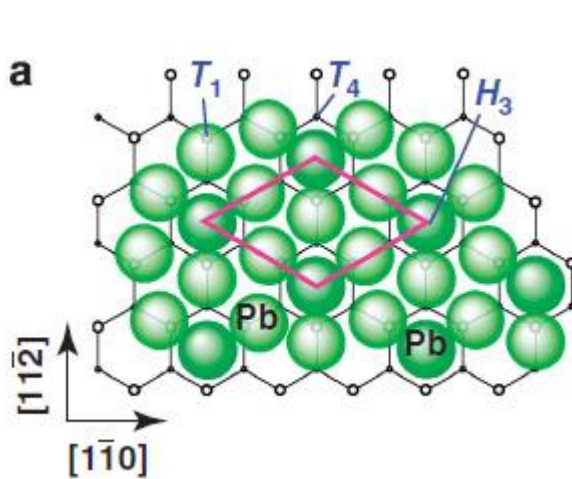
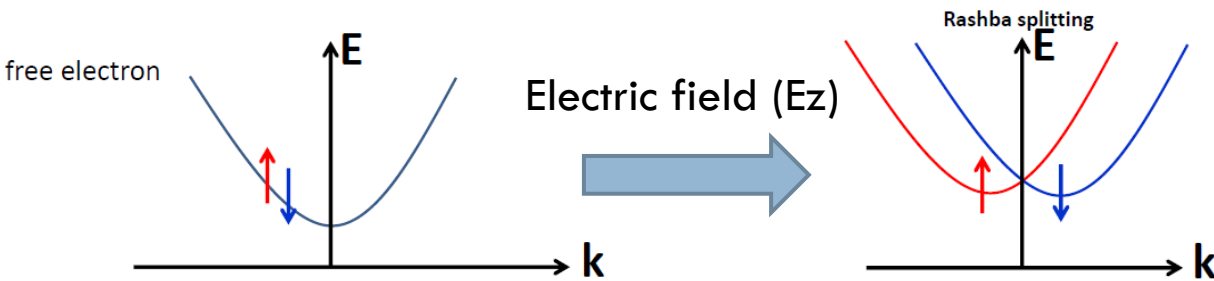
Condensed matter physics: band theory



Condensed matter physics: band theory

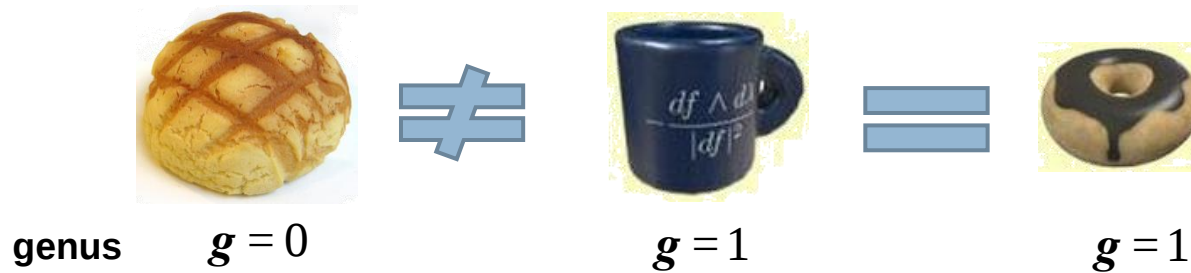
Example: surface Rashba effect

Nat. commun. **1**, 17 (2010)



Topology in condensed matter physics

Math $\Rightarrow$ real space

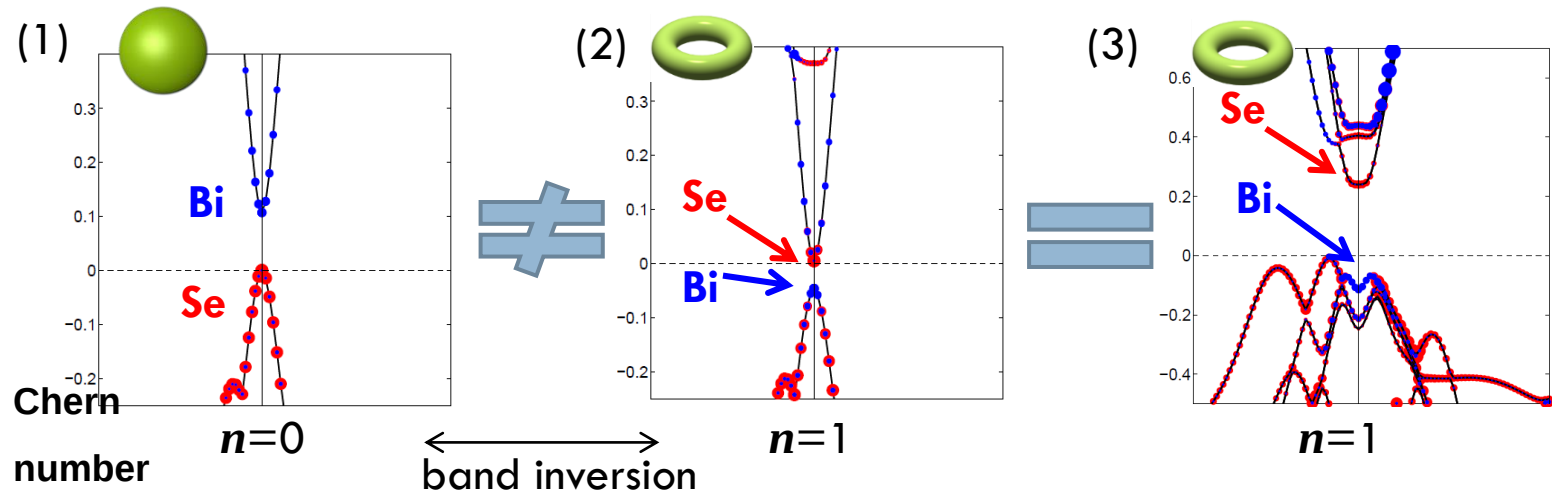


Gauss-Bonnet Theorem:

$$\oint_S K_{\text{Gauss}} ds = 2\pi(1 - g)$$

$\nearrow$ Gauss curvature $\nearrow$ genus

Topology in condensed matter physics



TKNN theory:

$$\sum_m \frac{1}{2\pi} \int_{BZ} d^2k \nabla \times i \langle u_m | \nabla | u_m \rangle = n$$

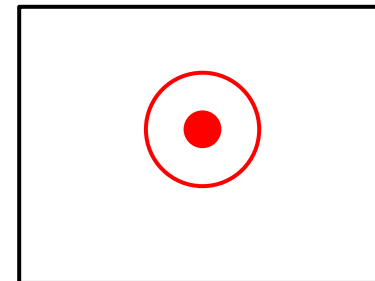
Berry curvature

Chern number

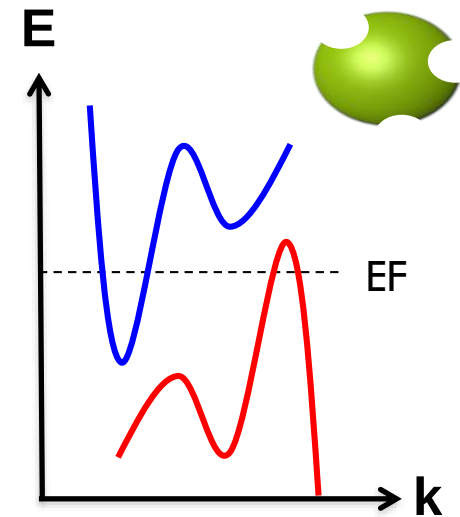
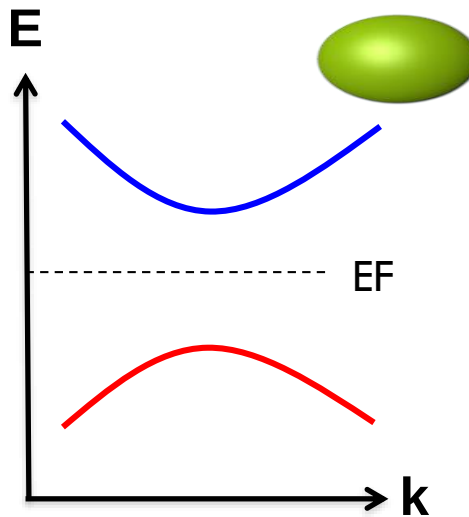
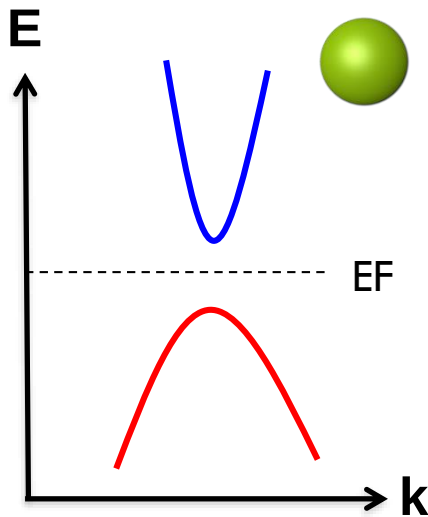
Thouless, Kohmoto, Nightingale, and den Nijs,
Phy. Rev. Lett. **49**, 405 (1982).

Berry curvature(flux)

BZ

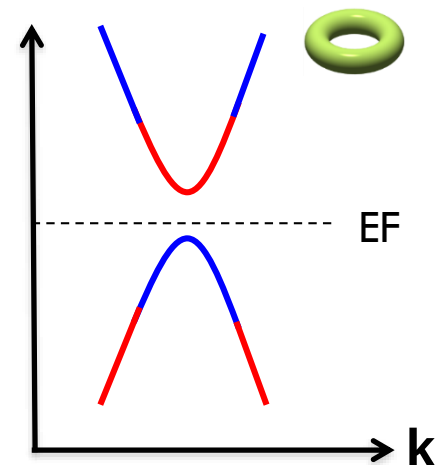


Topology in condensed matter physics



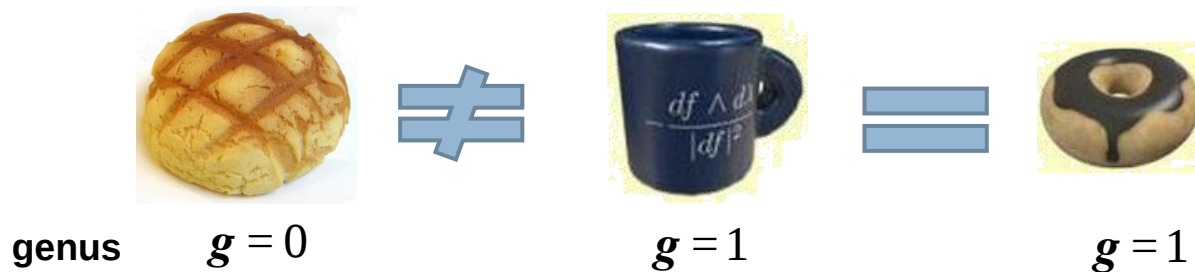
A. Bansil, Hsin Lin, Tanmoy Das, arXiv:1603.03576 (2016)

The point is that we can obtain the genus of the crumpled ball from that of the spherical ball so long as we can smoothly or adiabatically deform one into the other without introducing holes. Similarly, changes in the Hamiltonian, which do not induce a band inversion anywhere in the BZ, will not change the value of Z_2 .



Topology in condensed matter physics

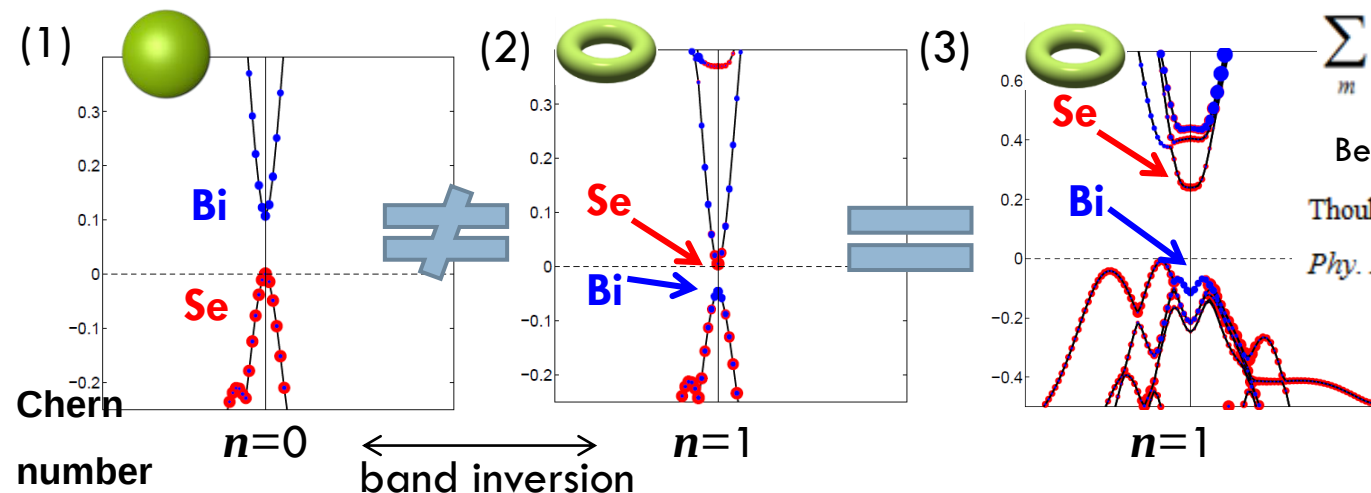
Math => real space



Gauss-Bonnet Theorem:

$$\oint_S \overset{\text{Gauss curvature}}{\underbrace{\kappa_{\text{Gauss}}}} ds = 2(1 - \underset{\text{genus}}{\underbrace{g}})$$

Phys => momentum space

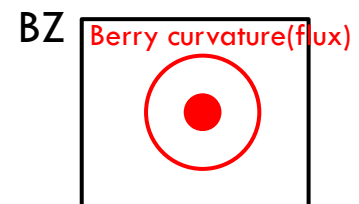


TKNN theory:

$$\sum_m \frac{1}{2\pi} \int_{\text{BZ}} d^2k \nabla \times i \langle u_m | \nabla | u_m \rangle = n$$

Berry curvature $\uparrow$ Chern number $\uparrow$

Thouless, Kohmoto, Nightingale, and den Nijs,
Phy. Rev. Lett. **49**, 405 (1982).



Topological phase transition

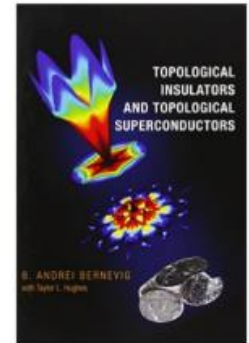
Berry connection $\mathbf{A}_n(\mathbf{k}) = i\langle u_{n\mathbf{k}} | \nabla_{\mathbf{k}} | u_{n\mathbf{k}} \rangle$

Berry curvature $\Omega_n(\mathbf{k}) = \nabla_{\mathbf{k}} \times \mathbf{A}_n(\mathbf{k})$

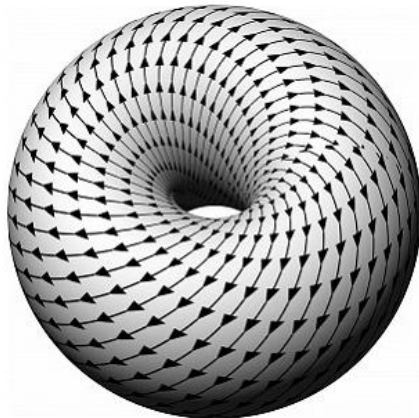
Chern invariant $\gamma_n = \oint_C \mathbf{A}_n(\mathcal{R}) \cdot d\mathcal{R} = \int_S \Omega_n(\mathcal{R}) \cdot d\mathcal{S}$

Topological Insulators and Topological Superconductors

B. Andrei Bernevig & Taylor L. Hughes
p.30

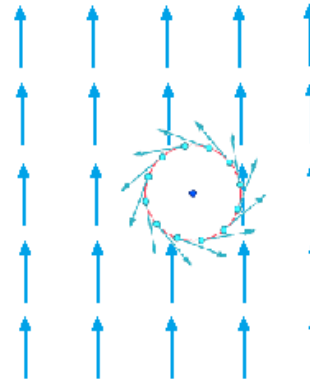


把BZ捲成甜甜圈(no boundary)



波函數平滑: $\gamma_n = 0$

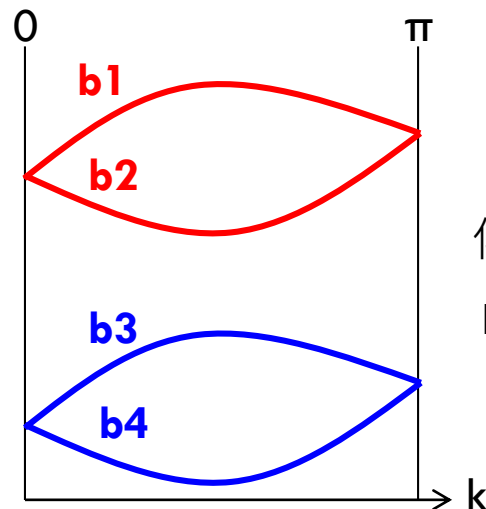
波函數有singularity



$\gamma_n \neq 0$

Topological phase transition

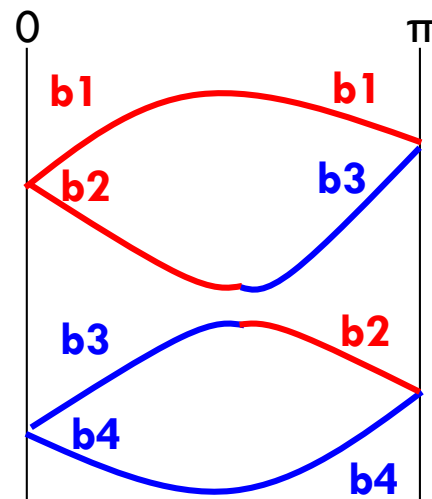
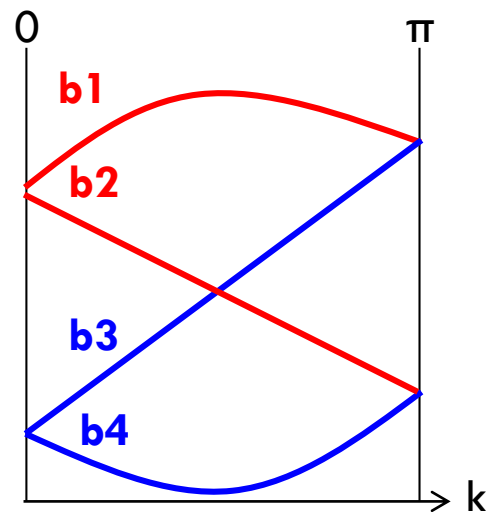
case 1



伴侶相同

Band insulator

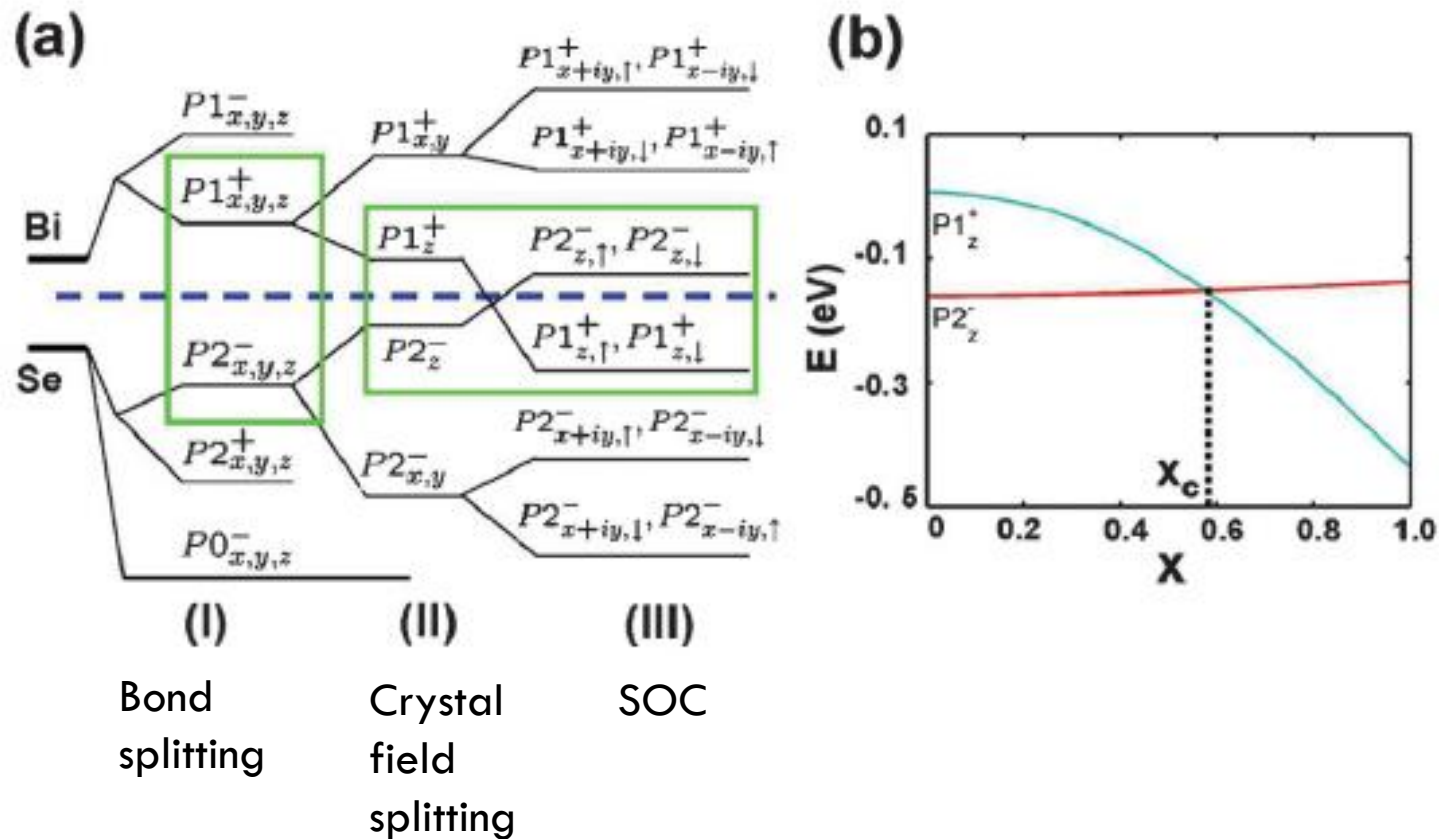
case 2



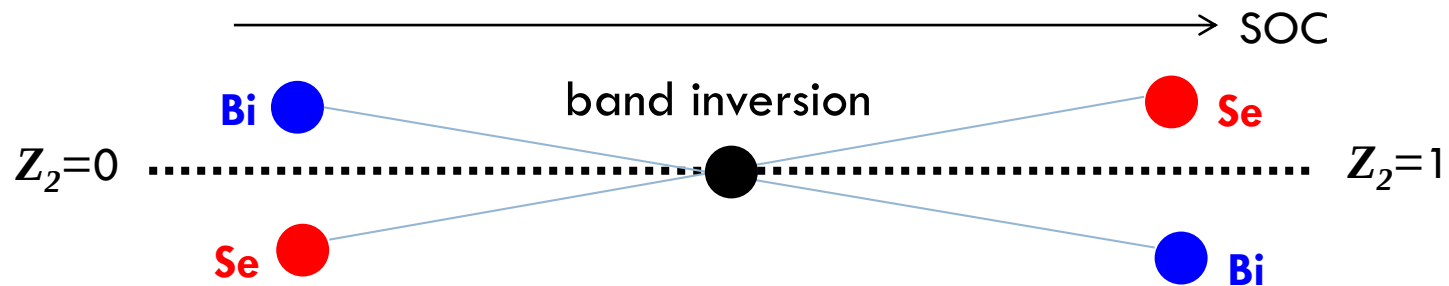
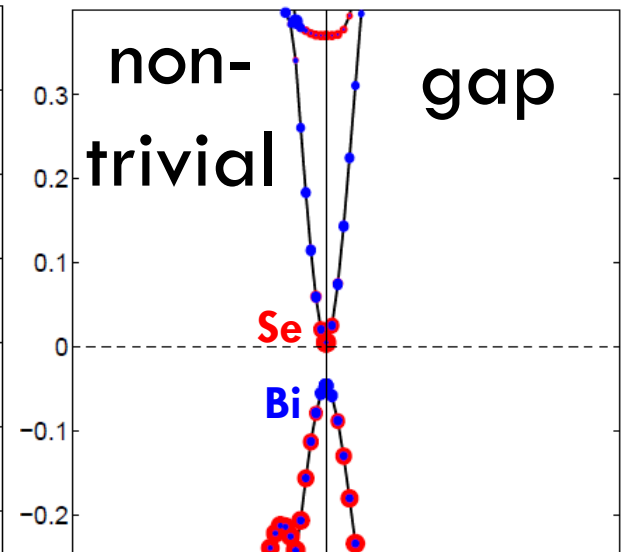
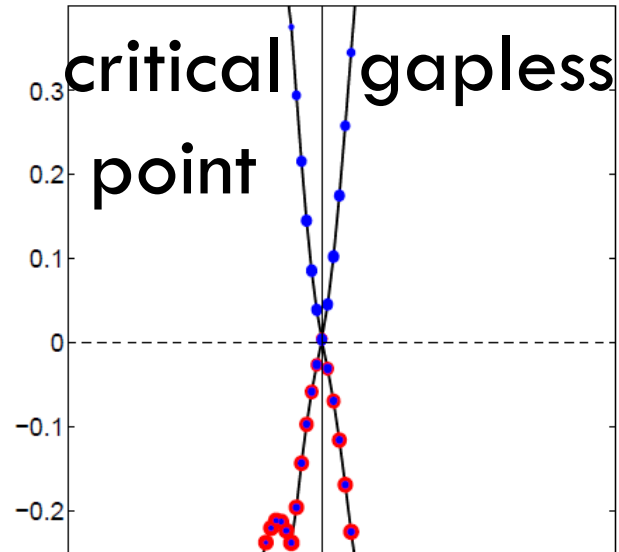
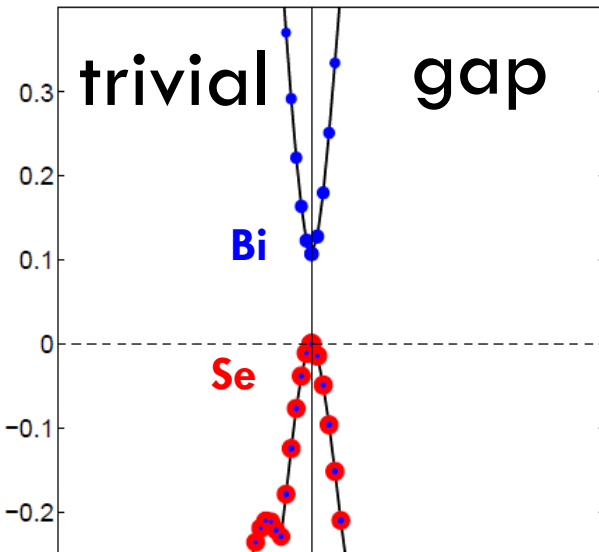
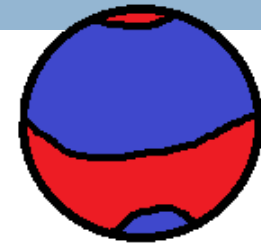
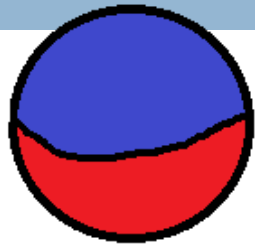
交換伴侶

Topological insulator

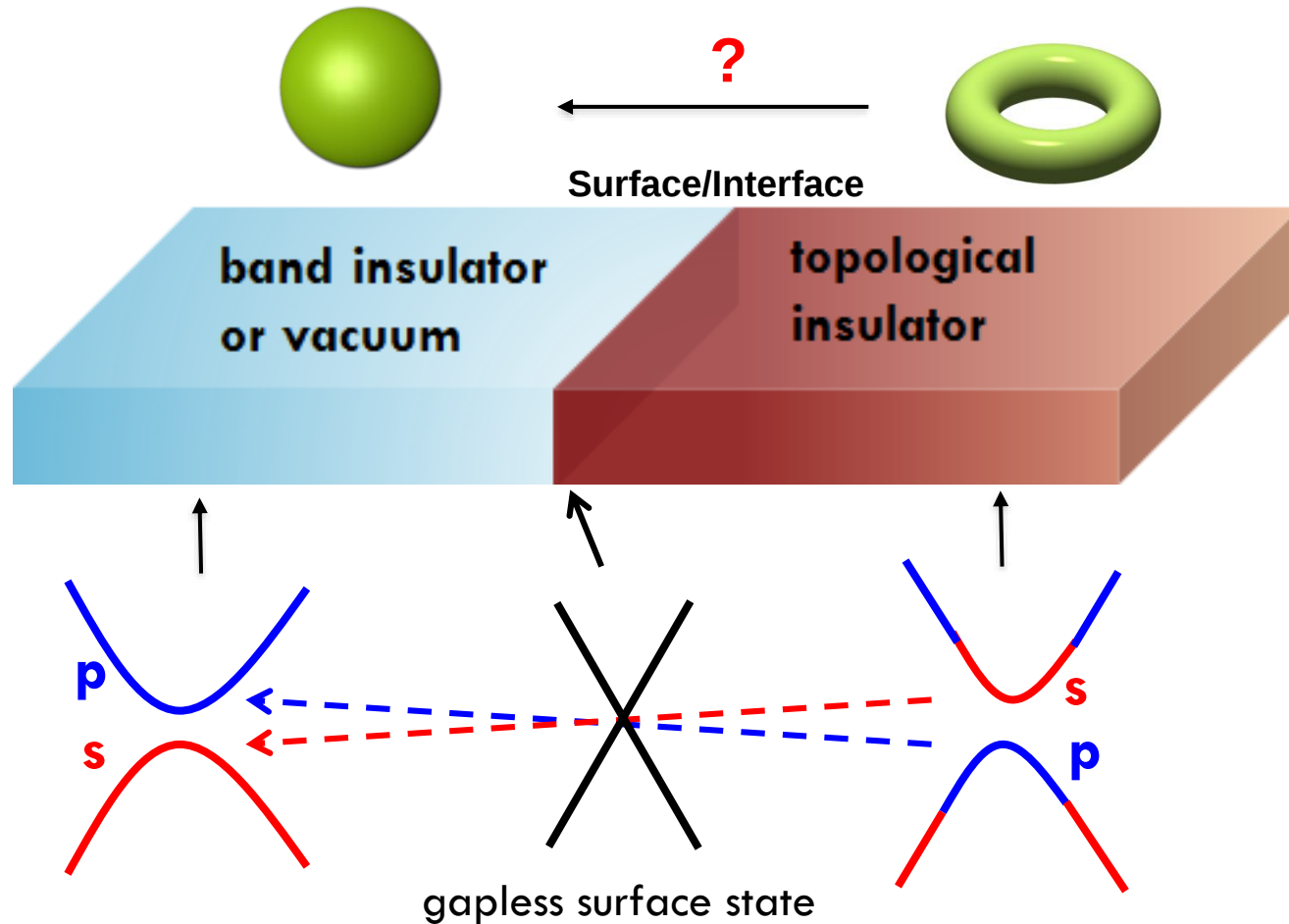
Topological phase transition



Topological phase transition

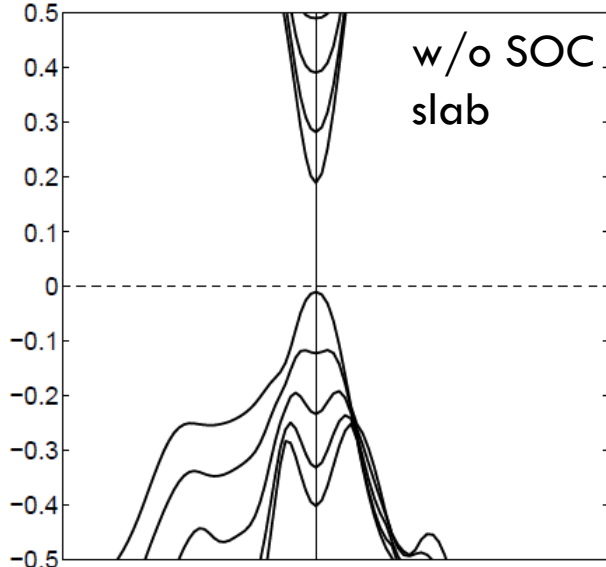
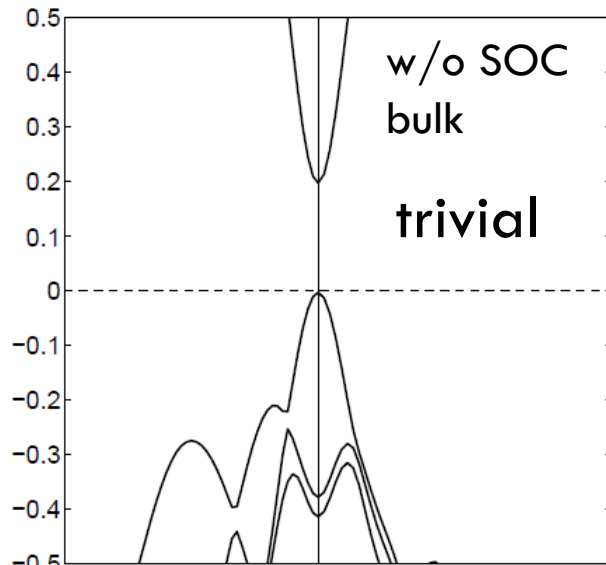


Topology in condensed matter physics (bulk-edge correspondence)

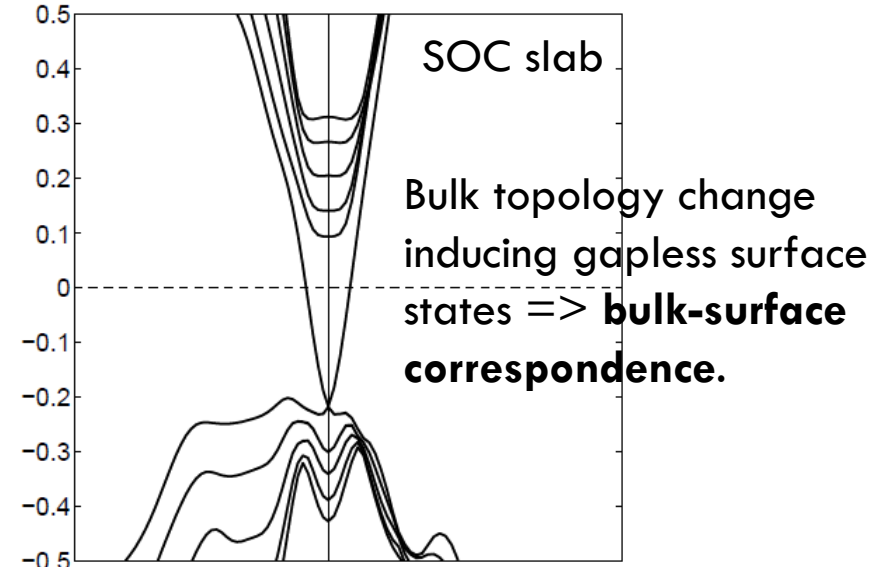
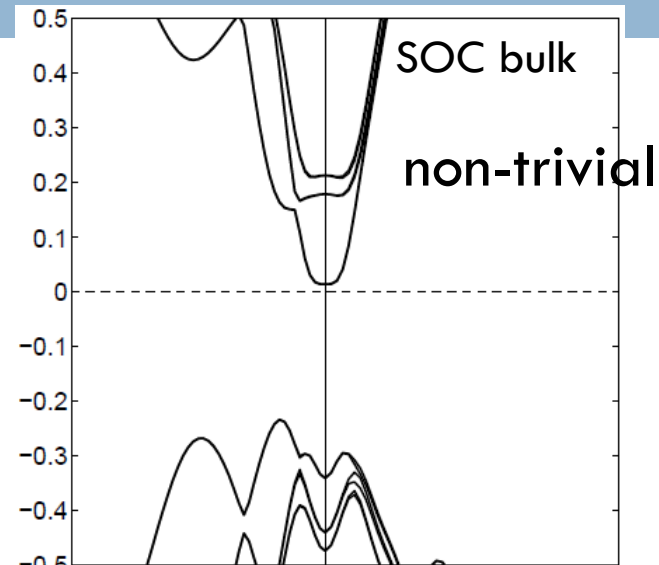
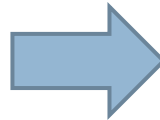


The gapless surface state is the hallmark of topological phase.

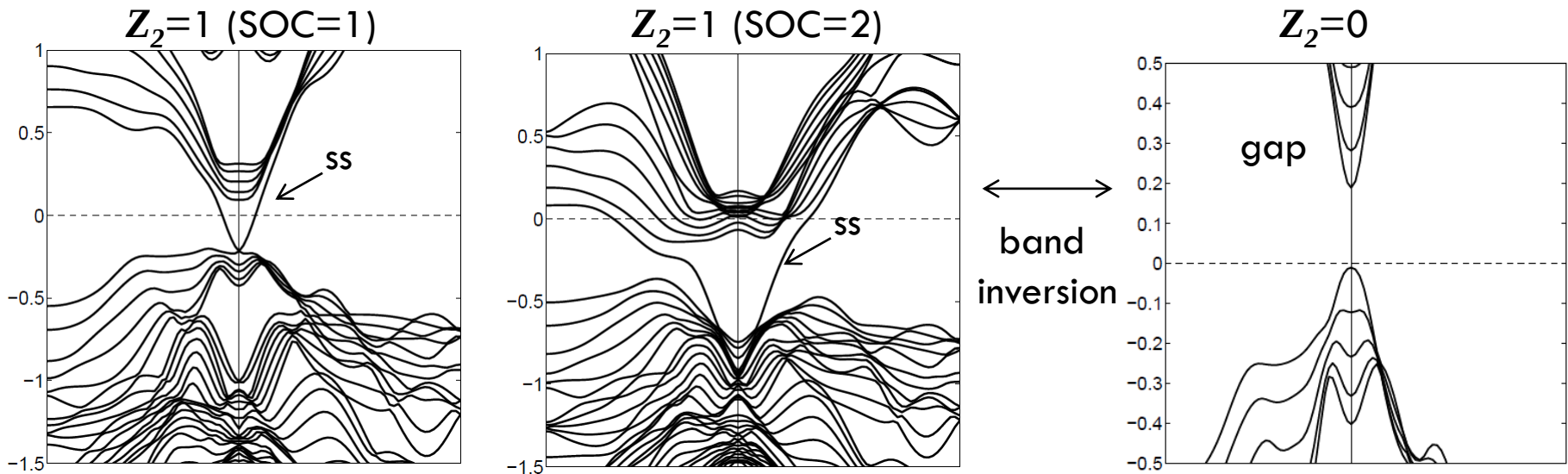
Topology in condensed matter physics (bulk-edge correspondence)



**band
inversion**

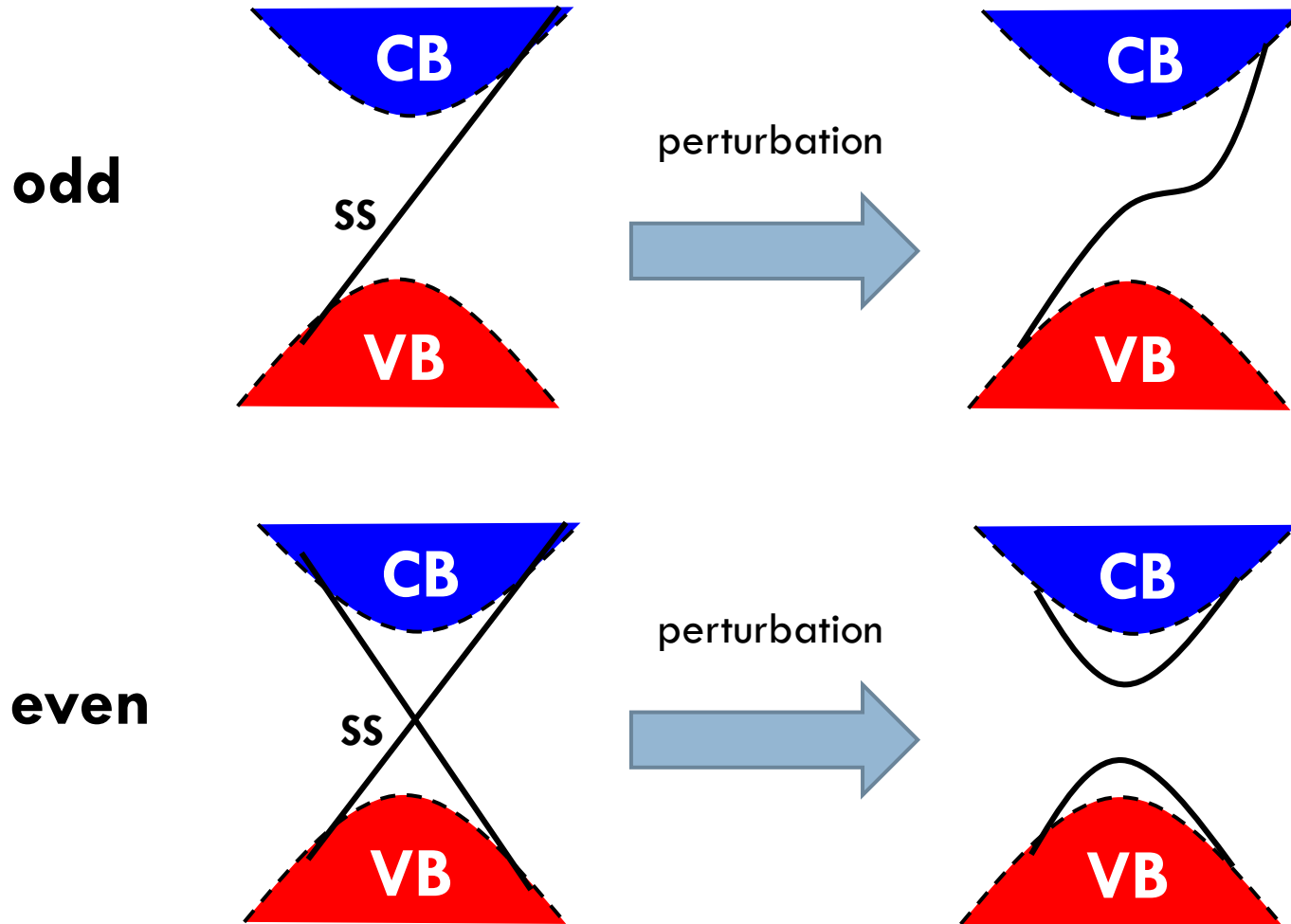


Topology in condensed matter physics (bulk-edge correspondence)



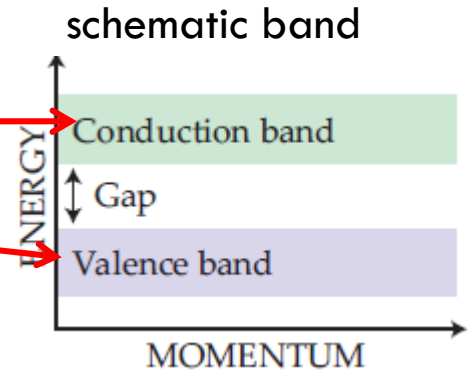
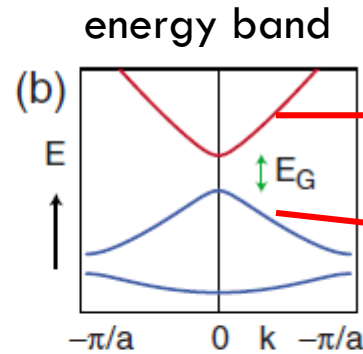
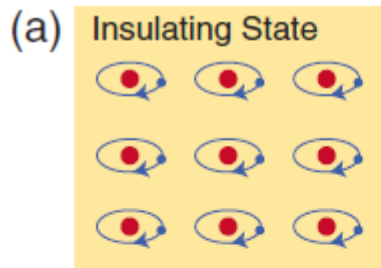
Small perturbation cannot destroy the topological surface states.

Topology in condensed matter physics (bulk-edge correspondence)

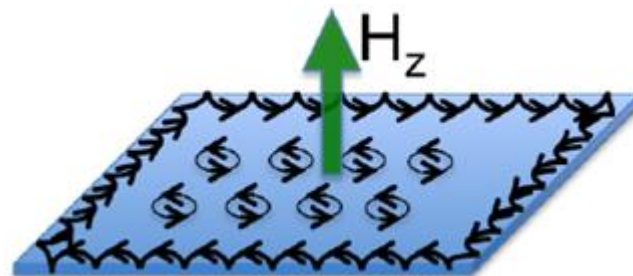
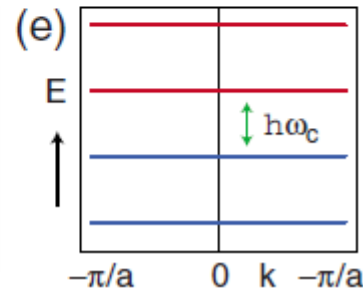
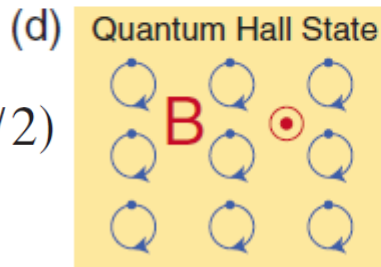


Integer quantum Hall effect (QHE)

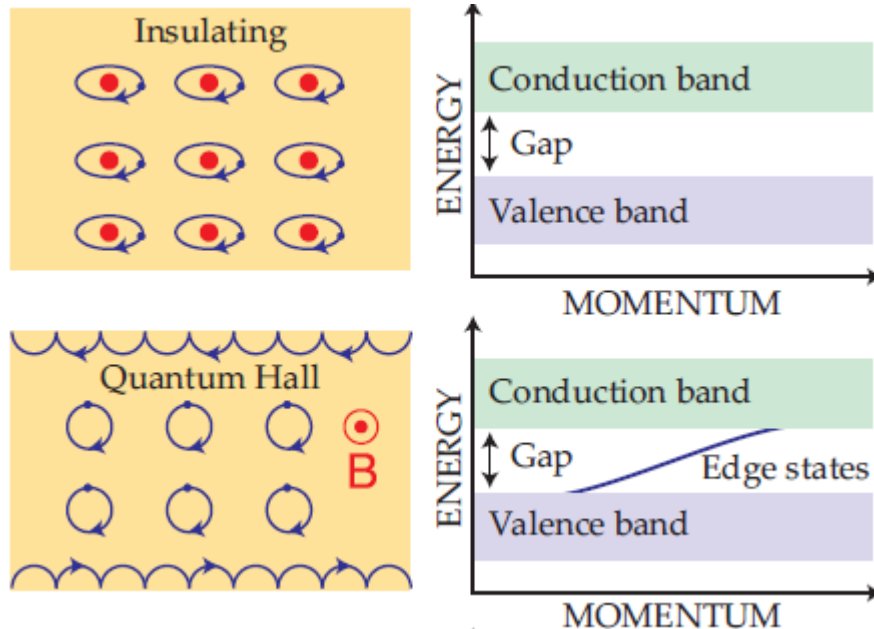
$$E_n(\vec{k})$$



$$\epsilon_m = \hbar \omega_c (m + 1/2)$$



Integer quantum Hall effect (QHE)

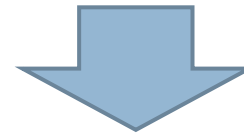


Berry connection $\mathcal{A}_m = i\langle u_m | \nabla_k | u_m \rangle$

Berry flux $\mathcal{F}_m = \nabla \times \mathcal{A}_m$

Chern invariant $n_m = \frac{1}{2\pi} \int d^2\mathbf{k} \mathcal{F}_m$

Chern number
 (陳省身) $N = n = \sum_1^N n_m$



Kubo formula

$$\sigma_{xy} = N e^2 / h.$$

Chern number

Landau's approach (order parameter)

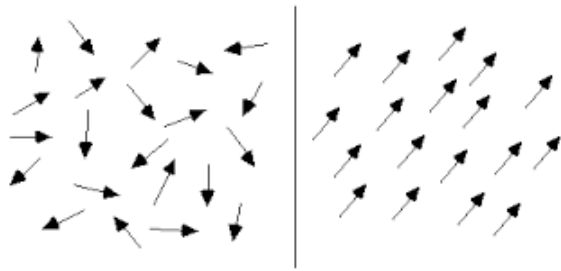
Landau's approach: spontaneous symmetry breaking (order parameter)

Magnet



$$\langle M \rangle = 0$$

$$\langle M \rangle \neq 0$$



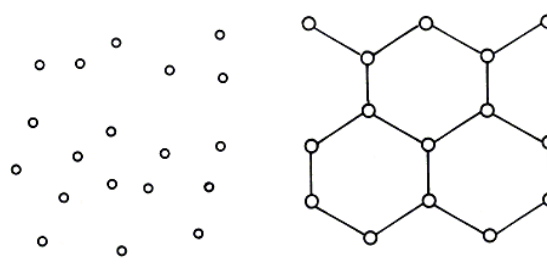
broken rotational symmetry

Crystal



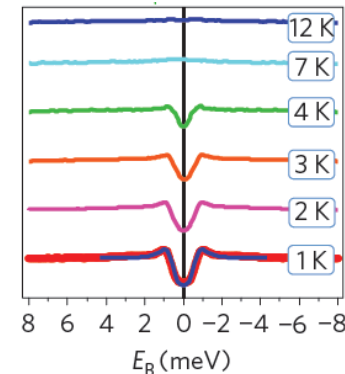
$$\langle \rho \rangle = 0$$

$$\langle \rho \rangle \neq 0$$



broken translational symmetry

Superconductor



$$\Delta = 0$$

$$\Delta \neq 0$$

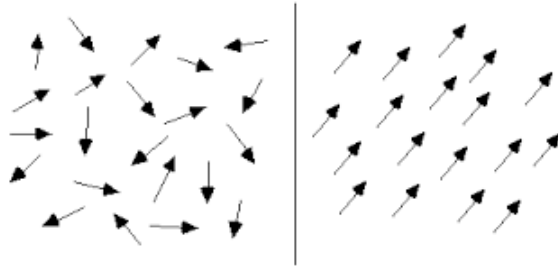
broken U(1) gauge symmetry

Topology in condensed matter physics

Landau approach: order parameter
(symmetry breaking)

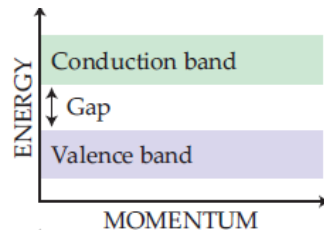
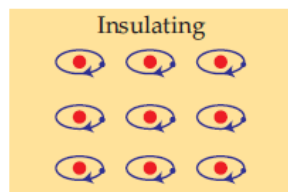
measurable
properties

High-T $\langle M \rangle = 0$ $\langle M \rangle \neq 0$ Low-T

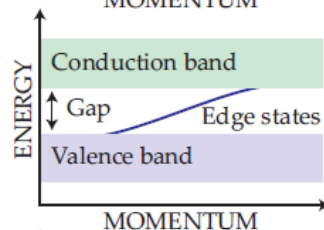
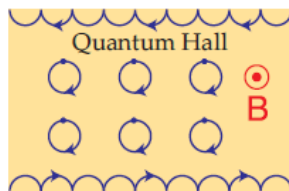


Bulk

Topology : topological invariant number



$$\nu = 0$$



$$\nu = \text{integer}$$

Surface

Density functional theory (DFT)

P. Hohenberg and W. Kohn

Phys. Rev. **136**, B864 (1964) Cited : 35015 times

W. Kohn and L. J. Sham

Phys. Rev. **140**, A1133 (1965) Cited : 39490 times

W. Kohn

Rev. Mod. Phys. **71**, 1253 (1998) (**Nobel Lecture**)

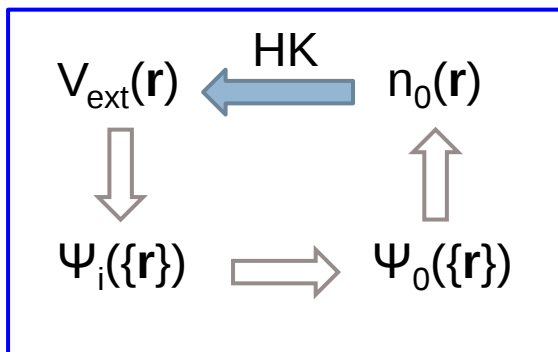
R. Martin

Electronic Structure (CAMBRIDGE 2004)

Density functional theory (DFT)

Hohenberg-Kohn Theorem

- (1) For any system of interacting particles in an external potential $V_{\text{ext}}(\mathbf{r})$, the potential $V_{\text{ext}}(\mathbf{r})$ is determined uniquely, except for a constant, by the ground state particle density $n_0(\mathbf{r})$.
- (2) A universal functional for the energy $E[n]$ in terms of the density $n(\mathbf{r})$ can be defined, valid for any external potential $V_{\text{ext}}(\mathbf{r})$. For any particular $V_{\text{ext}}(\mathbf{r})$, the exact ground state energy of the system is the global minimum value of this functional, and the density $n(\mathbf{r})$ that minimizes the functional is the exact ground state density $n_0(\mathbf{r})$.



$$\hat{H}\Psi = [\hat{T} + \hat{V} + \hat{U}] \Psi = \left[\sum_i^N \left(-\frac{\hbar^2}{2m_i} \nabla_i^2 \right) + \sum_i^N V(\vec{r}_i) + \sum_{i < j}^N U(\vec{r}_i, \vec{r}_j) \right] \Psi = E\Psi$$

$$n(\vec{r}) = N \int d^3r_2 \cdots \int d^3r_N \Psi^*(\vec{r}, \vec{r}_2, \dots, \vec{r}_N) \Psi(\vec{r}, \vec{r}_2, \dots, \vec{r}_N)$$

$$E[n] = \underbrace{T[n] + U[n]}_{\text{Universal functional}} + \int V(\vec{r}) n(\vec{r}) d^3r$$

$T[n]$ Kinetic energy

$U[n]$ e-e interaction

Density functional theory (DFT)

Kohn-Sham ansatz

The exact ground state density can be represented by the ground state density of an auxiliary system of non-interacting particles. This is called “non-interacting-V-representability”, although there are no rigorous proofs for real systems of interest, we will proceed assuming its validity.

$$H_{\text{aux}} = -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r})$$

$$n(\vec{r}) = \sum_{i=1}^N |\psi_i(\vec{r})|^2 \quad \text{where } \psi_i(\vec{r}) \text{ are orthonormal orbitals}$$

$$T_0[n] = -\frac{\hbar^2}{2m} \sum_i \langle \psi_i | \nabla^2 | \psi_i \rangle \quad \text{the independent particle kinetic energy}$$

$$V_H[n] = \frac{1}{2} \int d\vec{r} d\vec{r}' \frac{n(\vec{r})n(\vec{r}')}{|\vec{r} - \vec{r}'|} \quad \text{Hartree potential}$$

Density functional theory (DFT)

$$E_{\text{KS}} = T_0[n] + V_{\text{H}}[n] + \int d\vec{r} V_{\text{ext}}(\vec{r})n(\vec{r}) + E_{\text{xc}}[n]$$

where $E_{\text{xc}}[n] = F_{\text{HK}}[n] - (T_0[n] + V_{\text{H}}[n])$ ← approximation
LDA, GGA ...etc

functional derivative to minimize E_{KS}

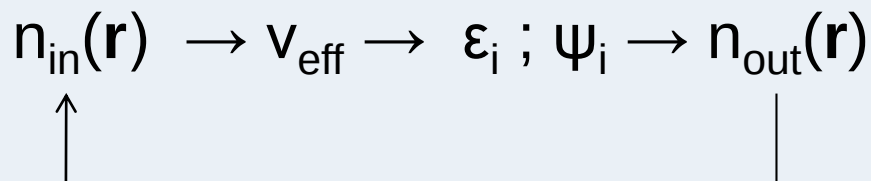
$$\left\{ -\frac{\hbar^2}{2m} \nabla^2 + v_{\text{eff}}(\vec{r}) \right\} \psi_i(\vec{r}) = \varepsilon_i \psi_i(\vec{r})$$

which is the **single-particle Kohn-Sham equation**

Local density approximation (LDA)

$$E_{\text{xc}}^{\text{LDA}}[n] = \int d\vec{r} v_{\text{xc}}(n(\vec{r})) n(\vec{r})$$

Self-consistent scheme



Method

Step 1 Density functional theory (DFT)

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V_s(\vec{r}) \right] \phi_i(\vec{r}) = \epsilon_i \phi_i(\vec{r}) \quad \text{where} \quad V_s(\vec{r}) = V(\vec{r}) + \int \frac{e^2 n_s(\vec{r}')}{|\vec{r} - \vec{r}'|} d^3 r' + V_{XC}[n_s(\vec{r})]$$



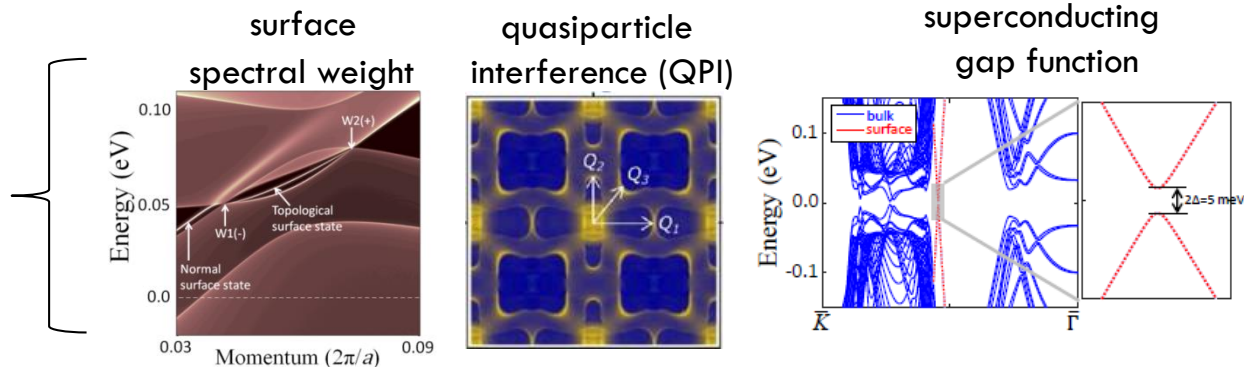
Step 2 ab-initio tight-binding model (Wannier function)

$$\underbrace{w_{n\mathbf{R}}(\mathbf{r})}_{\text{Wannier}} = \frac{V}{(2\pi)^3} \int_{\text{BZ}} \left[\sum_m U_{mn}^{(\mathbf{k})} \underbrace{\psi_{m\mathbf{k}}(\mathbf{r})}_{\text{Bloch}} \right] e^{-i\mathbf{k} \cdot \mathbf{R}} d\mathbf{k}$$

hopping parameters from first-principles



Step 3 Electronic structures



Density functional theory (DFT)

Total Energy and magnetic moment of Fe

Structure,
lattice constant, and
magnetic moment
all agree well with
experiments

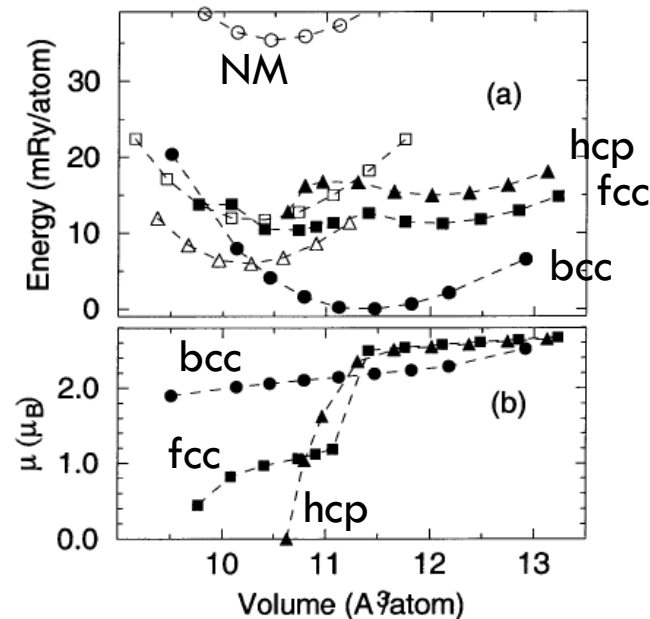
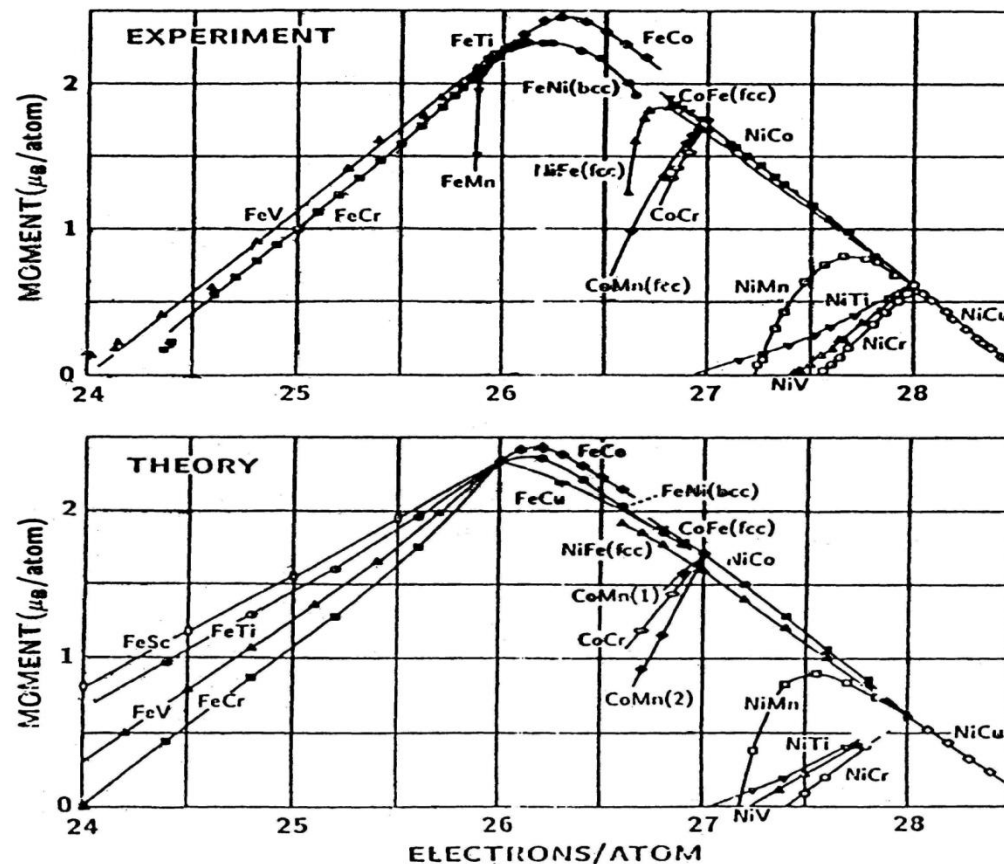


FIG. 1. (a) Total energy (relative to -2545.611 Ry/atom) of Fe as a function of volume per atom for bcc (circles), fcc (squares) and hcp (triangles). The curves are a polynomial fit to the total energies. Solid symbols denote the ferromagnetic states and open symbols, the nonmagnetic states. (b) Magnetic moment (μ) of bcc, fcc and hcp Fe as a function of volume per atom.

Density functional theory (DFT)

Slater-Pauling Curve: Experiment and L(S)DA Theory
LDA gives very good results for weakly correlated system

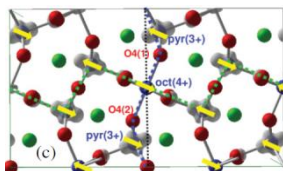


Density functional theory (DFT)

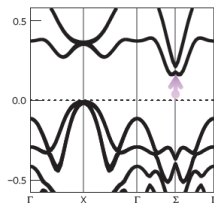
Density functional theory (DFT) + ab-initio tight-binding model:

Transition metal oxides

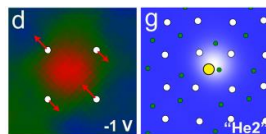
multiferroic: TbMn_2O_5
PRB



Iridate: $\text{Sr}_3\text{Ir}_2\text{O}_7$
Nat. Mat.

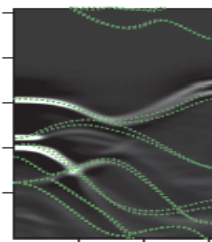


Cuprate: Bi2212
Nano Lett.

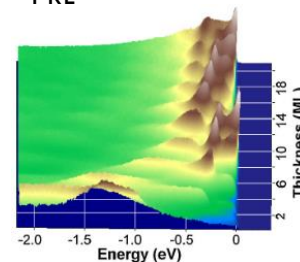


2D materials (TMDC and thin-film)

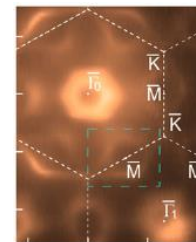
TMDC: MoSe_2
Nat. Nano.



Pb/Ge
PRL

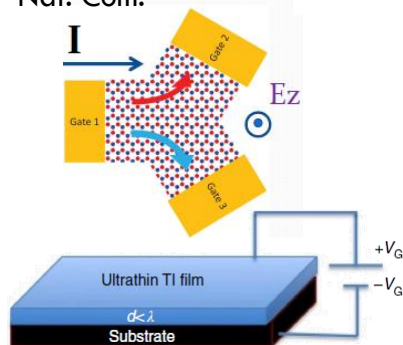


PbAu/Pb
NJP

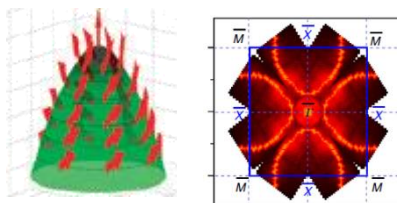


Topological insulator

2D Topological insulator
Nat. Com.

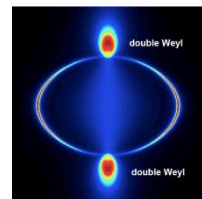


3D Topological insulator
Nat. Phys.
Nat. Com.
PRL

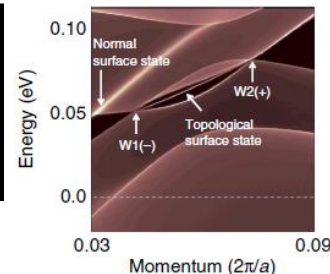


Topological semimetals

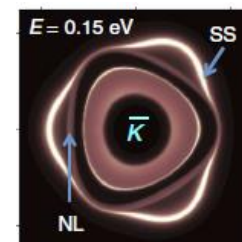
3D Dirac
Science
Nat. Com.



Weyl semimetals
Nat. Phys.
Nat. Com.
PRL



Nodal-line: PbTaSe_2
Nat. Com.



Density functional theory (DFT)

Insufficient of LDA

- Gaps too small or no gap, PRB44, 943 (1991)
- Spin and orbital **moment too small**, PRB44, 943 (1991)
- Especially for **transition metal oxides**

Attempts on improving LDA

- Hartree-Fock (HF) method, PRB48(1993)5058
- GW approximation (GWA), PRB46(1992)13051,
- **LDA+Hubbard U (LDA+U) method, PRB44(1991)943**
- DMFT, TDDFT, ...

Density functional theory (DFT)

TABLE II. Experimental (expt) and calculated (LDA + U) spin moments (m , in μ_B) and energy gaps (E , in eV) of the late-3d-transition-metal monoxides. For comparison, we also show these quantities as calculated from LSDA (Ref. 1).

	E_{LSD}	$E_{\text{LSD}+U}$	E_{expt}	m_{LSD}	$m_{\text{LSD}+U}$	m_{expt}
CaCuO ₂	0.0	2.1	1.5 ^a	0.0	0.66	0.51 ^b
CuO	0.0	1.9	1.4 ^c	0.0	0.74	0.65 ^d
NiO	0.2	3.1	4.3, ^e 4.0 ^f	1.0	1.59	1.77, ^g 1.64, ^h 1.90 ⁱ
CoO	0.0	3.2	2.4 ^{j,k}	2.3	2.63 (3.60)	3.35, ^l 3.8 ^m
FeO	0.0	3.2	2.4 ⁿ	3.4	3.62 (4.59)	3.32 ^m
MnO	0.8	3.5	3.6–3.8 ^o	4.4	4.61	4.79, ^s 4.58 ⁱ

^aY. Tokura, T. Arima, S. Koshihara, T. Ido, S. Ishibashi, H. Takagi, and S. Uchida, *Proceedings of the Second International Symposium on Superconductivity*, Tsukuba (Springer, New York, in press).

^bD. Vaknin, E. Cougnol, P. K. Davies, J. E. F. *et al.*, *Phys. Rev. B* **39**, 9122 (1989).

^cF. P. Koffyberg and F. A. Benko, *J. Appl. Phys.*

^dJ. B. Forsyth, P. J. Brown, and B. M. Wankly

^eG. A. Sawatzky and J. W. Allen, *Phys. Rev. L*

^fS. H fner, J. Osterwalder, T. Riesterer, and F.

^gB. E. F. Fender, A. J. Jacobson, and F. A. We

^hH. A. Alperin, *J. Phys. Soc. Jpn. Suppl. B* **17**,

ⁱA. K. Cheetham and D. A. O. Hope, *Phys. Re*

^jJ. van Elp *et al.* (unpublished).

^kR. J. Powell and W. E. Spicer, *Phys. Rev. B* **2**, 2182 (1970).

^lD. C. Kahn and R. A. Ericson, *Phys. Rev. B* **1**, 2243 (1970).

^mW. L. Roth, *Phys. Rev.* **110**, 1333 (1958); D. Hermann-Ronzaud, P. Burlet, and J. Rossat Mignod, *J. Phys. C* **11**, 2123 (1978).

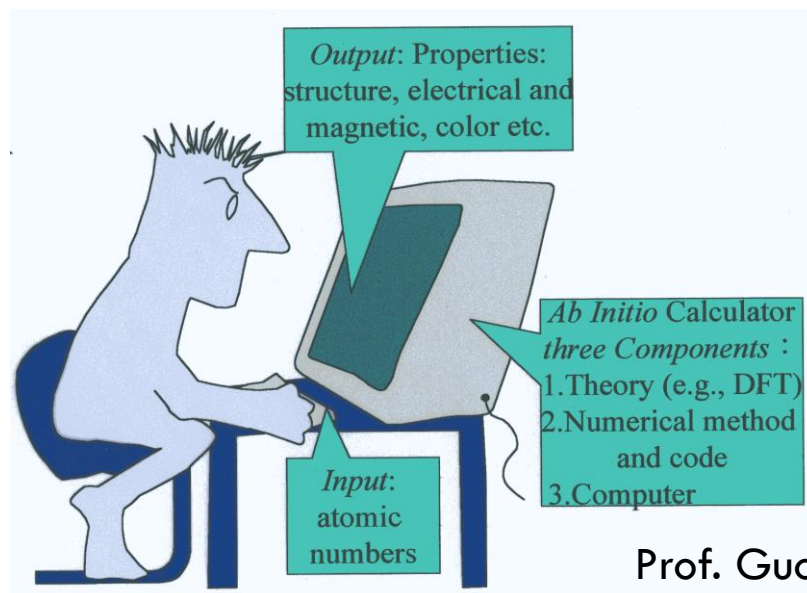
ⁿH. K. Bowen, D. Adler, and B. H. Auken, *J. Solid State Chem.* **12**, 355 (1975).

^oR. N. Iskenderov, I. A. Drabkin, L. T. Emel'yanova, and Ya. Ksendzov, *Fiz. Tverd. Tela (Leningrad)* **10**, 2573 (1968) [*Sov. Phys.—Solid State* **10**, 2031 (1969)]; L. Messick, W. C. Walker, and R. Glosser, *Phys. Rev. B* **6**, 3941 (1972).

Gaps too small or no gap
Spin and orbital moment too small
PRB 44 (1991) 943

Density functional theory (DFT)

DFT package: VASP, OpenMX, Quantum Espresso ...etc
Ab-initio tight-binding model



Prof. Guo (NTU)

Ab-initio: 只要給定元素種類和原子排列位置,理論上可以得到所有物理量.

Topological Insulator

1. Introduction

Band theory

Topology in condensed matter physics

Basics properties: Robust, invariant number, gapless surface states

Comparing with Landau's approach

Density functional theory (DFT)

2. Topological insulator (quantum spin Hall insulator)

Strong topological insulator, weak topological insulator, topological crystalline insulator, topological Kondo insulator...etc

3. Topological semimetal

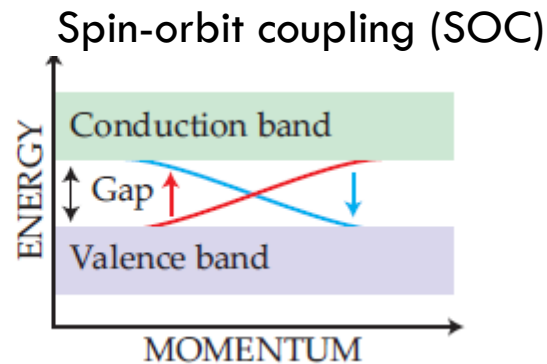
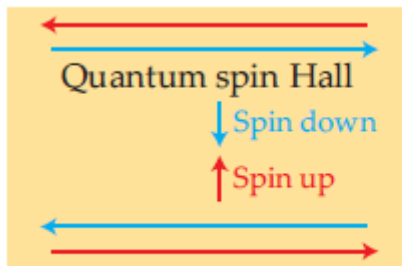
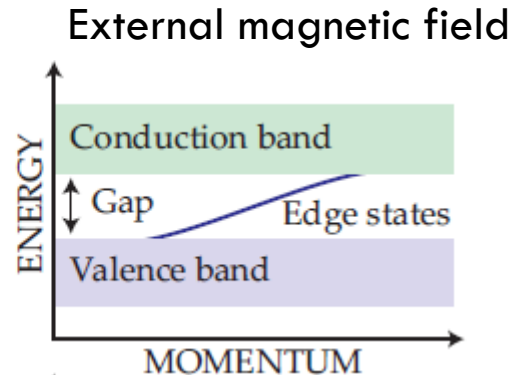
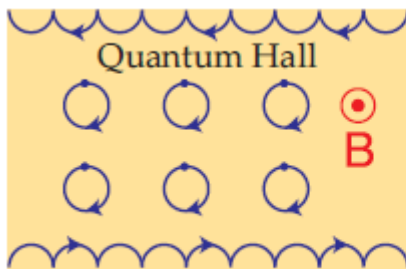
3D Dirac semimetal, Weyl semimetal, Nodal semimetal, New Fermion

Topological insulator

- (1) M. Z. Hasan and C. L. Kane , Rev. Mod. Phys. **82**, 3045 (2010)
- (2) X.-L. Qi and S.-C. Zhang, Rev. Mod. Phys. **83**, 1057 (2011)
- (3) A. Bansil, Hsin Lin, Tanmoy Das, arXiv:1603.03576 (2016)
- (4) Hongming Weng et al., Advances in Physics **64**, 227 (2015)
- (5) Chao-Xing Liu, Shou-Cheng Zhang and Xiao-Liang Qi, arXiv:1508.07106 (2015)
- (6) M. Z. Hasan, S.-Y. Xu, G. Bian, *Phys. Scr.* **T164**, 014001 (2015)
- (7) Hongming Weng et al., arXiv:1603.04744 (2016)

Quantum spin Hall (QSH)

L. Fu, Phys. Rev. B **76**, 045302 (2007)



$$\text{TRS} : E(k, \uparrow) = E(-k, \downarrow)$$

$$n_{\uparrow} + n_{\downarrow} = 0,$$

$$n_{\sigma} = (n_{\uparrow} - n_{\downarrow}) / 2$$

$\mathbb{Z}_2$ invariant is

$$\nu = n_{\sigma} \bmod 2$$

$\nu_0 = 0$: normal insulator

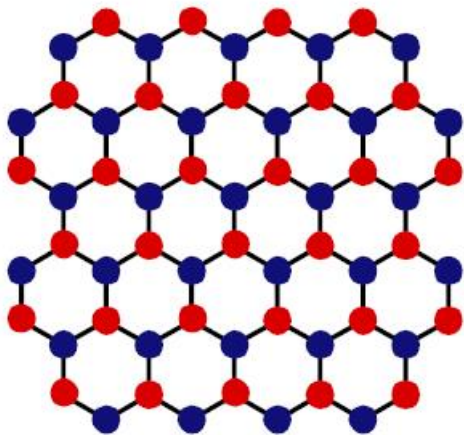
$\nu_0 = 1$: QSH insulator

T-breaking : Chern number

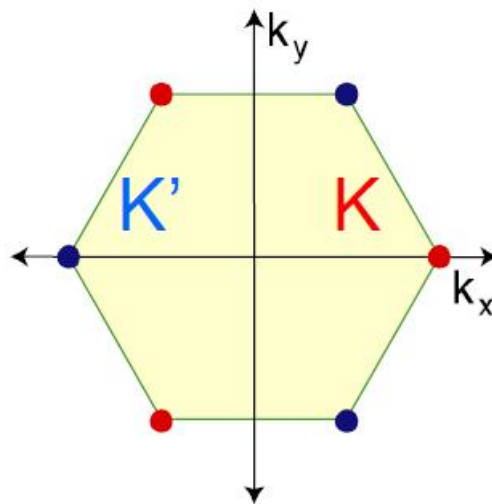
T-preserve : $\mathbb{Z}_2$ number (spin Chern number)

Quantum spin Hall (QSH)

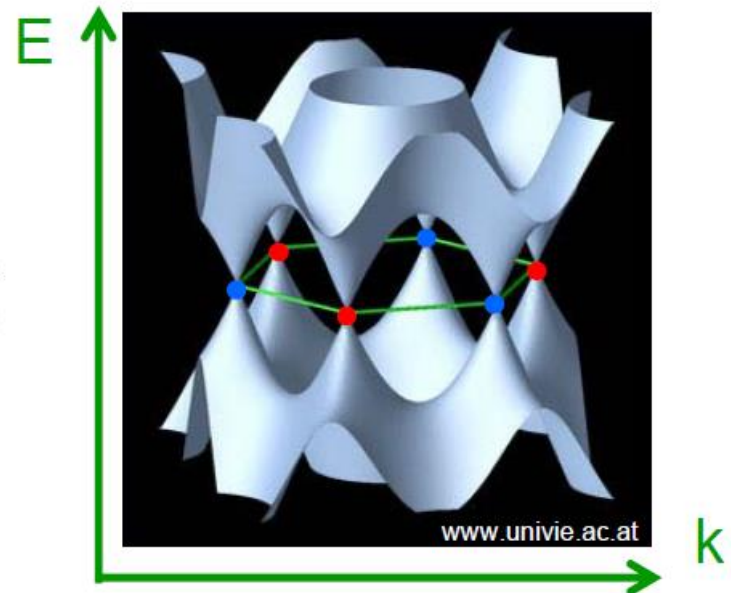
$$H = t \sum_{\langle i,j \rangle} c_i^\dagger c_j$$



Honeycomb Lattice

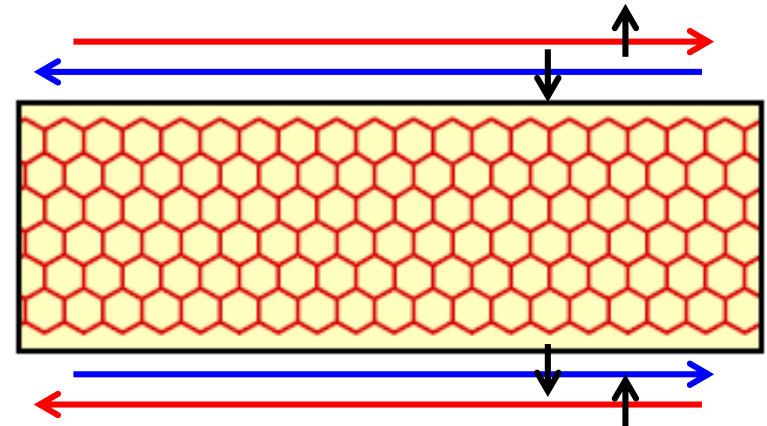
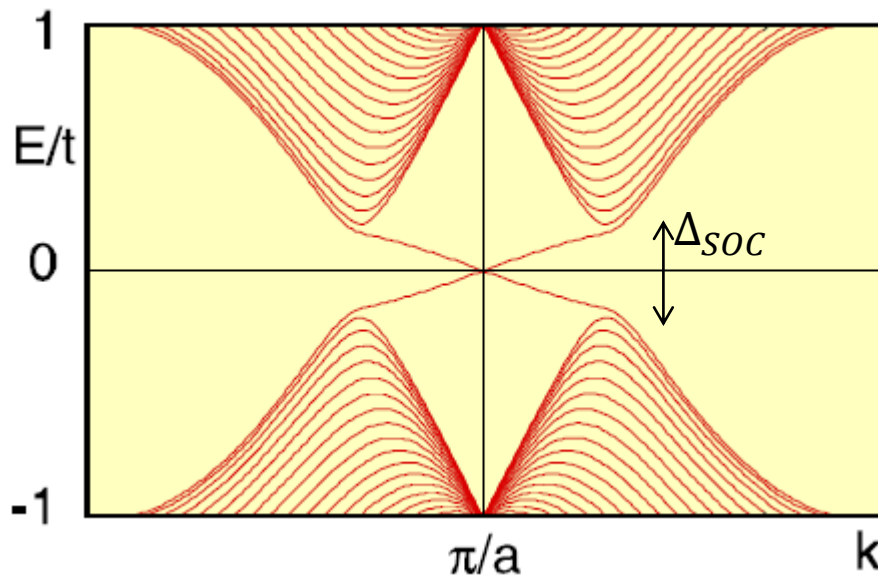


Brillouin Zone



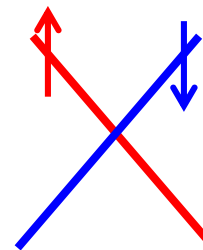
Quantum spin Hall (QSH)

$$H = t \sum_{\langle i,j \rangle} c_i^\dagger c_j + i\lambda_{SO} \sum_{\langle\langle i,j \rangle\rangle} v_{ij} c_i^\dagger s^z c_j$$

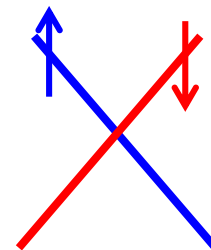


helical spin texture

Top edge



Bottom edge



gap $\sim 10^{-3}$ meV

Topological invariant and parity

method 1: berry phase

Berry connection $\mathcal{A}_n(\mathbf{R}) = i\langle n(\mathbf{R}) | \nabla_{\mathbf{R}} | n(\mathbf{R}) \rangle$

Berry curvature $\Omega_n(\mathbf{R}) = \nabla_{\mathbf{R}} \times \mathcal{A}_n(\mathbf{R})$

Chern invariant $\gamma_n = \int_S d\mathbf{S} \cdot \Omega_n(\mathbf{R})$

Chern number $N = \sum_{n=1}^{n=occ} \gamma_n$

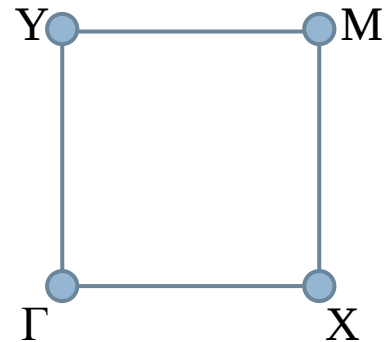
$$n_{\uparrow} + n_{\downarrow} = 0,$$

$$n_{\sigma} = (n_{\uparrow} - n_{\downarrow})/2$$

$\mathbb{Z}_2$ invariant is

$$\nu = n_{\sigma} \bmod 2$$

method 2: parity

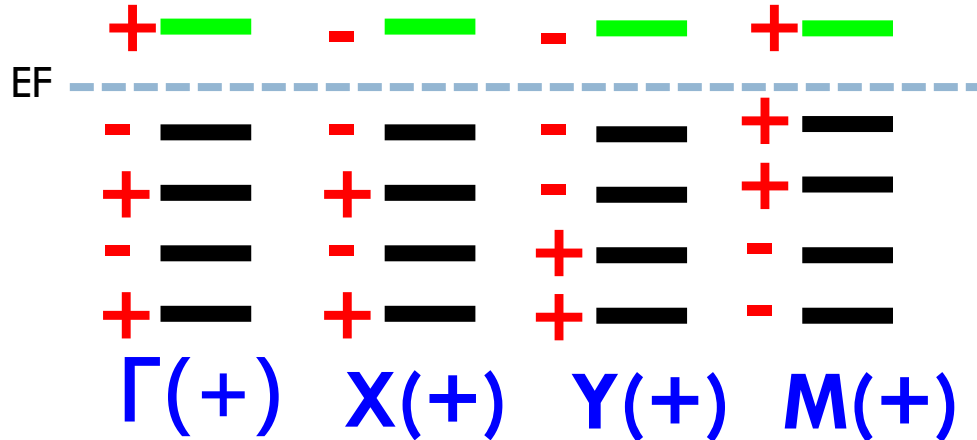


If the system preserves time-reversal and inversion symmetry

$$Z_2 = \delta_{\Gamma} \delta_X \delta_M \delta_Y = (-1)^{\nu}$$

L. Fu, Phys. Rev. B **76**, 045302 (2007)

Topological invariant and parity

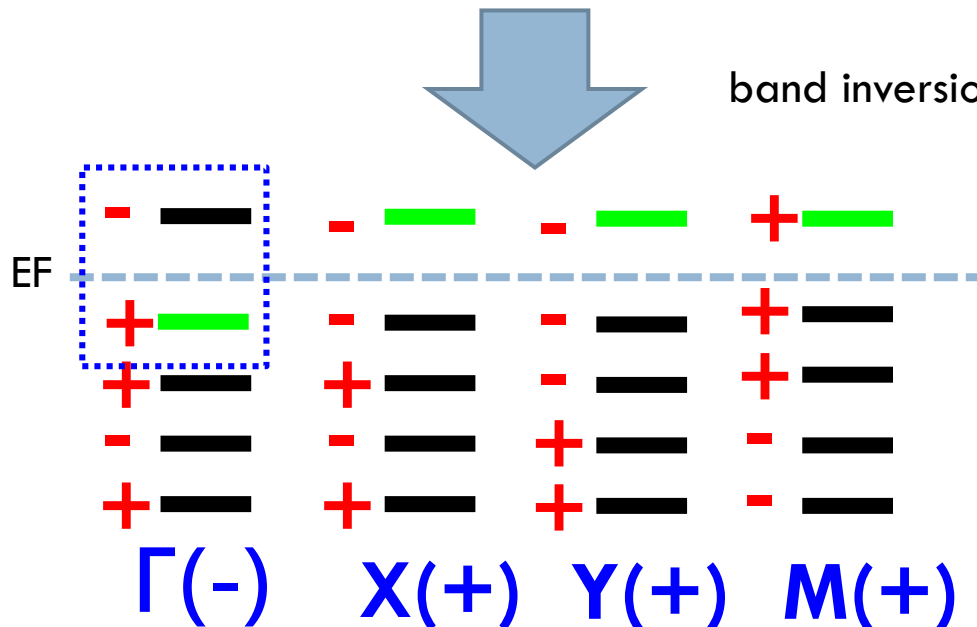


L. Fu, Phys. Rev. B **76**, 045302 (2007)

$$\delta_\Gamma \delta_X \delta_Y \delta_M = -1^0$$

$$1 * 1 * 1 * 1 = (-1)^0$$

$$Z_2 = 0$$



band inversion at Γ point

$$\delta_\Gamma \delta_X \delta_Y \delta_M = -1^1$$

$$-1 * 1 * 1 * 1 = (-1)^1$$

$$Z_2 = 1$$

Topological insulator

$2D: \nu_0$

Quantum spin Hall insulator

$3D: (\nu_0; \nu_1, \nu_2, \nu_3)$

Topological insulator

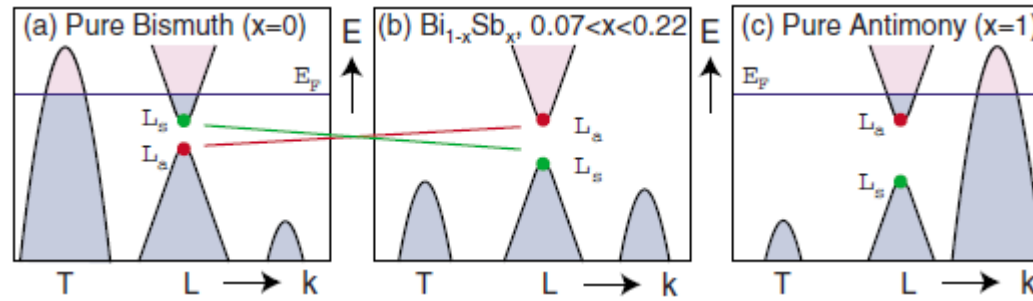
$\uparrow$
strong index

$\underbrace{\hspace{1.5cm}}$
weak index

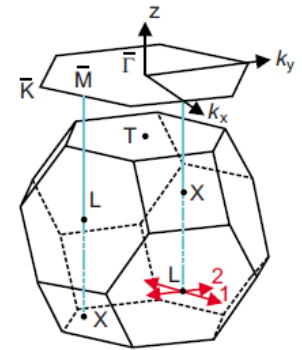
$\nu_0 \neq 0$: *strong topological insulator*

$\nu_i \neq 0$: *weak topological insulator*

Topological insulator ($\text{Bi}_{1-x}\text{Sb}_x$)



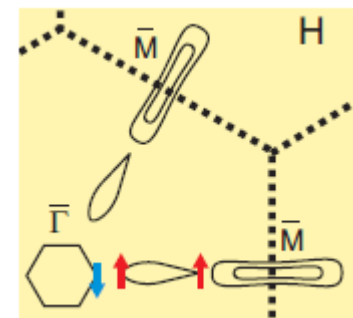
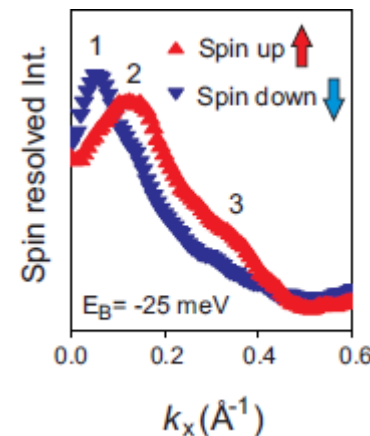
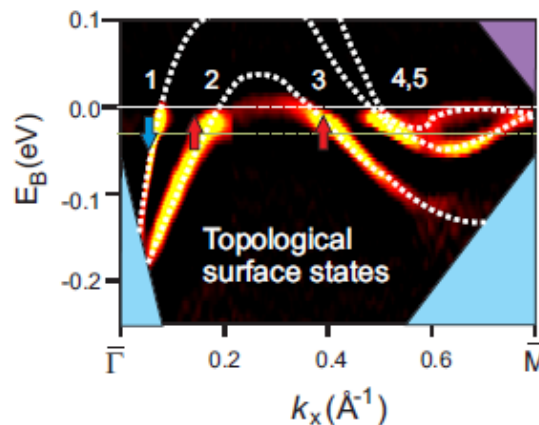
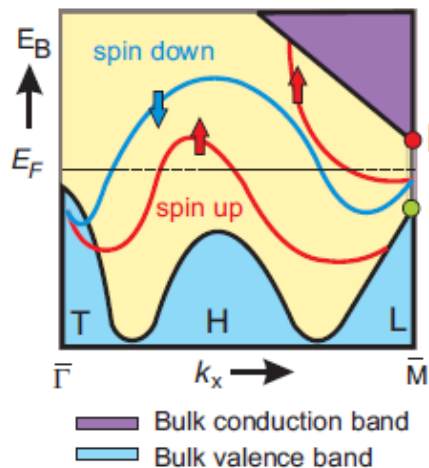
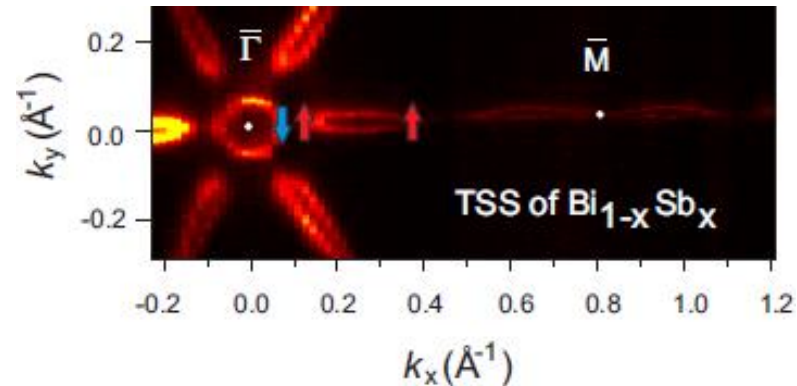
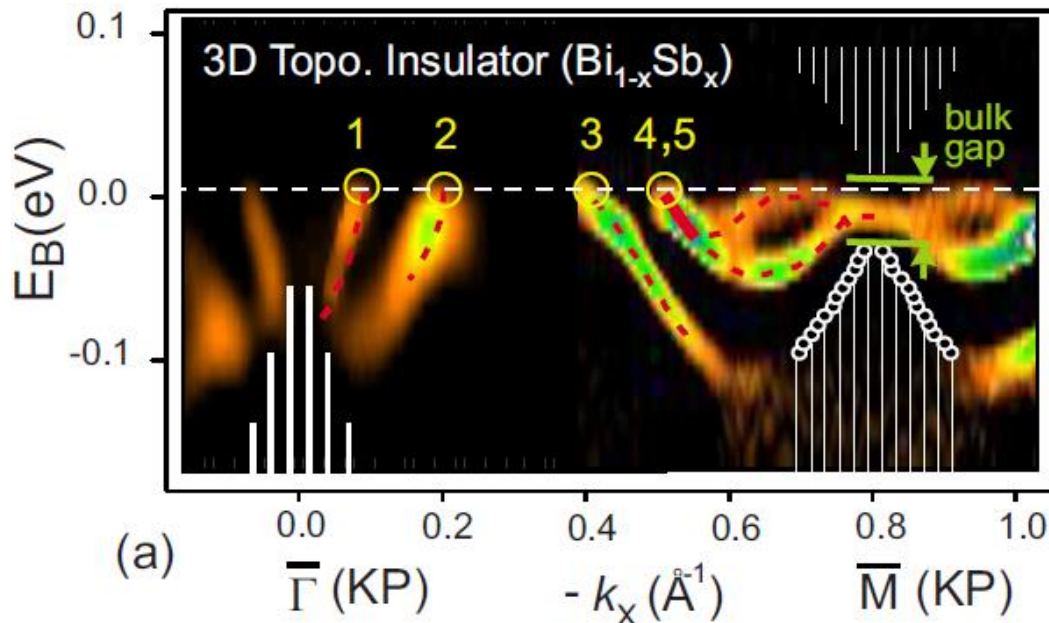
Sb doping concentration $\rightarrow$



Bi: Class (0;000)							Sb: Class (1;111)						
Λ_a	Symmetry label					δ_a	Λ_a	Symmetry label					δ_a
1Γ	Γ_6^+	Γ_6^-	Γ_6^+	Γ_6^+	Γ_{45}^+	-1	1Γ	Γ_6^+	Γ_6^-	Γ_6^+	Γ_6^+	Γ_{45}^+	-1
$3L$	L_s	L_a	L_s	L_a	L_a	-1	$3L$	L_s	L_a	L_s	L_a	L_s	+1
$3X$	X_a	X_s	X_s	X_a	X_a	-1	$3X$	X_a	X_s	X_s	X_a	X_a	-1
$1T$	T_6^-	T_6^+	T_6^-	T_6^+	T_{45}^-	-1	$1T$	T_6^-	T_6^+	T_6^-	T_6^+	T_{45}^-	-1

D. Hsieh et al., Nature **452**, 970 (2008)

Topological insulator ($\text{Bi}_{1-x}\text{Sb}_x$)

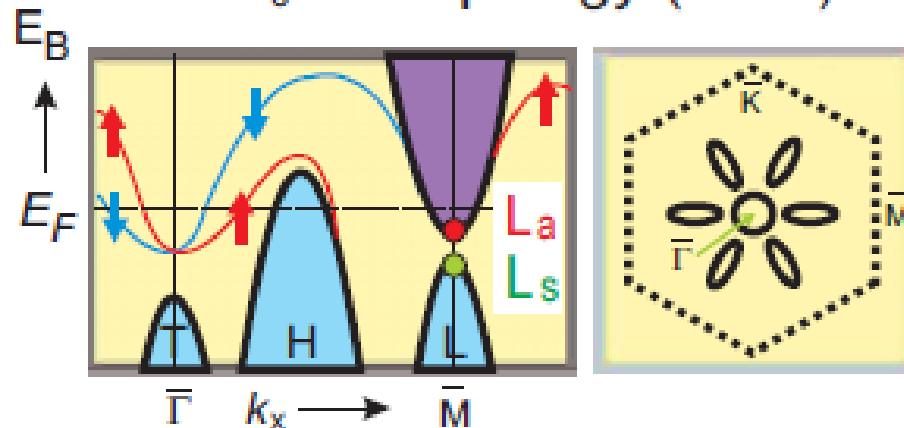


D. Hsieh et al., Nature **452**, 970 (2008)

D. Hsieh et al., Science **323**, 919 (2009)

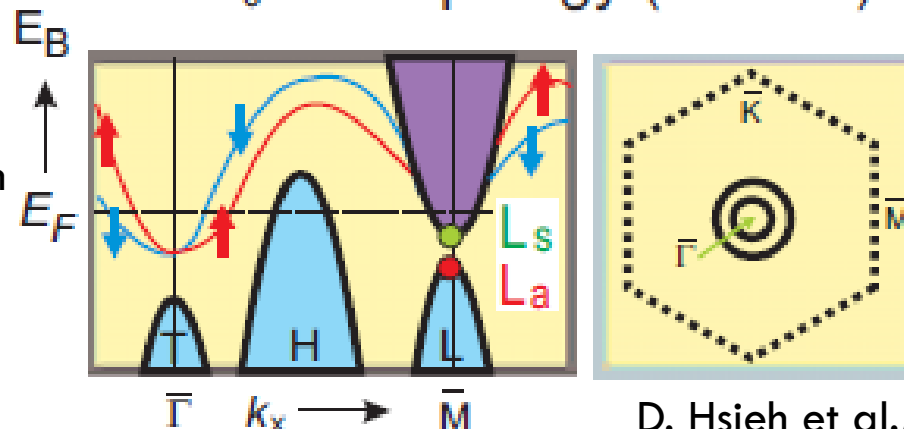
Topological insulator ($\text{Bi}_{1-x}\text{Sb}_x$)

A $\nu_0 = 1$ topology (BiSb)



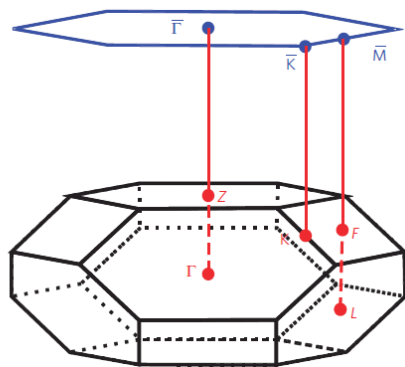
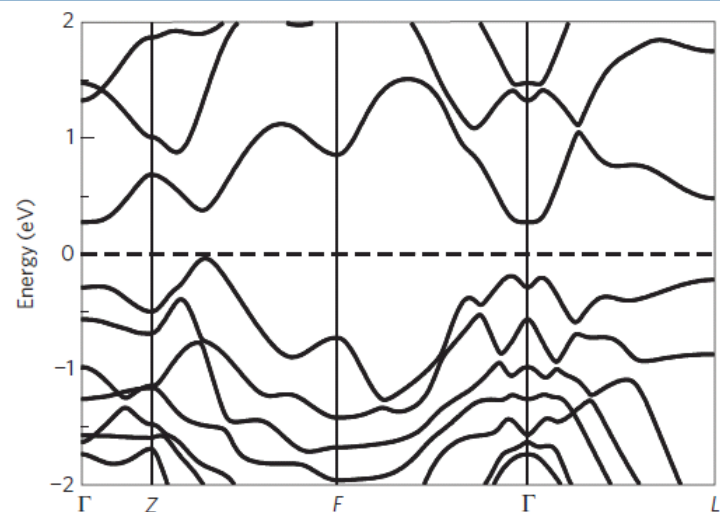
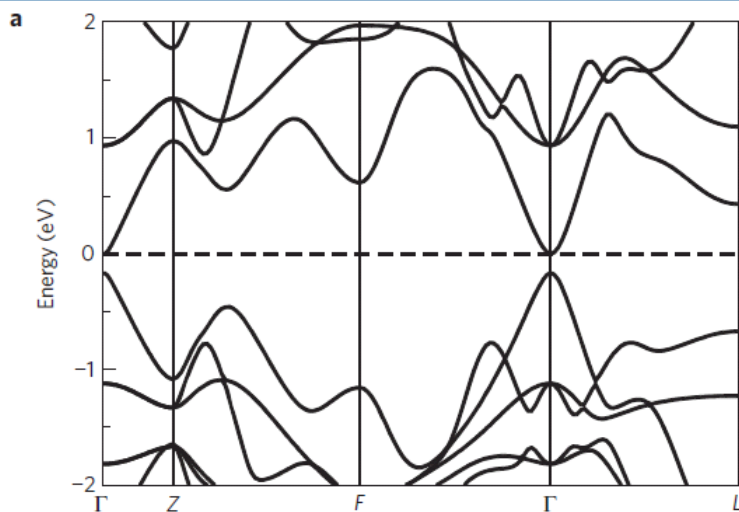
Odd number of FS

B $\nu_0 = 0$ topology (Au-like)

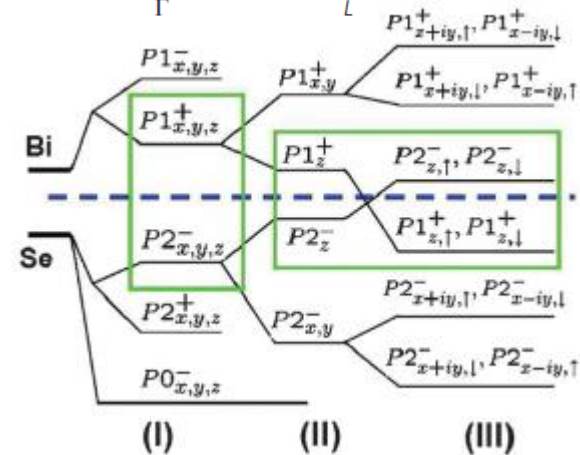


Even number of FS

Topological insulator (Bi_2Se_3)



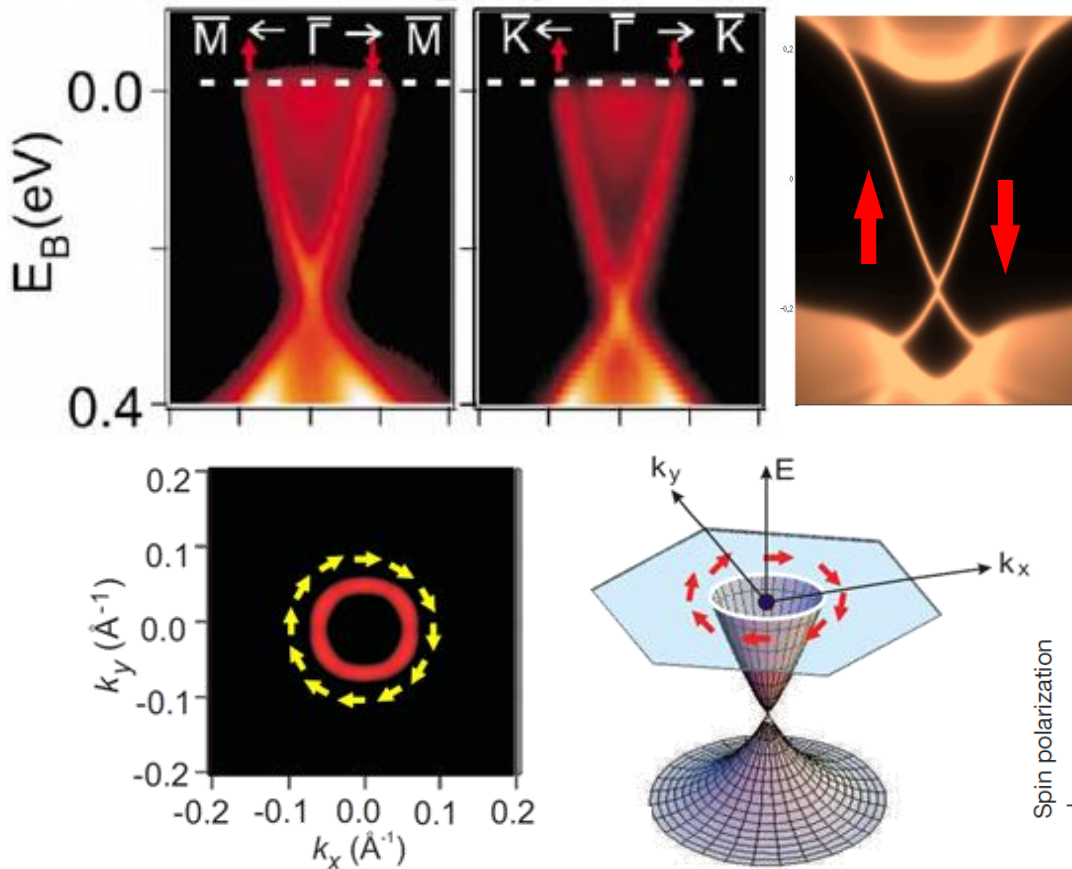
Sb_2Se_3	+ - + - + - + - + - + - - - ; +	(+)
Sb_2Te_3	+ - + - + + - + - + - - - + ; -	(-)
Bi_2Se_3	+ - + - + - + - + - + - - + ; -	(-)
Bi_2Te_3	+ - + - + - + + - + - - - + ; -	(-)

H. Zhang et al. Nat. Phys. **5**, 438 (2009)

Topological insulator (Bi_2Se_3)

ARPES

Theory

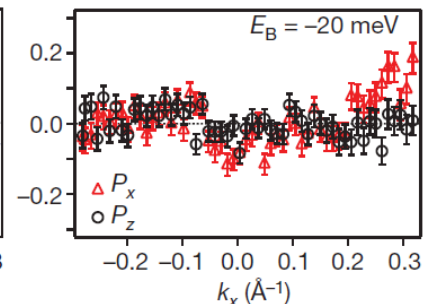
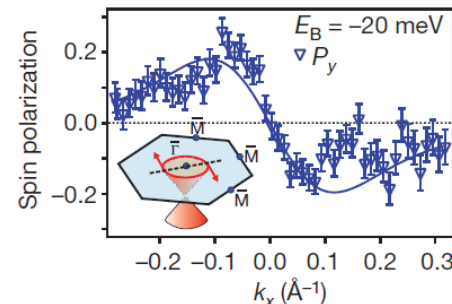


Bulk: insulating gap
topological Z_2 invariant



**odd/even number
surface states**

Surface: gapless surface states
spin-momentum locked

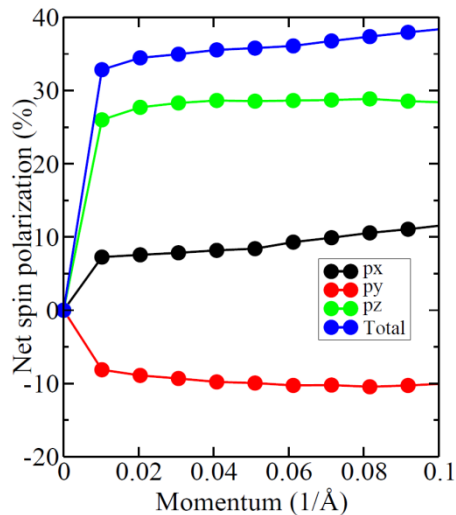
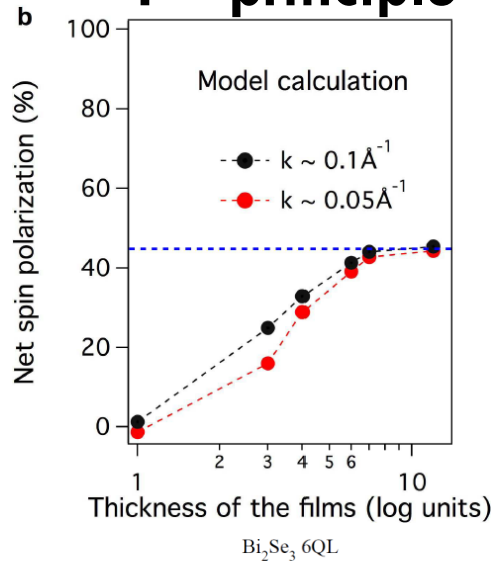


Y. Xia et al. Nature Physics **5**, 398 (2009)

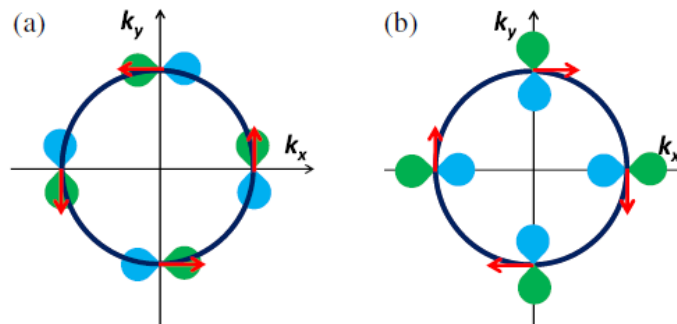
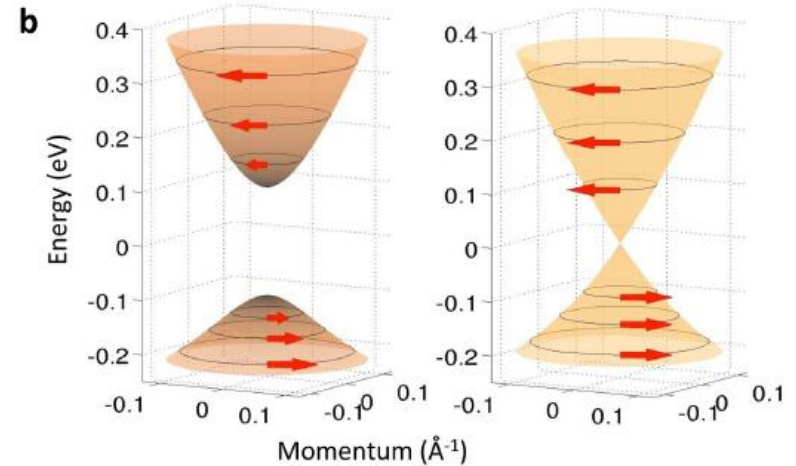
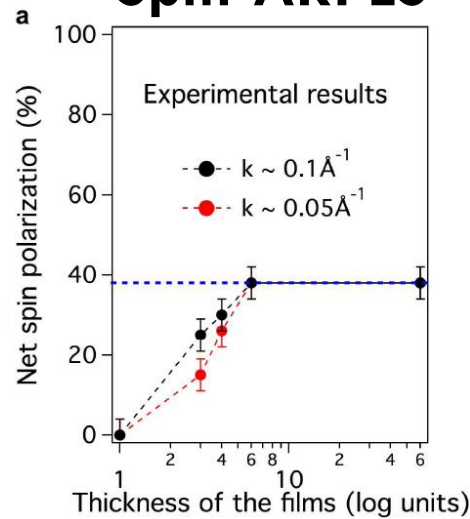
D. Hsieh et al. Nature **460**, 1101 (2009)

Topological insulator (Bi_2Se_3)

1st -principle

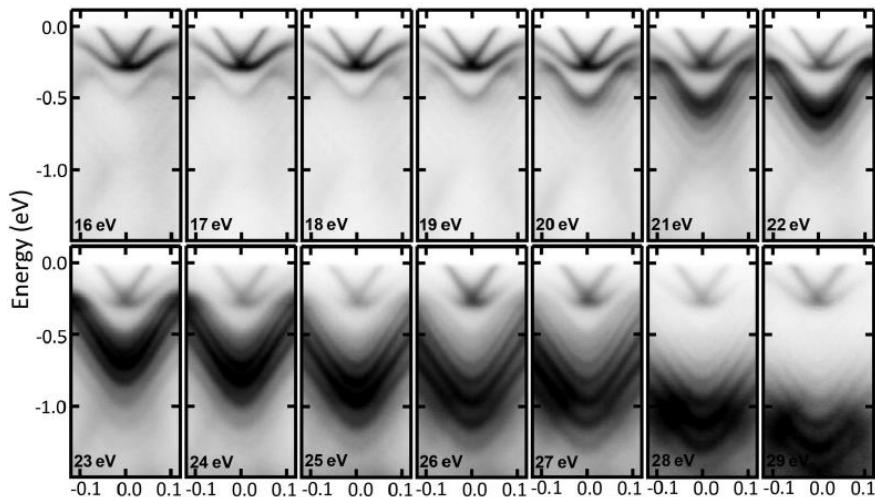
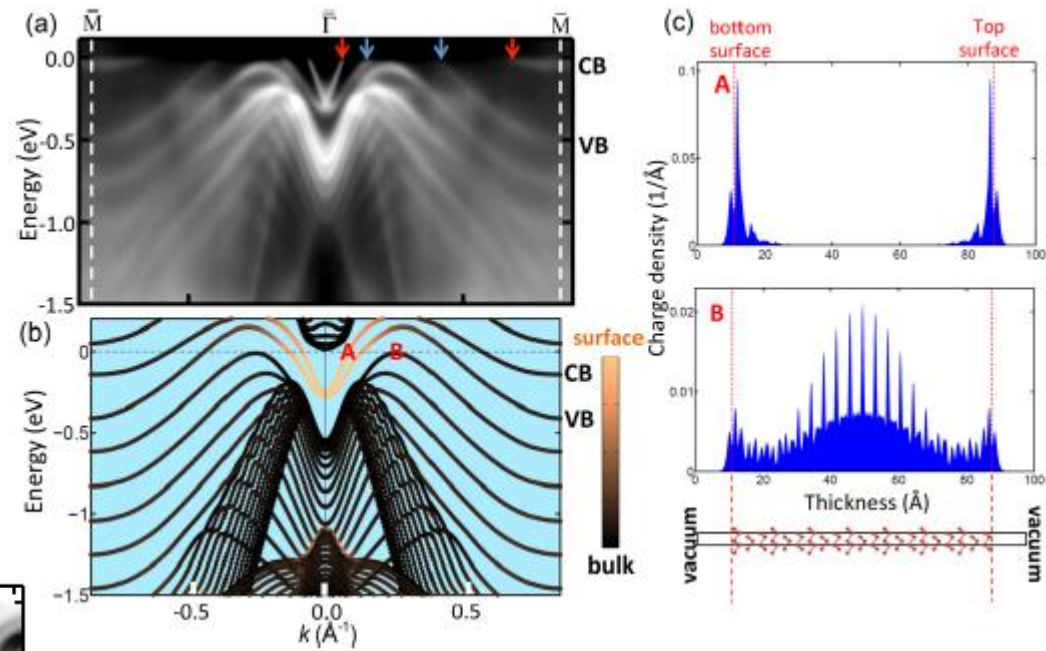
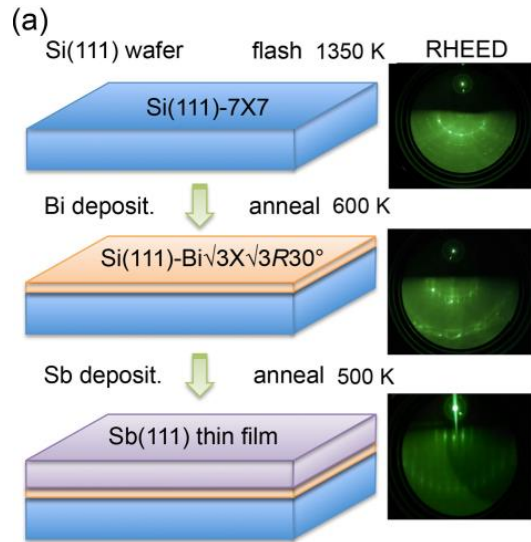


Spin-ARPES



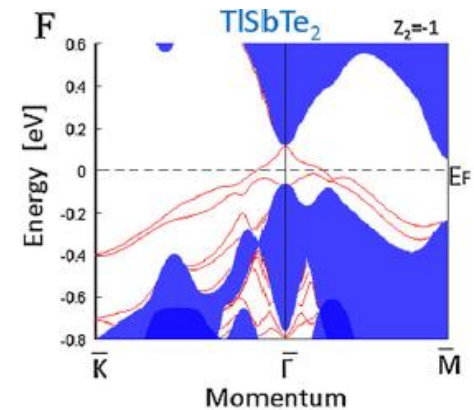
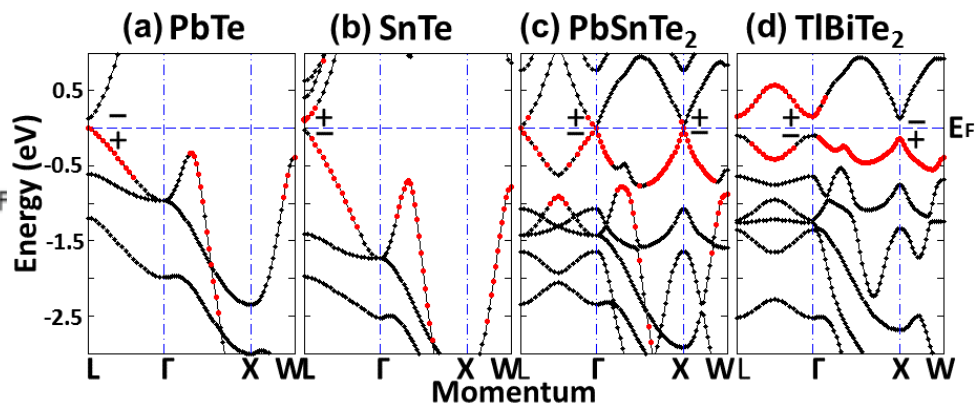
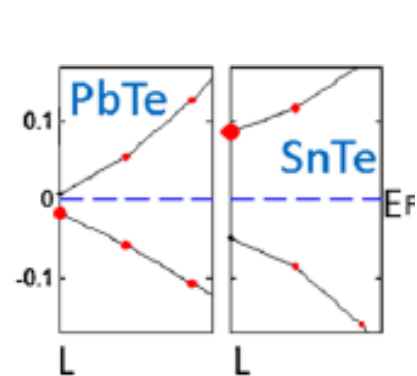
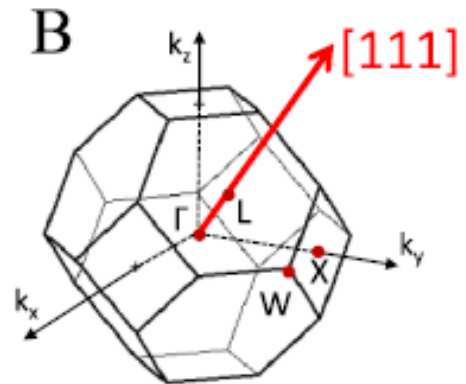
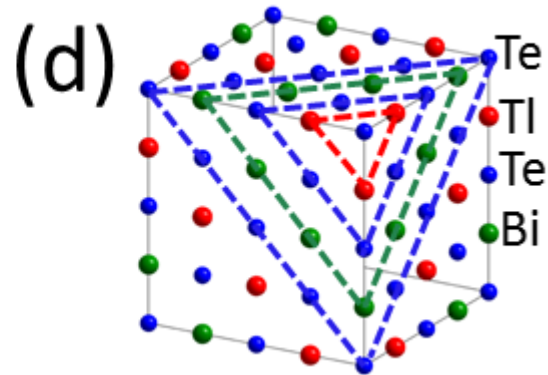
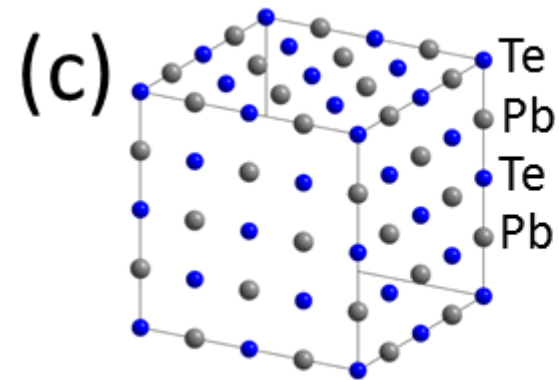
M. Neupane... T.-R. Chang et al., Nat. comm. **5**, 3841 (2014)

Topological insulator



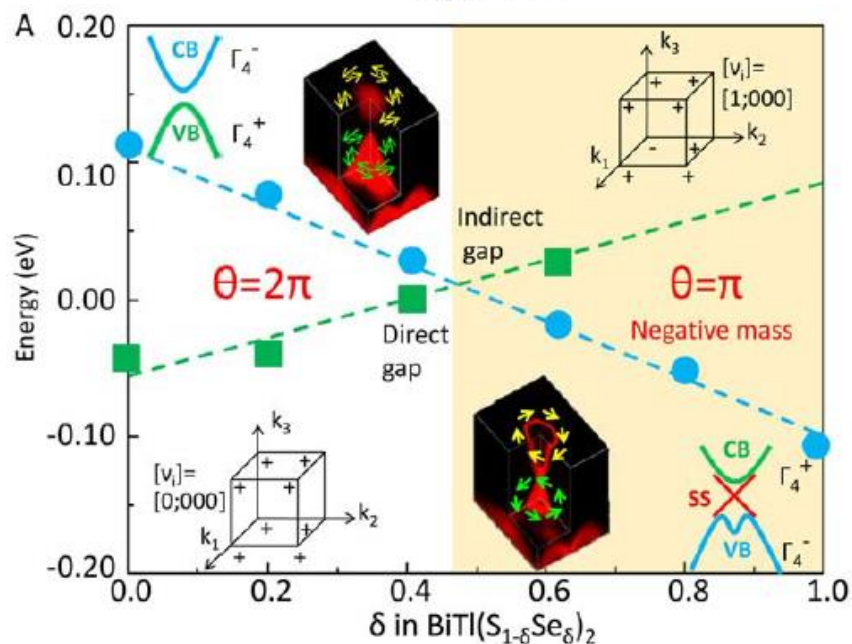
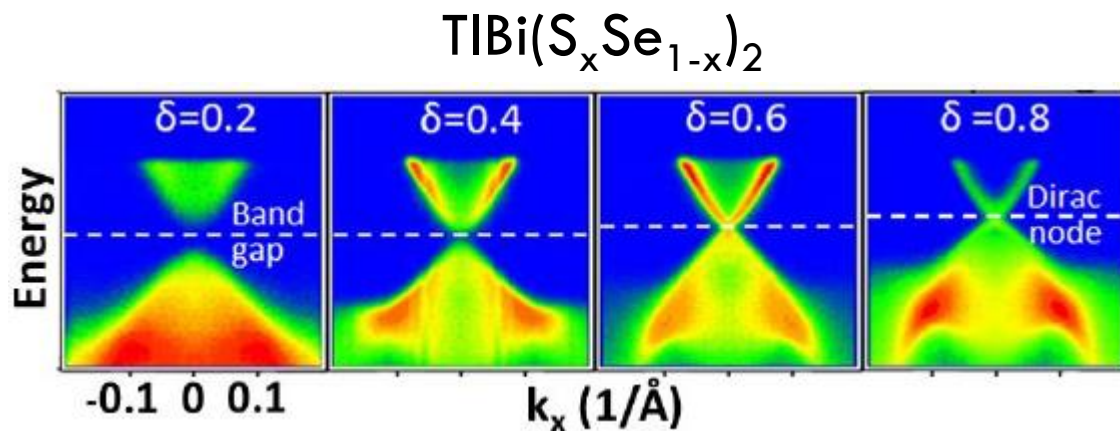
G. Bian, G. Xu, T.-R. Chang et al PRB **92**, 241401 (R) (2015)

Topological phase transition



H. Lin et al., PRL **105**, 036404 (2010)

Topological phase transition



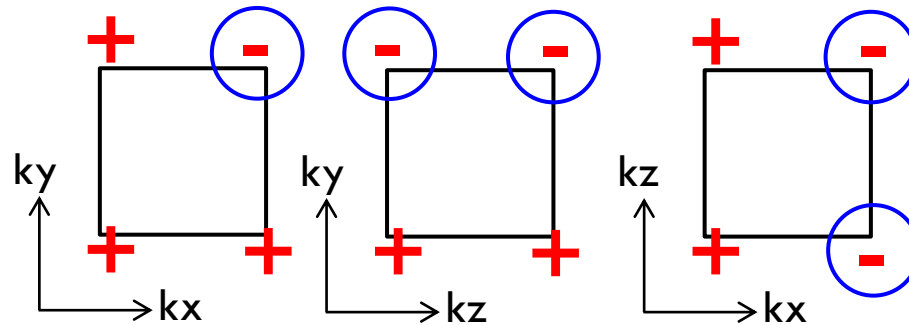
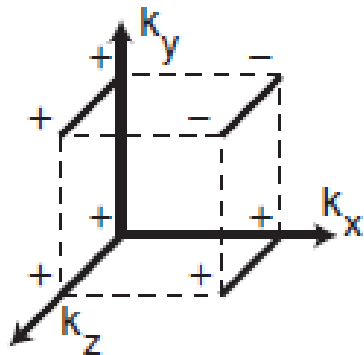
Su-Yang Xu et al.,
Science **332**, 560 (2011)

Weak topological insulator

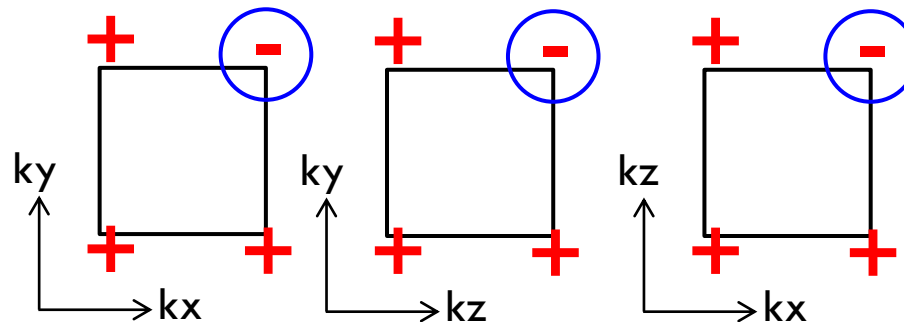
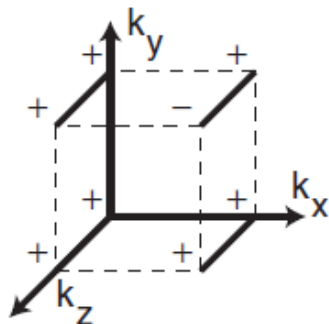
$$3D: (v_0; \underbrace{v_1, v_2, v_3}_{\text{weak index}})$$

$\uparrow$
 strong index

Weak topological insulator $Z_2 = (0; 0, 0, 1)$

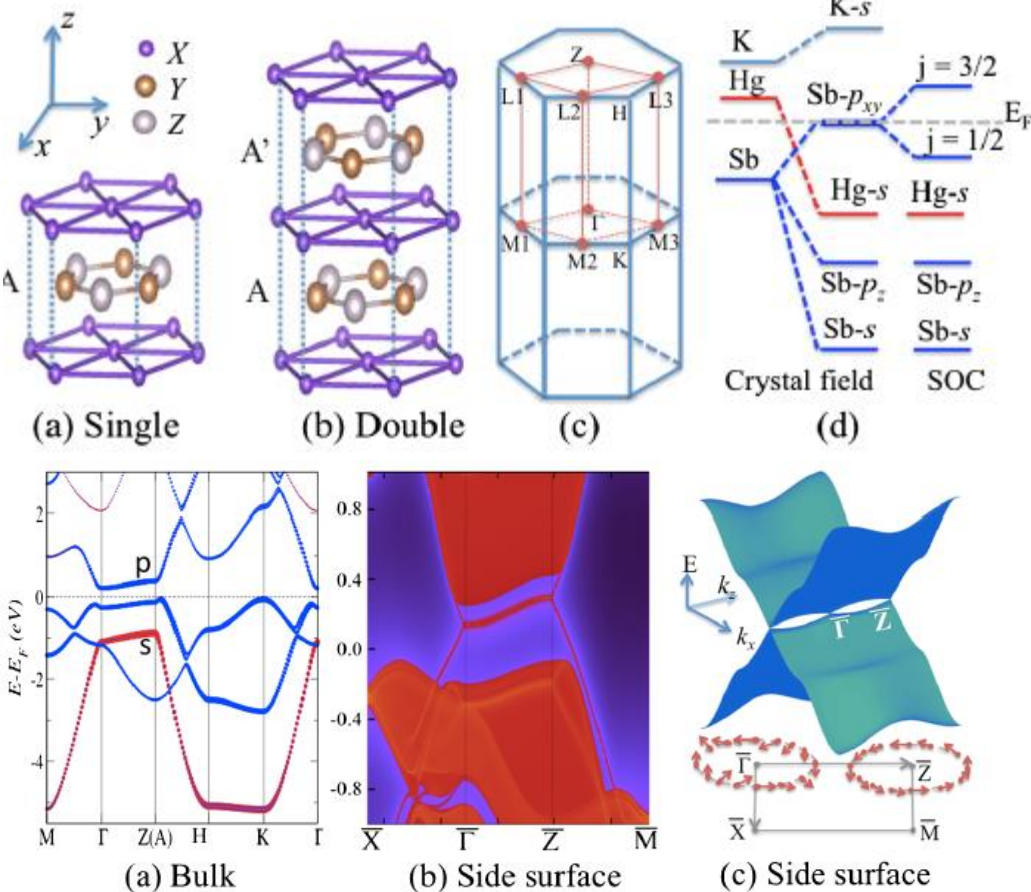


Strong topological insulator $Z_2 = (1; 1, 1, 1)$



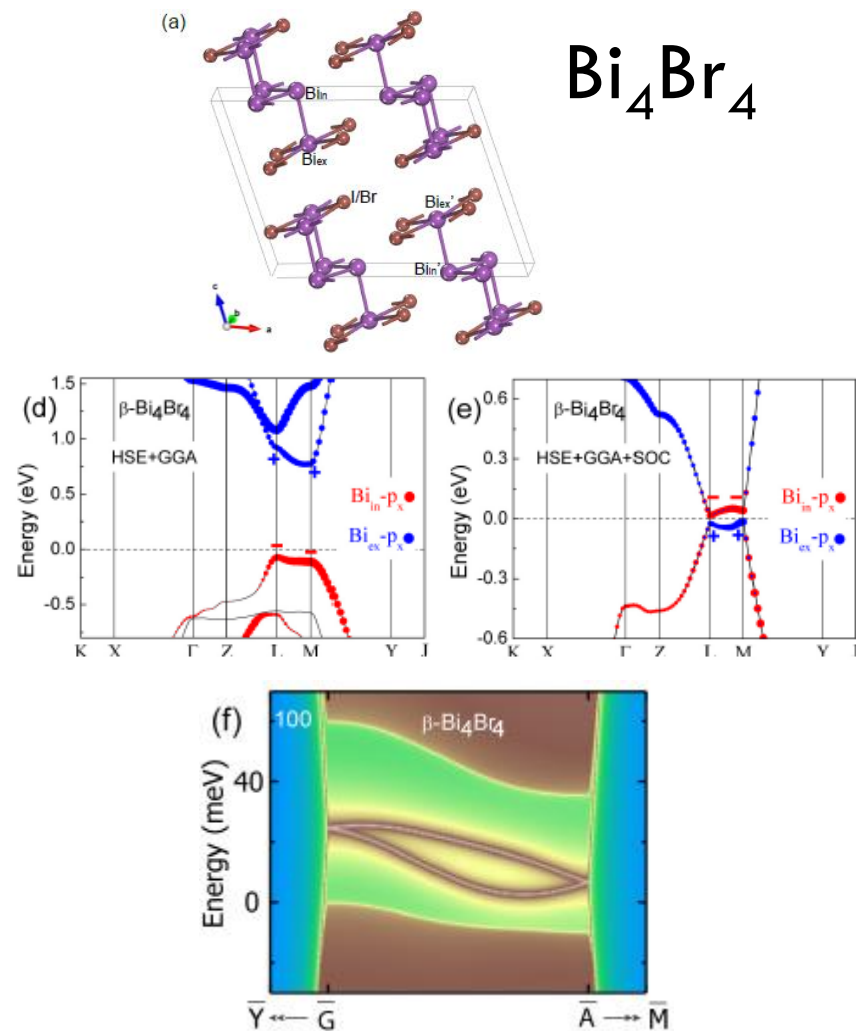
Weak topological insulator

KHgSb



B. Yan, PRL **109**, 116406 (2012)

Bi₄Br₄

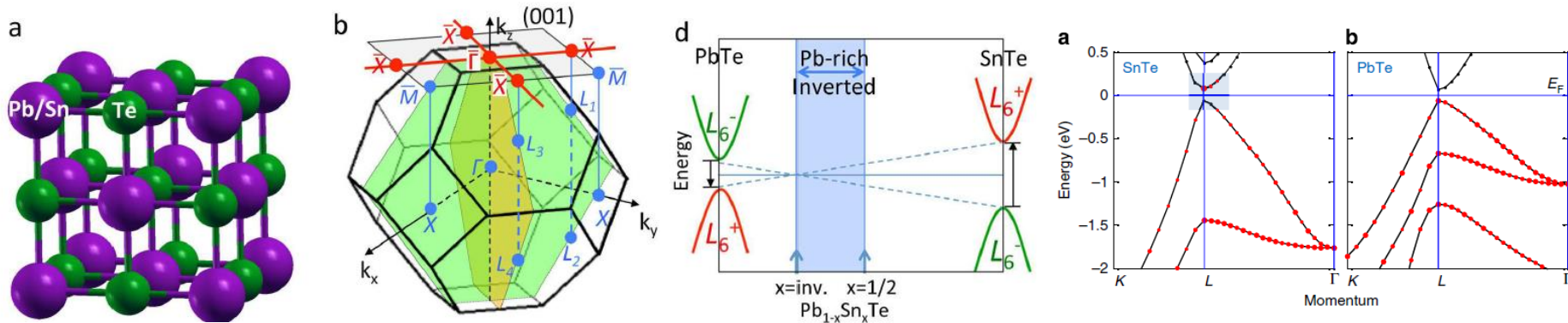


C.-C. Liu et al., PRL **116**, 066801 (2016)

Topological crystalline insulator

SnTe and PbTe

T. YH. Hsieh, Nat. comm **3**, 982 (2012)



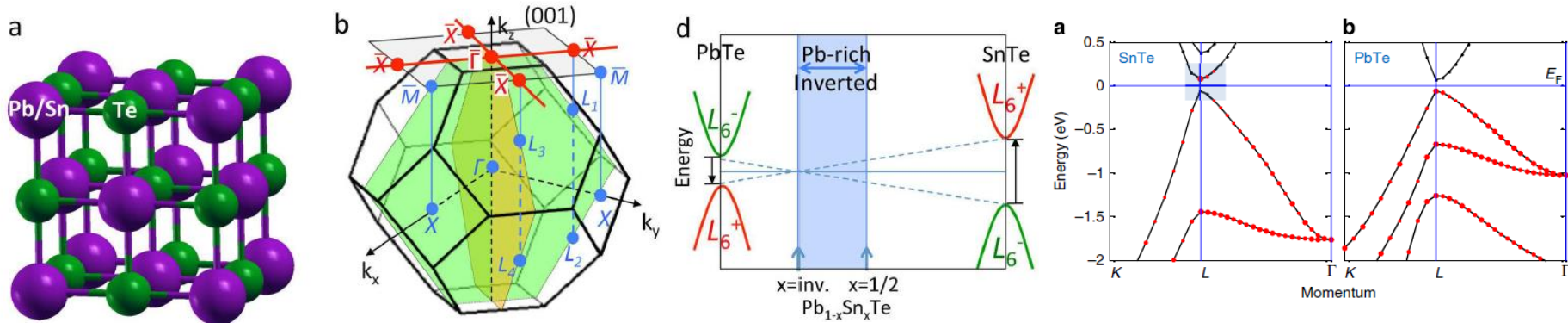
$$Z_2 = (0; 0,0,0)$$

Is SnTe (PbTe) a normal band insulator ?

Topological crystalline insulator

SnTe and PbTe

T. YH. Hsieh, Nat. comm **3**, 982 (2012)



$Z_2 = (0; 0,0,0)$ Is SnTe (PbTe) a normal band insulator ?

Bloch wavefunctions on the mirror plane $\Rightarrow$ mirror eigenvalue $M = \pm i$

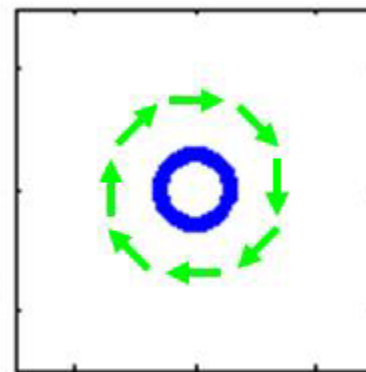
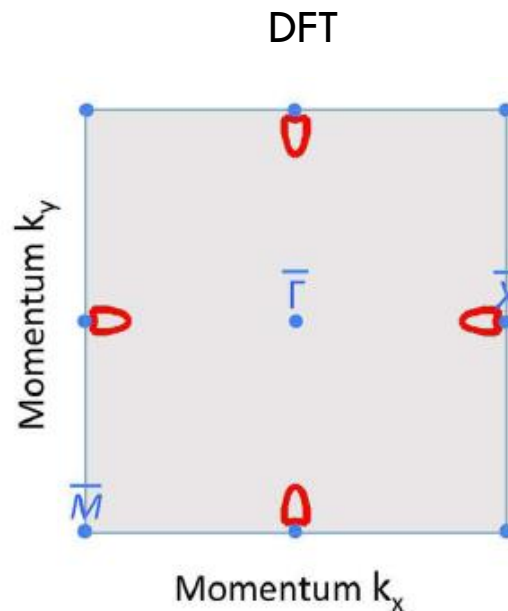
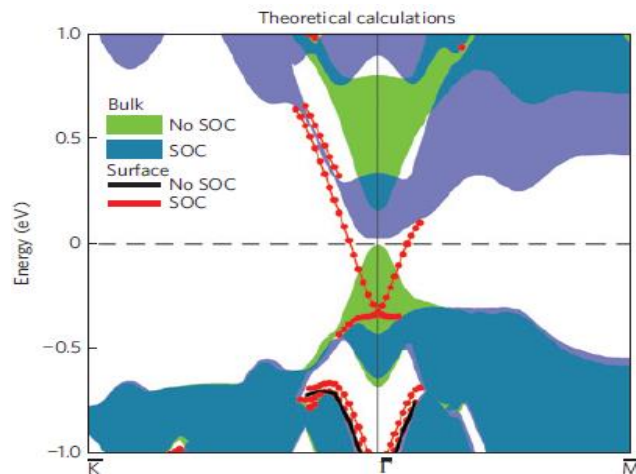
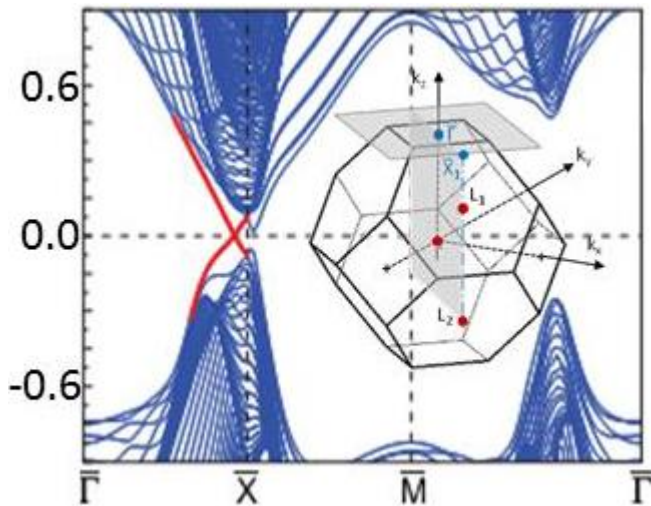
$M = \pm i \Rightarrow$ Chern number $n_{\pm i}$

Mirror Chern number $n_M = (n_{+i} - n_{-i})/2$

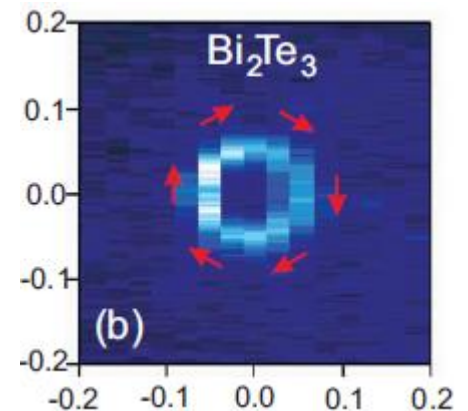
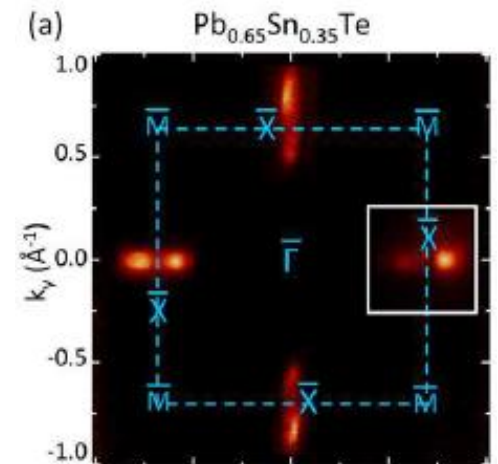
A non-zero mirror Chern number defines a topological crystalline insulator with mirror symmetry.

Topological crystalline insulator

S. Y. Xu, Nat. comm **3**, 1192 (2012)



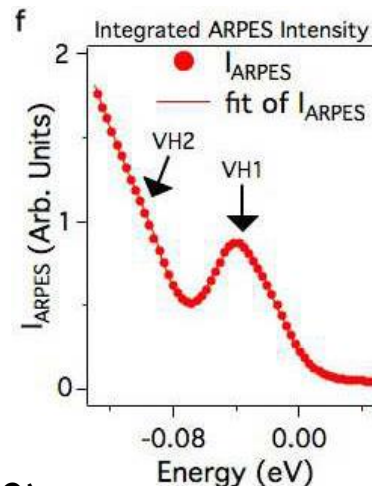
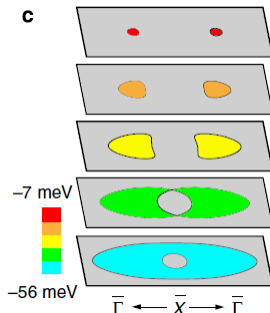
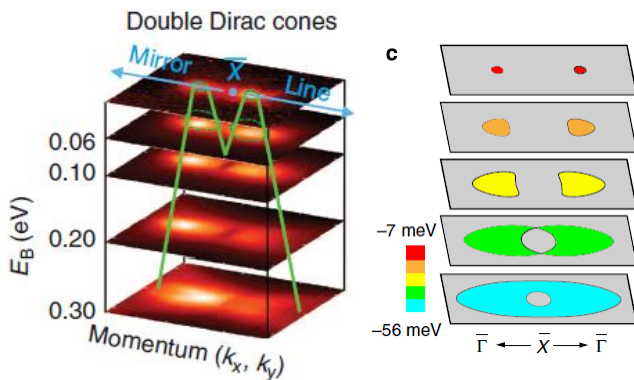
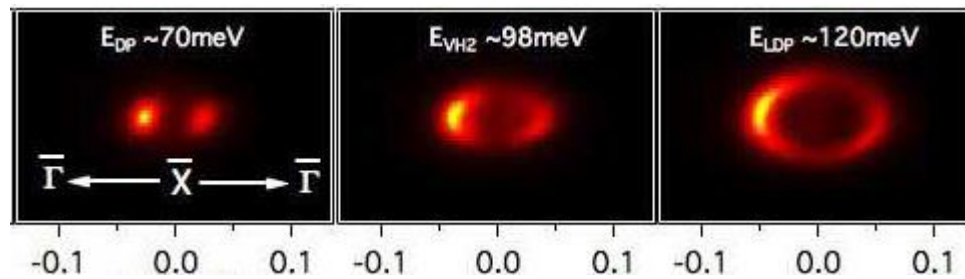
ARPES



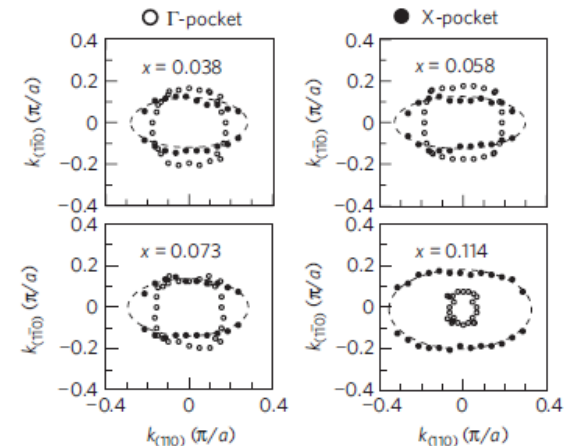
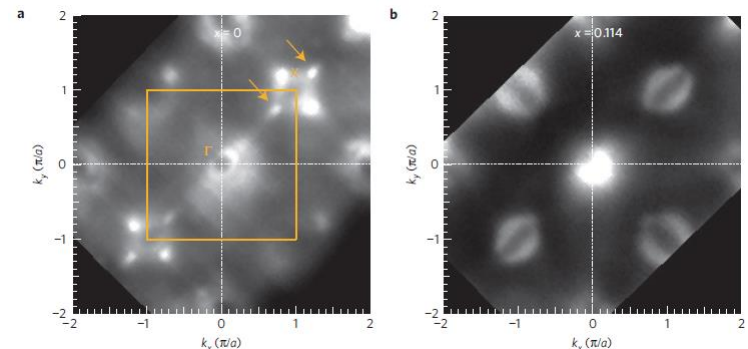
Lifshitz transition

What is Lifshitz transition ?

Lifshitz transition is a change of the topology of the Fermi surface.



Ba(Fe_{1-x}Co_x)₂As₂



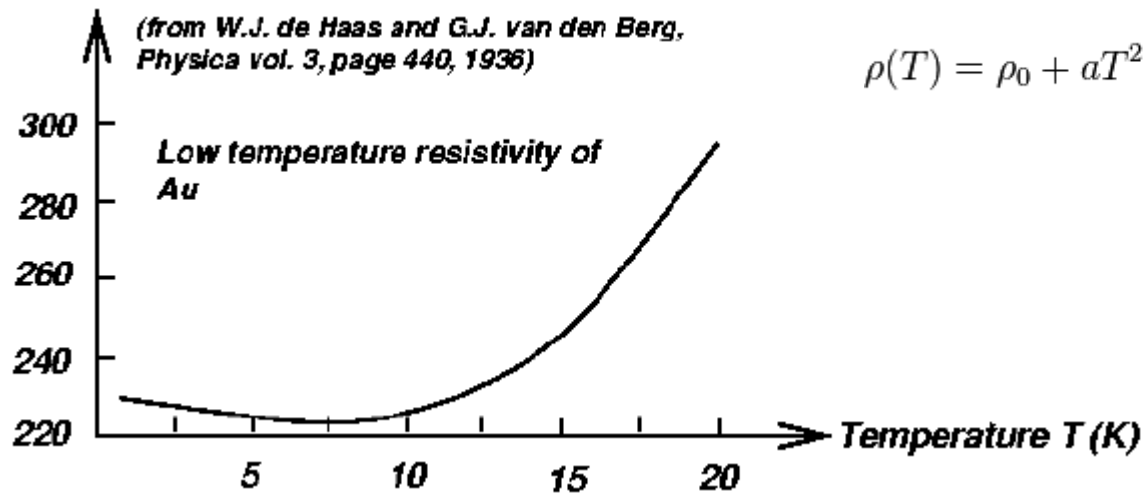
S. Y. Xu, Nat. comm **3**, 1192 (2012)

C. Liu, Nat. phys. **6**, 419 (2010)

Topological invariant number

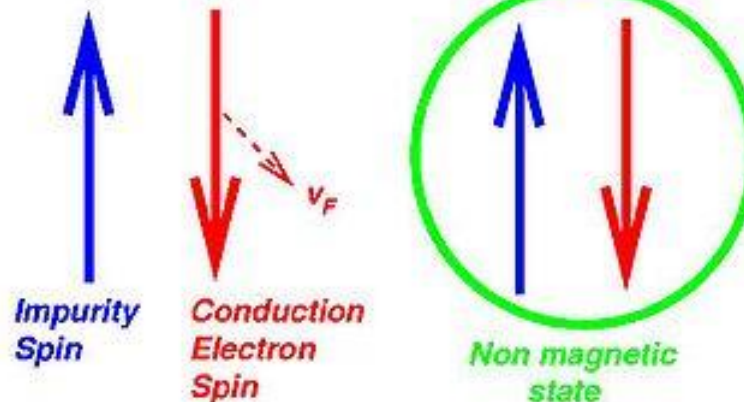
	Topological invariant	Gapless surface states
Topological insulator:	$Z_2 = (1; 0,0,0)$	odd
Weak topological insulator:	$Z_2 = (0; 0,0,1)$	odd (for two surface)
topological crystalline insulator:	$Z_2 = (0; 0,0,0) \quad n_M \neq 0$	even
Normal band insulator:	$Z_2 = (0; 0,0,0) \quad n_M = 0$	none

Topological Kondo insulator



$$\rho(T) = \rho_0 + aT^2 + c_m \ln \frac{\mu}{T} + bT^5,$$

High T – weak coupling Low T – strong coupling



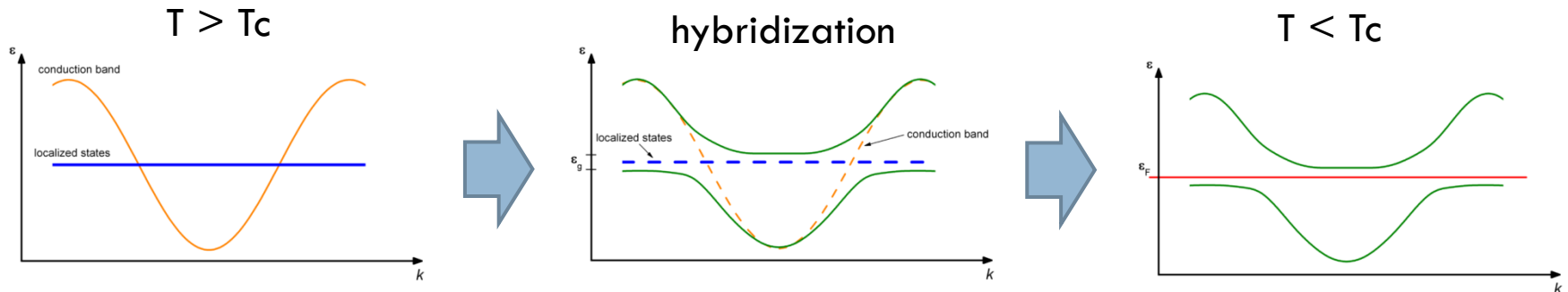
wiki: Kondo effect

Topological Kondo insulator

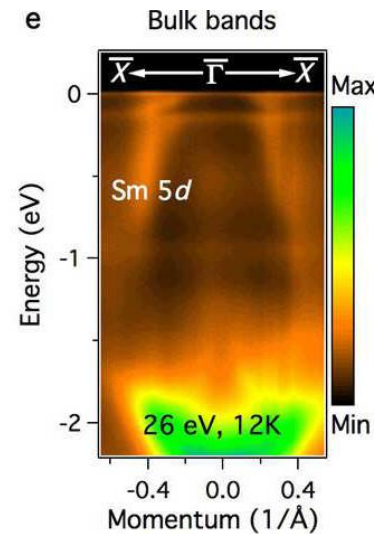
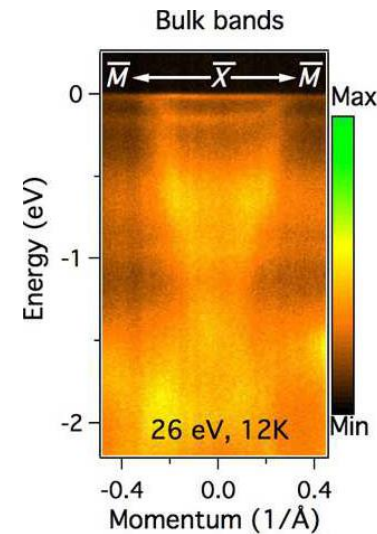
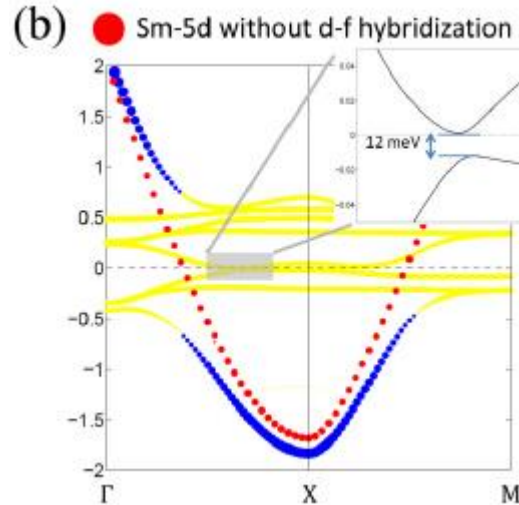
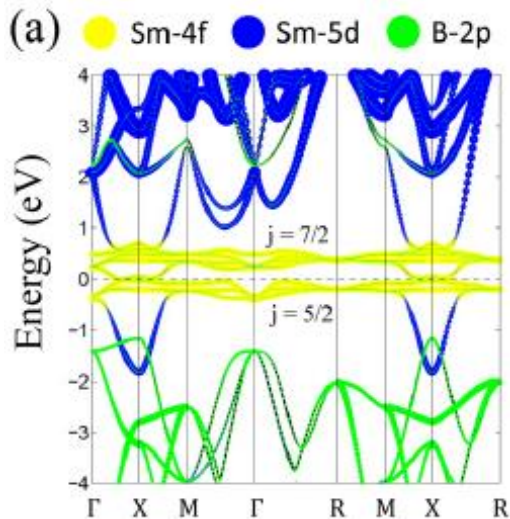
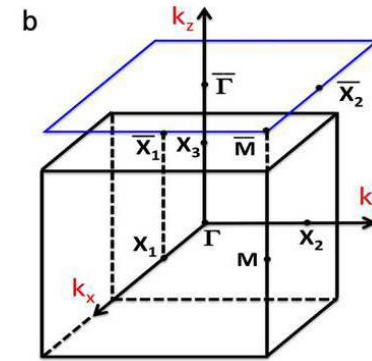
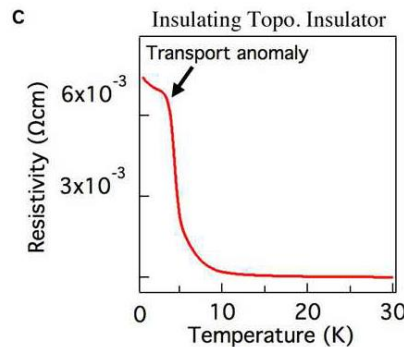
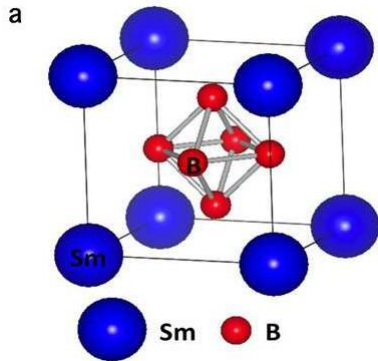
Kondo effect



Kondo insulator



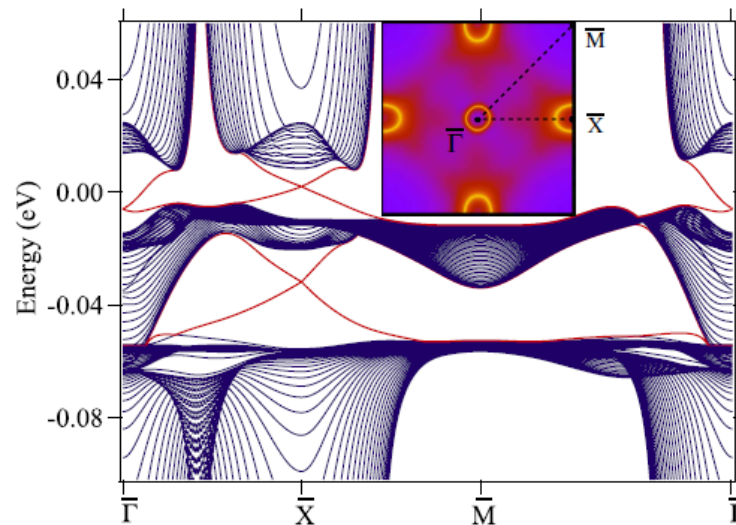
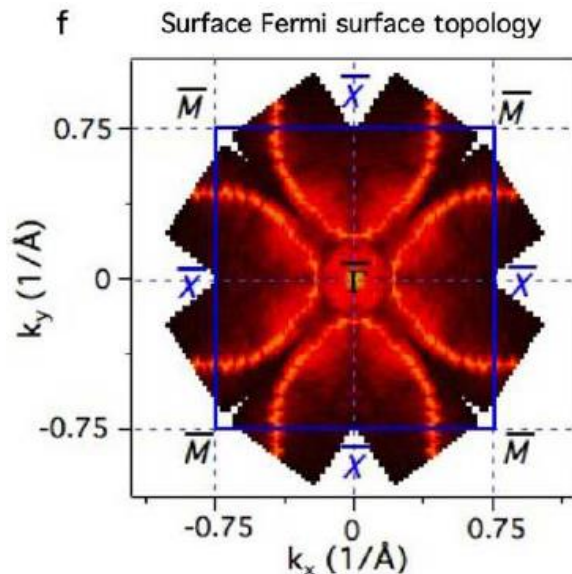
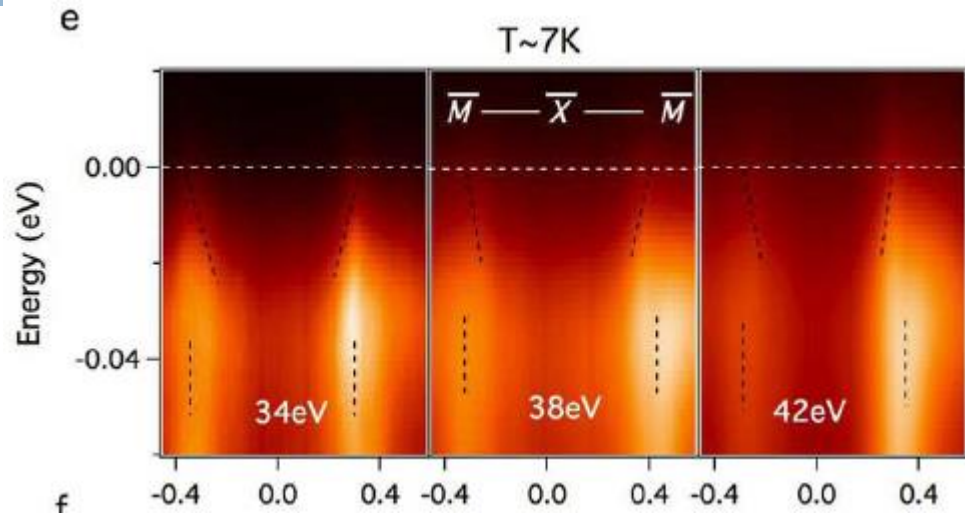
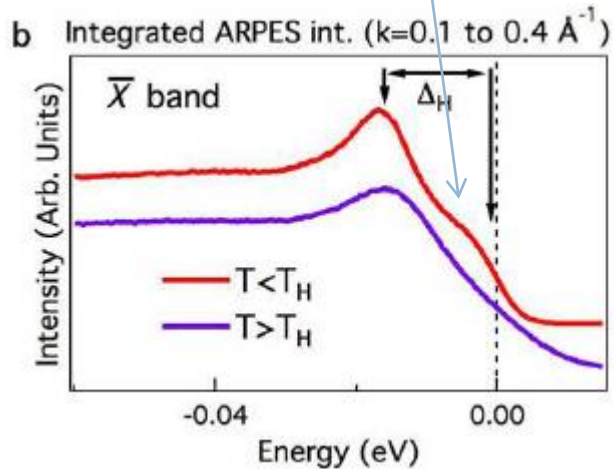
Topological Kondo insulator



M. Neupane... **T.-R. Chang** et al, Nat. comm. **4**, 2991 (2013)
T. R. Chang et al, PRB **91**, 155151 (2015)

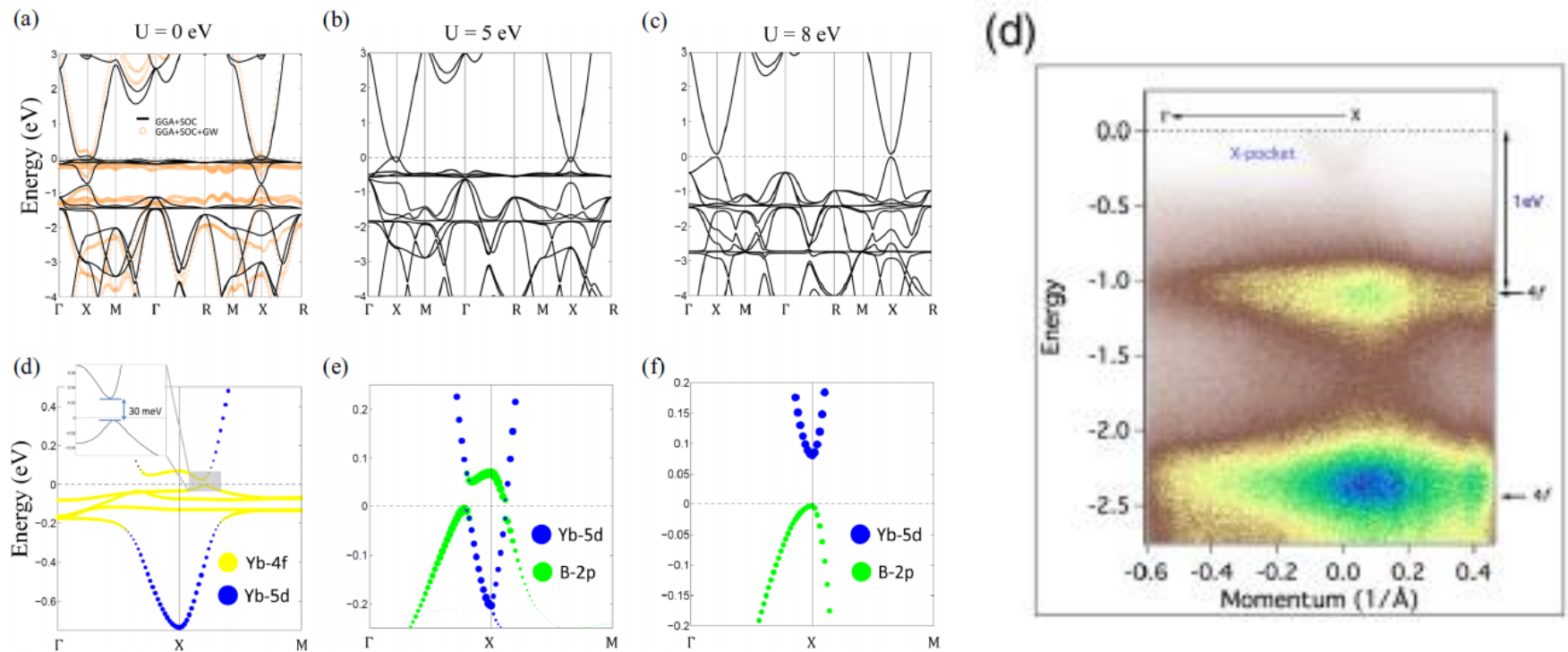
Topological Kondo insulator

in gap state



M. Neupane... **T.-R. Chang** et al,
Nat. comm. **4**, 2991 (2013)
L. Feng et al,
PRL **110**, 096401 (2013)

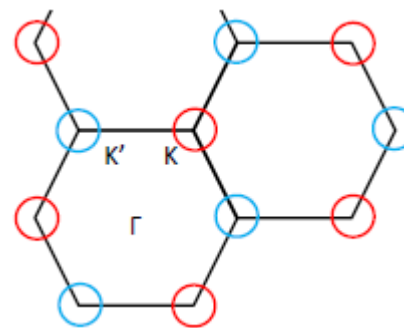
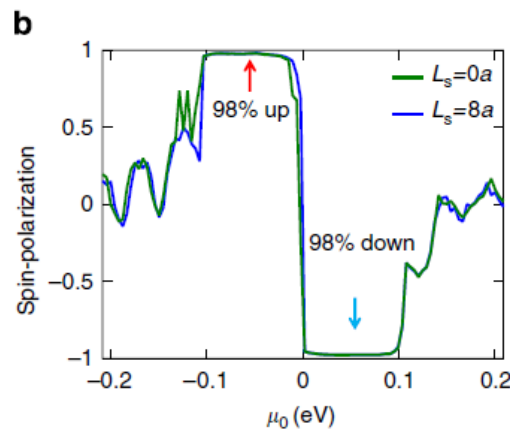
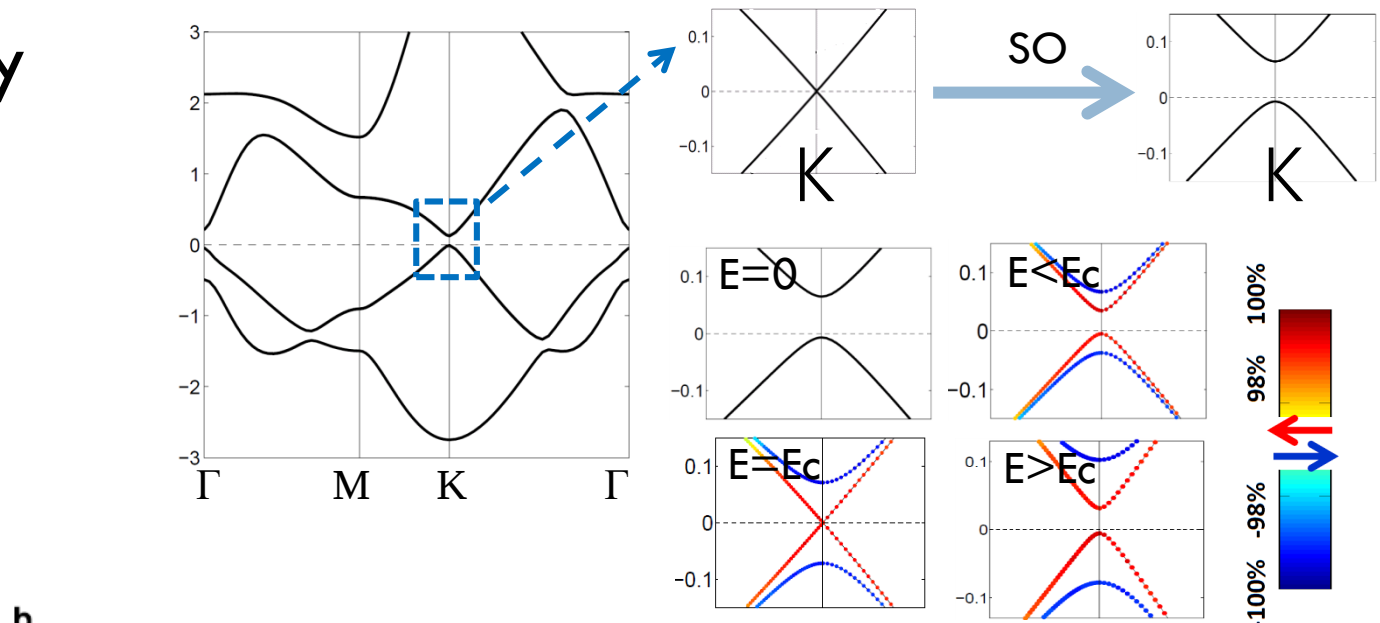
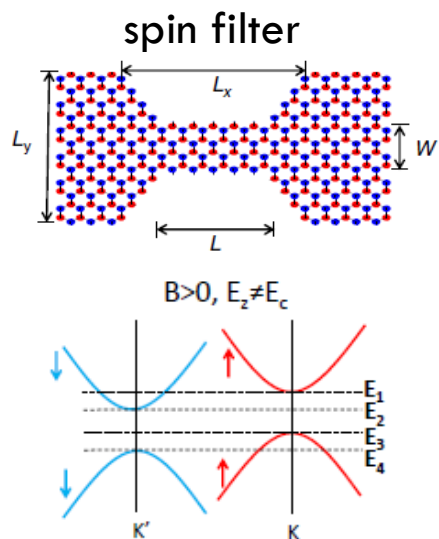
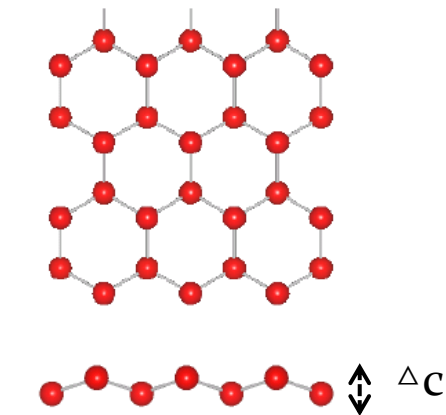
Topological Kondo insulator



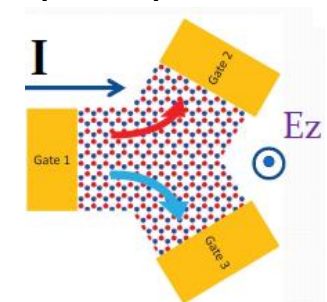
M. Neupane... **T.-R. Chang** et al, PRL **114**, 016403 (2015)
T. R. Chang et al, PRB **91**, 155151 (2015)

Possible applications

Silicene family

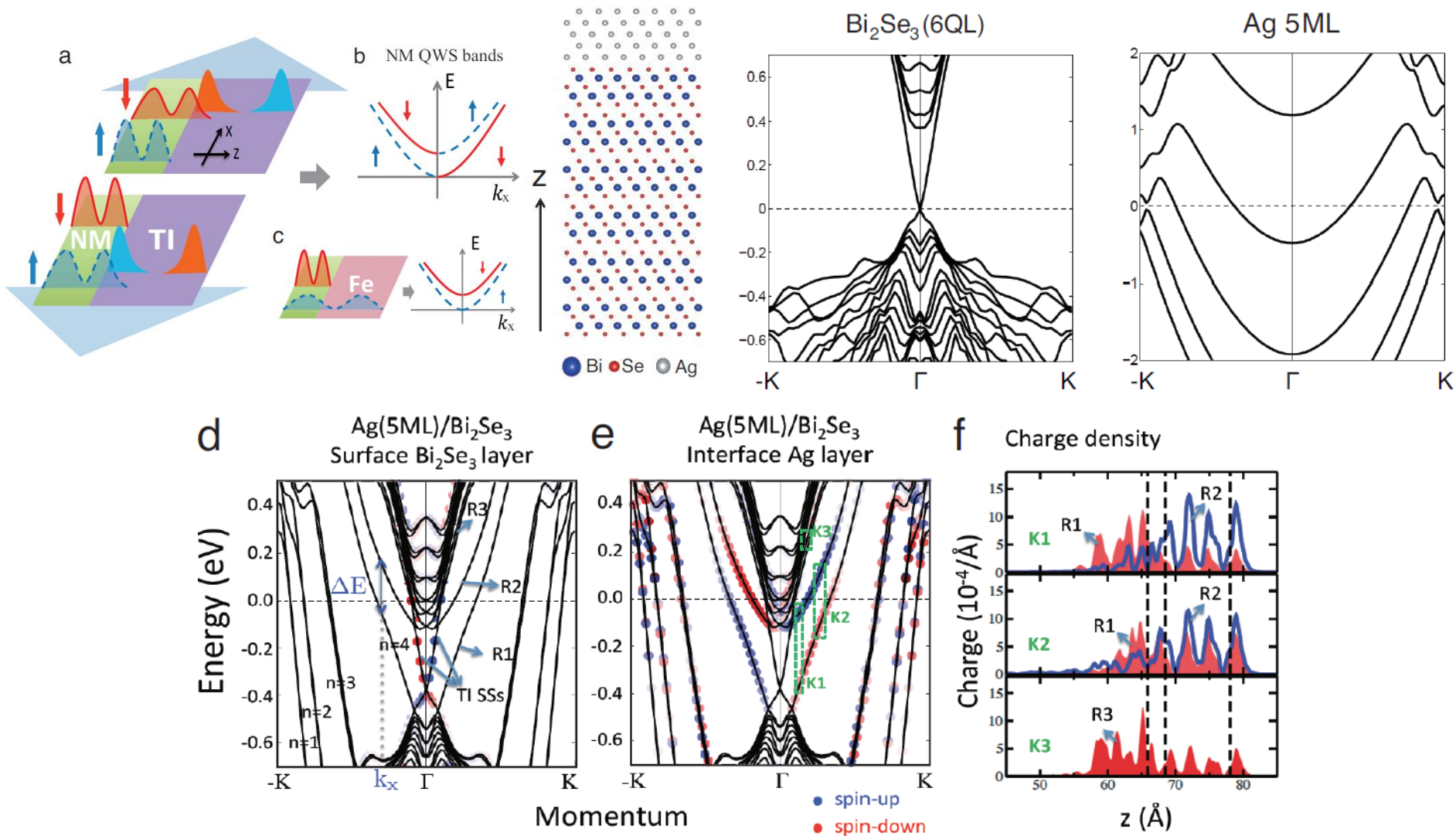


spin separator

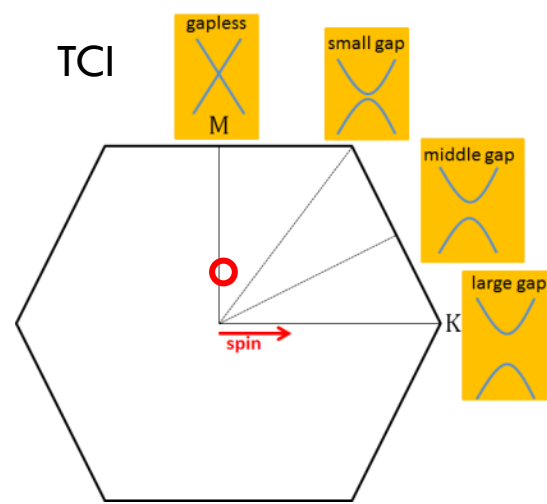
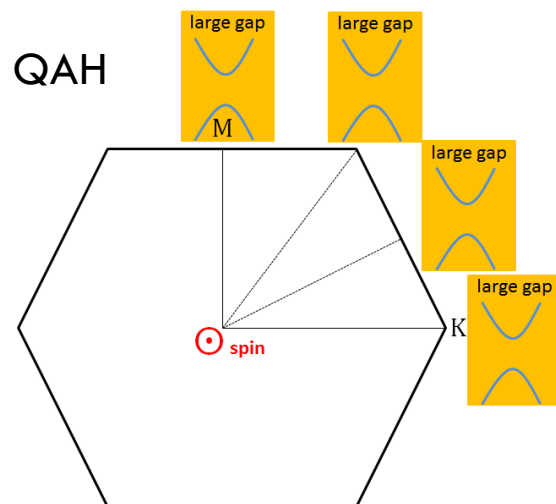
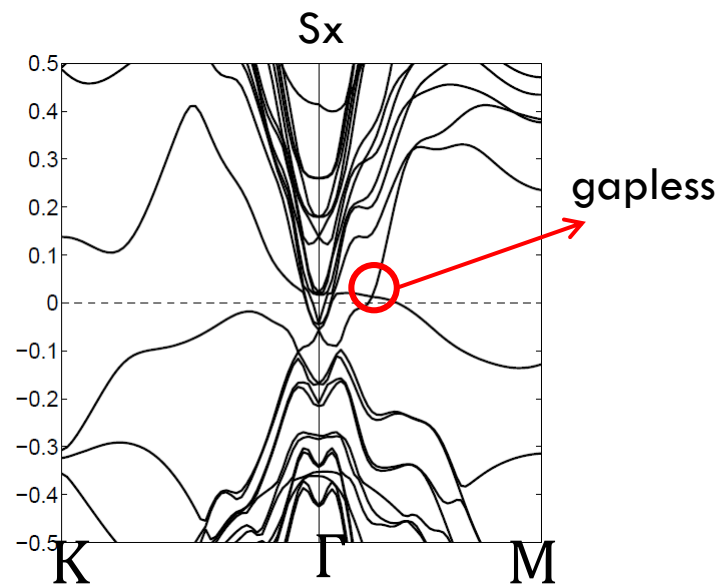
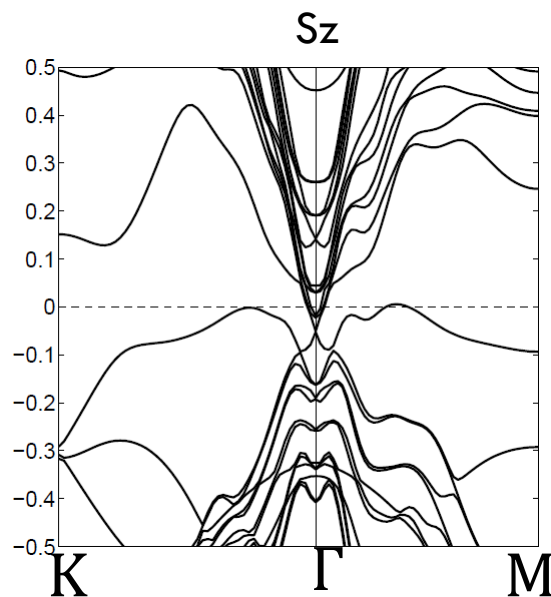
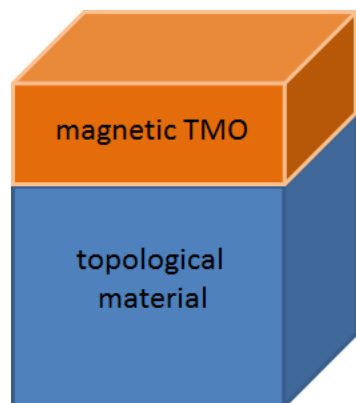


Tsai... T.-R. Chang et al. Nature Commun. 4, 1500 (2013)

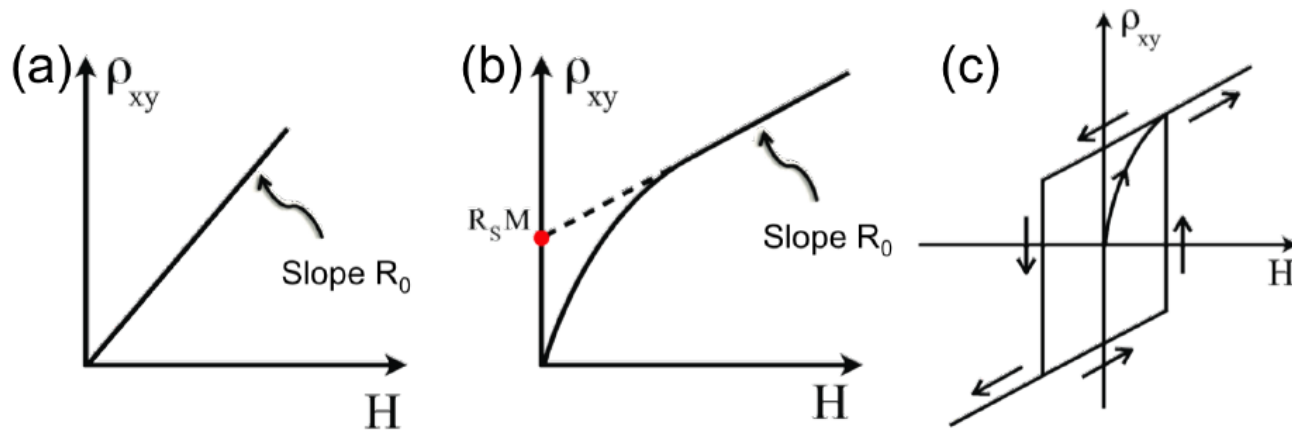
Possible applications



Possible applications



Anomalous Hall effect



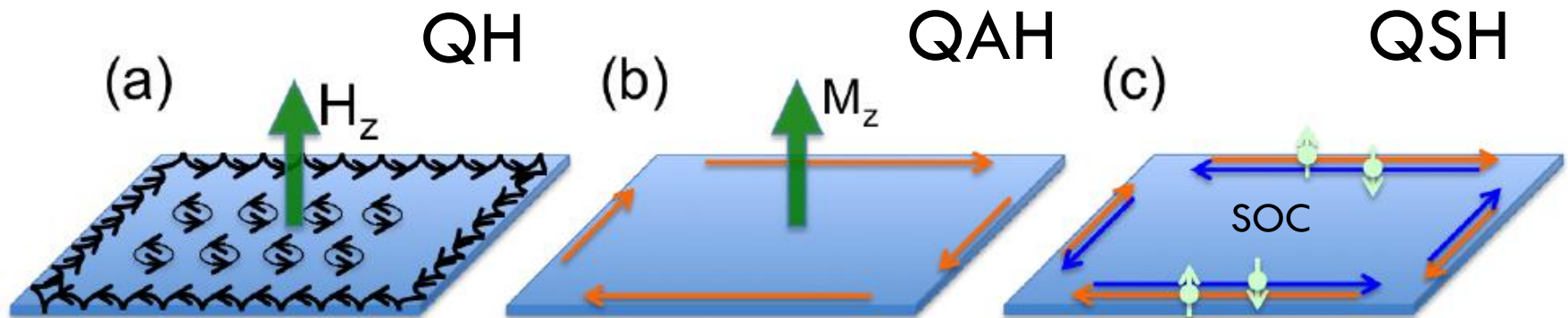
$$\rho_{xy} = R_0 H$$

$$\rho_{xy} = R_0 H + R_s M$$

$$\dot{\mathbf{r}} = \frac{1}{\hbar} \frac{\partial \epsilon_n(\mathbf{k})}{\partial \mathbf{k}} - \dot{\mathbf{k}} \times \boldsymbol{\Omega}_n(\mathbf{k}),$$

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

Quantum anomalous Hall effect



The quantum anomalous Hall effect is defined as a quantized Hall effect realized in a system without external magnetic field.

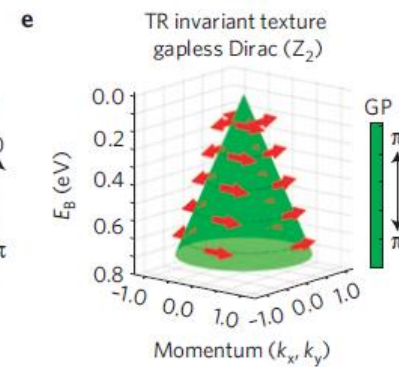
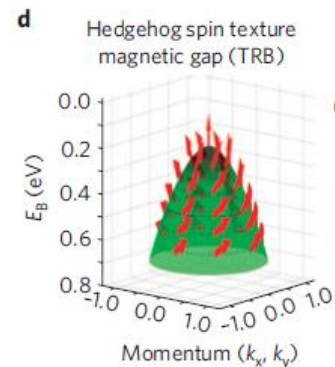
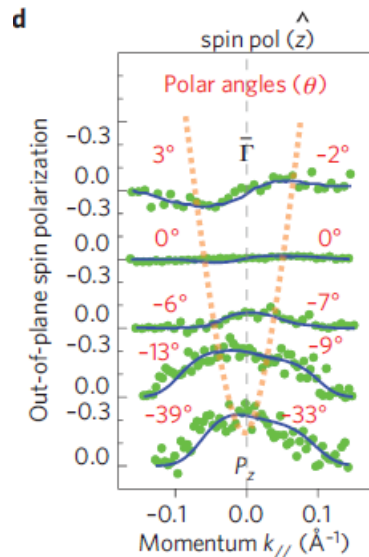
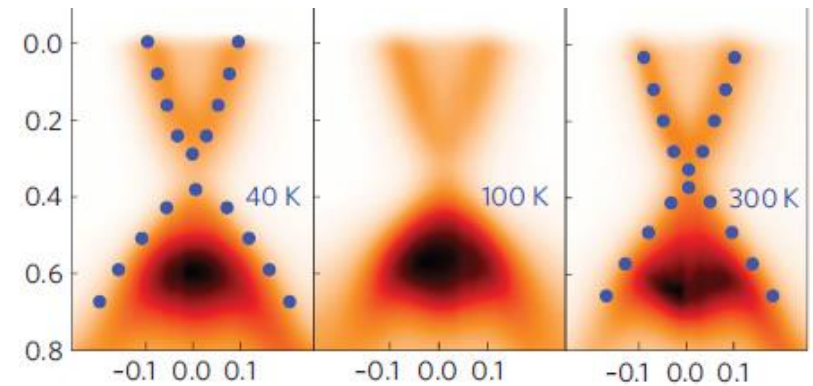
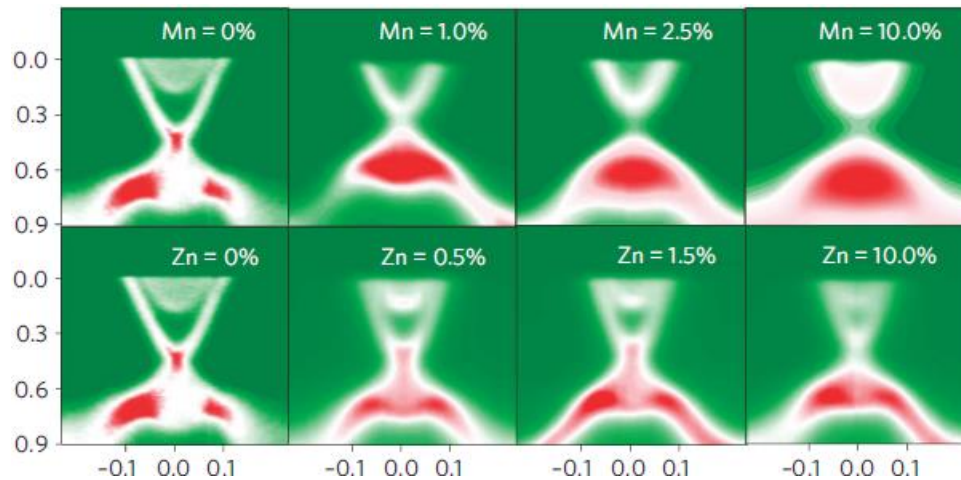
1. It must be two dimensional
2. It must be insulating in the bulk
3. It must break the TRS with a certain magnetic ordering
4. The occupied bands must carry a non-zero Chern number

Quantum anomalous Hall effect

2D topological insulator might be an answer

- To sandwich a TI thin film with FM insulators. The FM proximity effect will open up a gap for the Dirac surface states on both surfaces of the TI, which gives rise to the QAHE.
- To dope the magnetic ions into the TI thin film and make it a FM semiconductor. The QAHE can be obtained by proper control of the doping.
- To grow graphene, silicene, or other honeycomb lattice on top of magnetic insulators or with magnetic adsorbates. The low energy acquire both the Zeeman exchange-splitting and the SOC, which drive the system towards QAHE
- Other proposals, such as heavy metal on magnetic insulator substrate, strained epitaxial film with interface band inversion in EuO/GdN or CdO/EuO , etc.

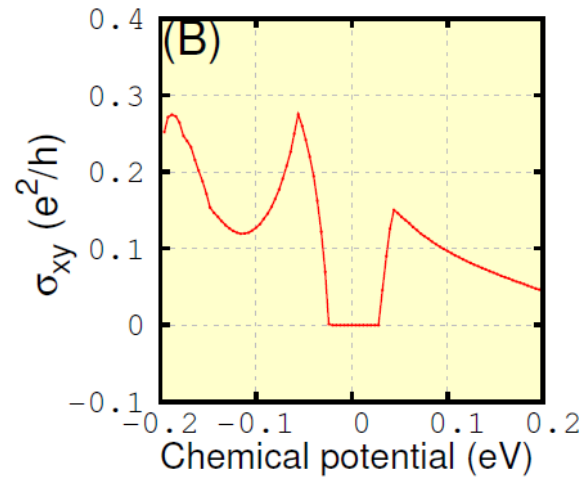
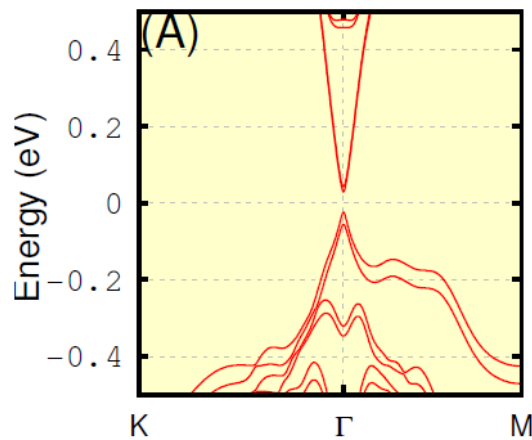
Quantum anomalous Hall effect



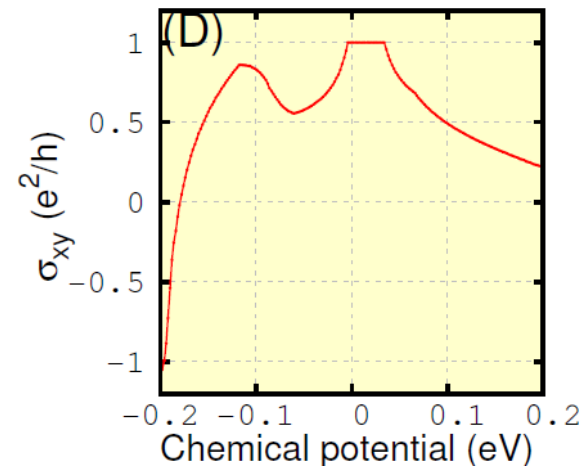
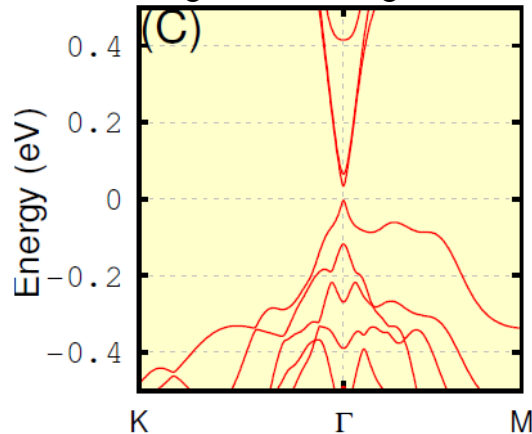
Su-Yang Xu... **T.-R. Chang** et al., Nature phys. **8**, 616 (2012)

Quantum anomalous Hall effect

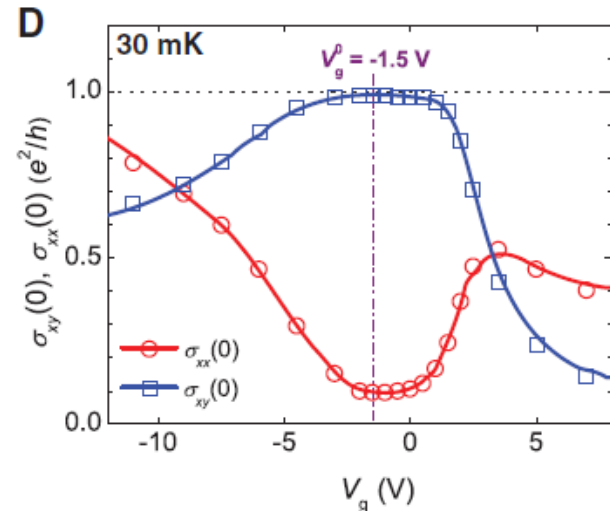
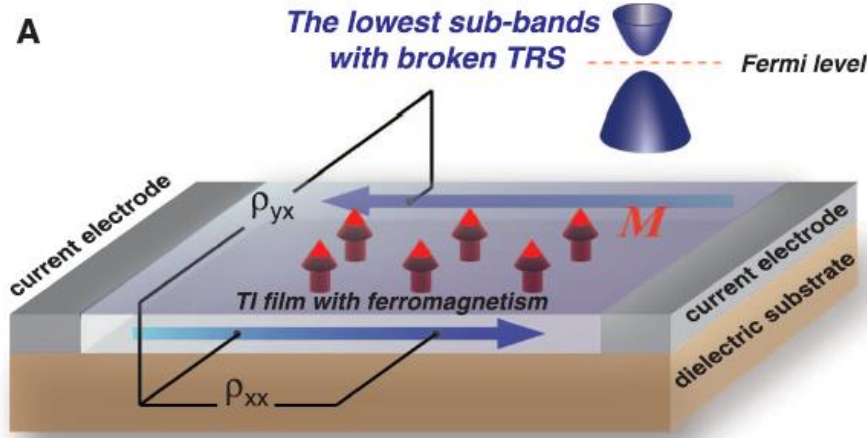
Small exchange field



Large exchange field



Quantum anomalous Hall effect



$$\begin{aligned}\sigma_{xy} &= -\frac{e^2}{\hbar} \sum_n \int_{BZ} \frac{d^2\mathbf{k}}{(2\pi)^2} f_n(\mathbf{k}) \Omega_{n,z}(\mathbf{k}) \\ &= -\frac{e^2}{2\pi\hbar} \int_{BZ} d^2\mathbf{k} \sum_{n(\text{occ})} \Omega_{n,z}(\mathbf{k}) \\ &= -\frac{e^2}{2\pi\hbar} \int_{BZ} d^2\mathbf{k} \Omega_z(\mathbf{k}),\end{aligned}$$

$$\int_S \Omega(\mathbf{k}) \cdot d\mathbf{S} = 2\pi Z$$

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