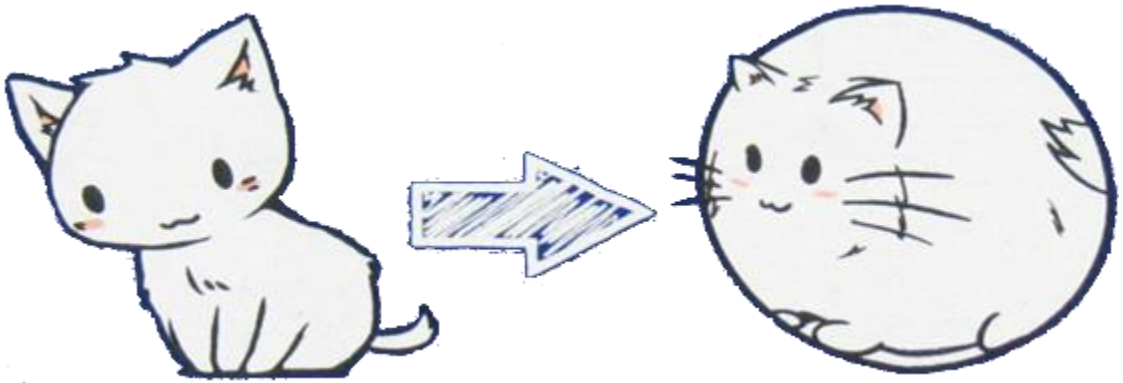
Topological Materials



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2016/May./19

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)

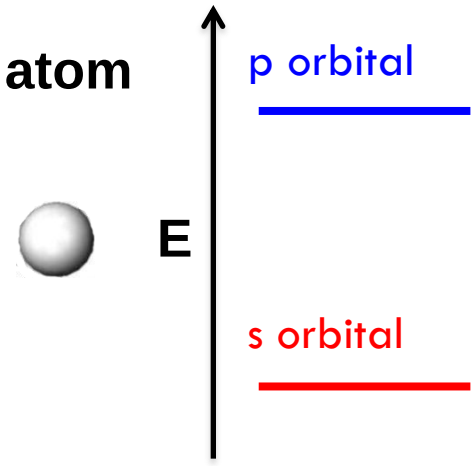
2. Topological insulator (quantum spin Hall insulator)

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

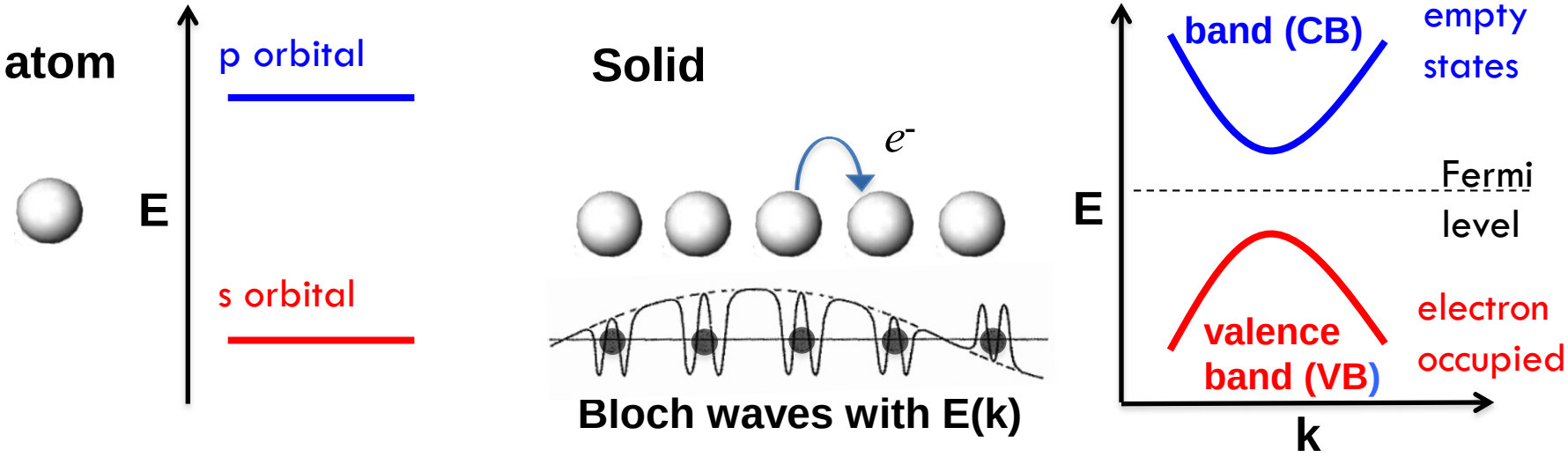
3. Topological semimetal

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

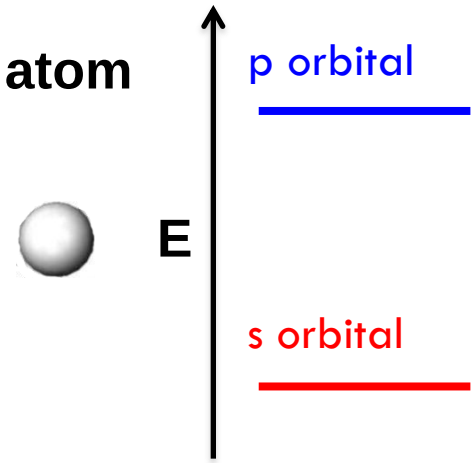
Condensed matter physics: band theory

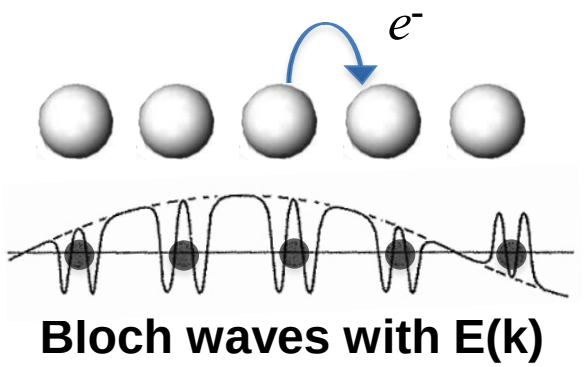


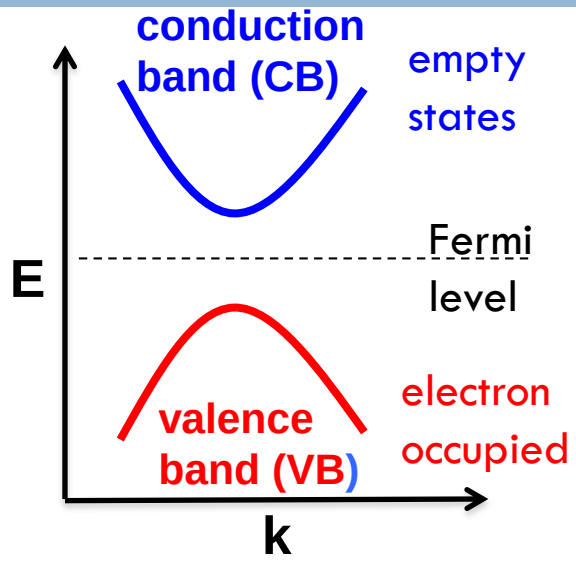
Condensed matter physics: band theory

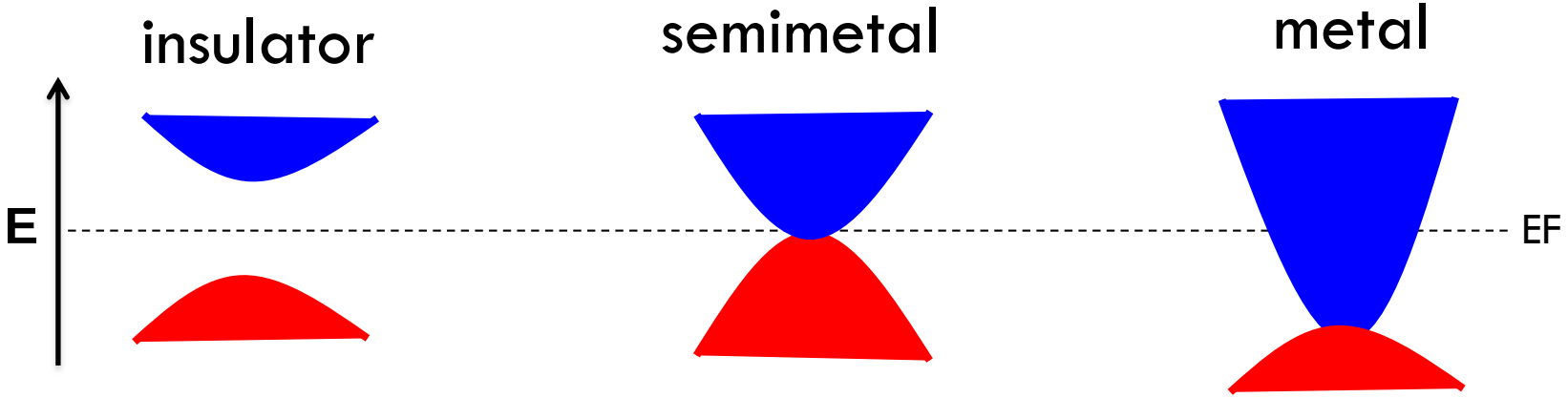


Condensed matter physics: band theory

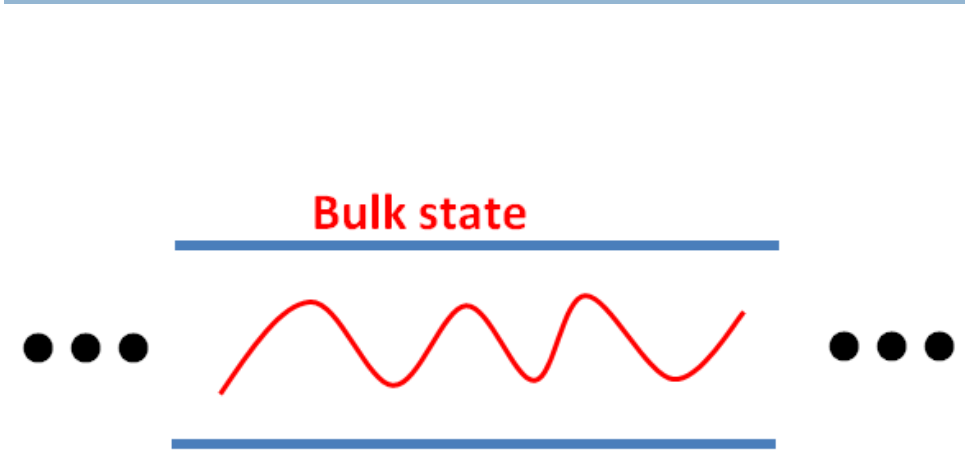


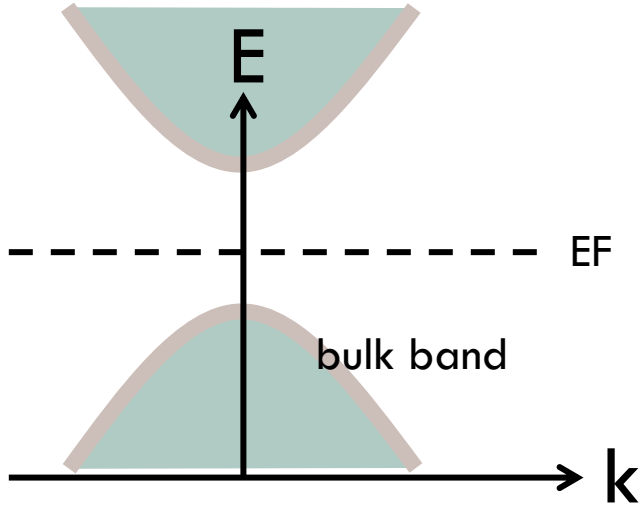


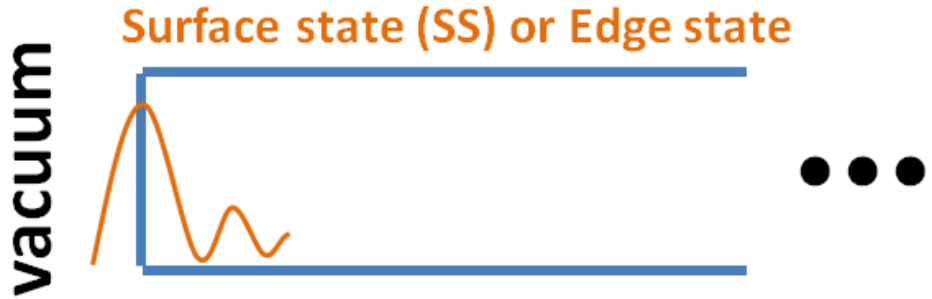


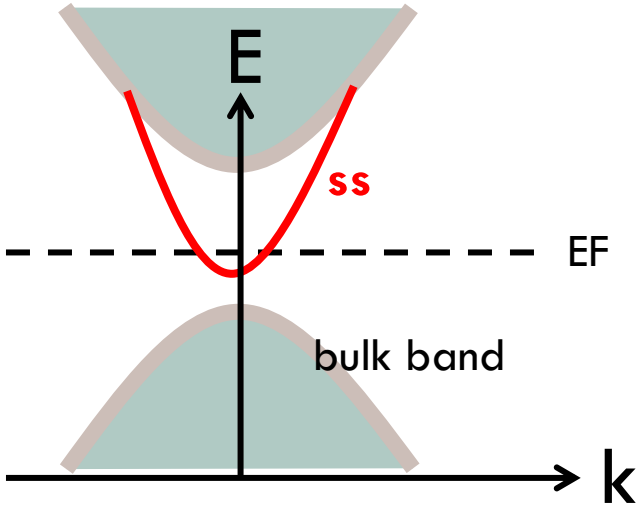


Condensed matter physics: band theory





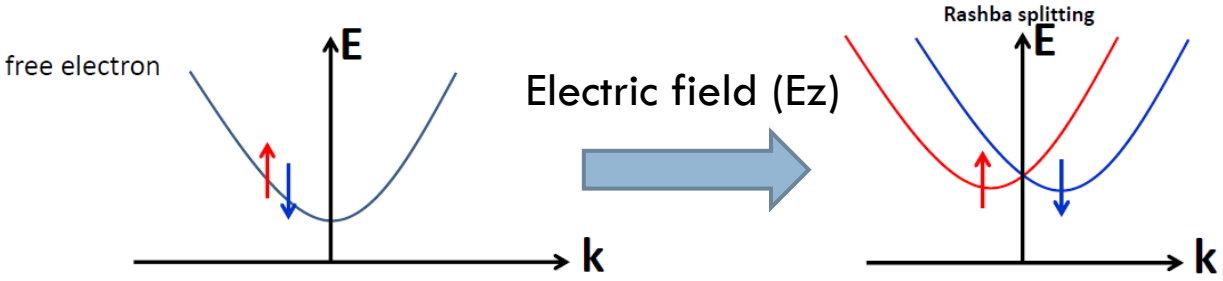


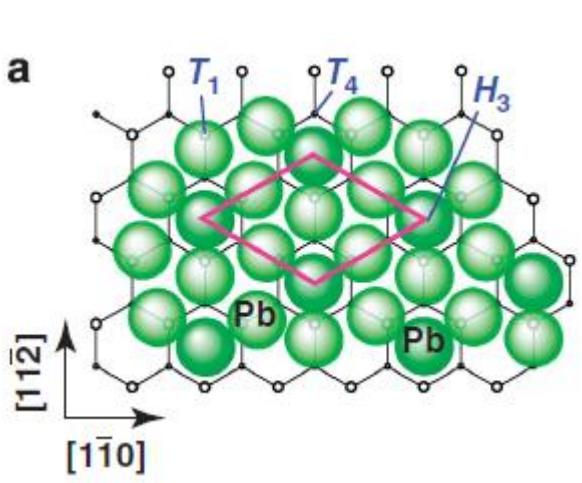


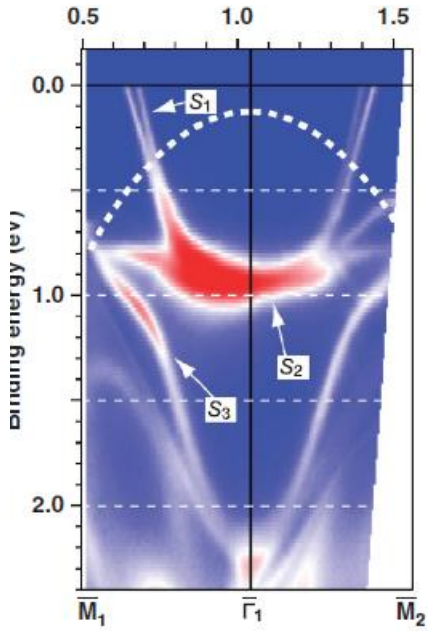
Condensed matter physics: band theory

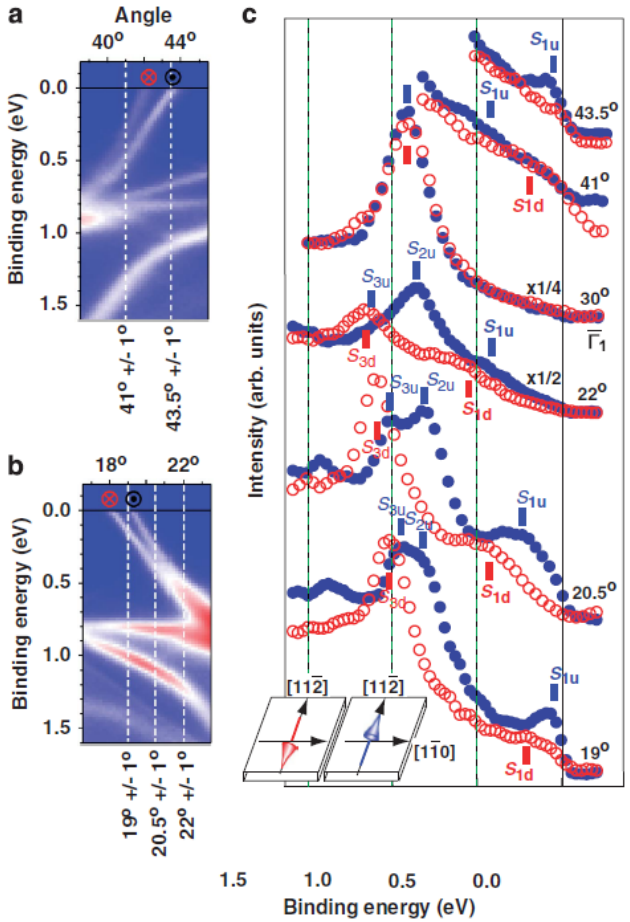
Example: surface Rashba effect

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









Topology in condensed matter physics

Math => real space

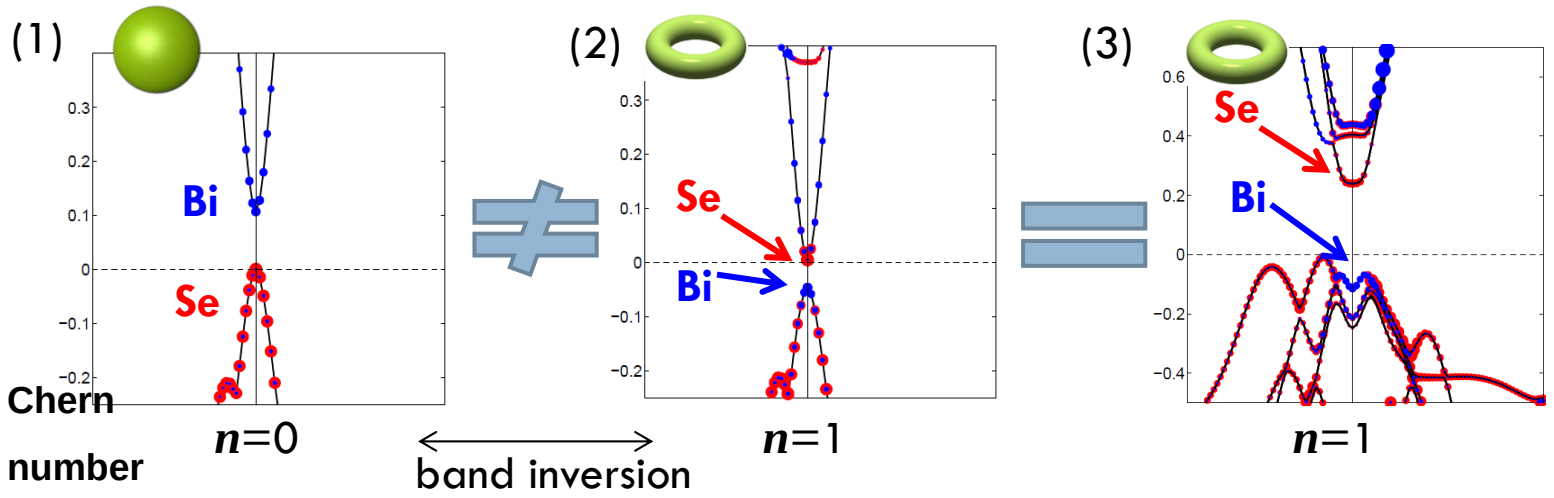
genus $g = 0$ $g = 1$ $g = 1$

Gauss-Bonnet Theorem:

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

Gauss curvature genus

Topology in condensed matter physics



TKNN theory:

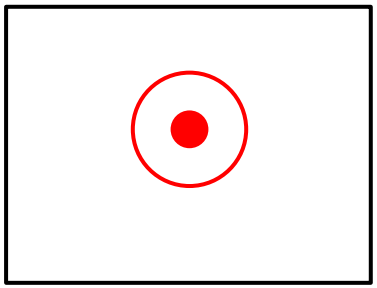
$$\sum_m \frac{1}{2\pi}\int_{BZ} d^2k \nabla \times i\left\langle u_m \middle| \nabla \middle| u_m \right\rangle = n$$

Berry curvature — **Chern number**

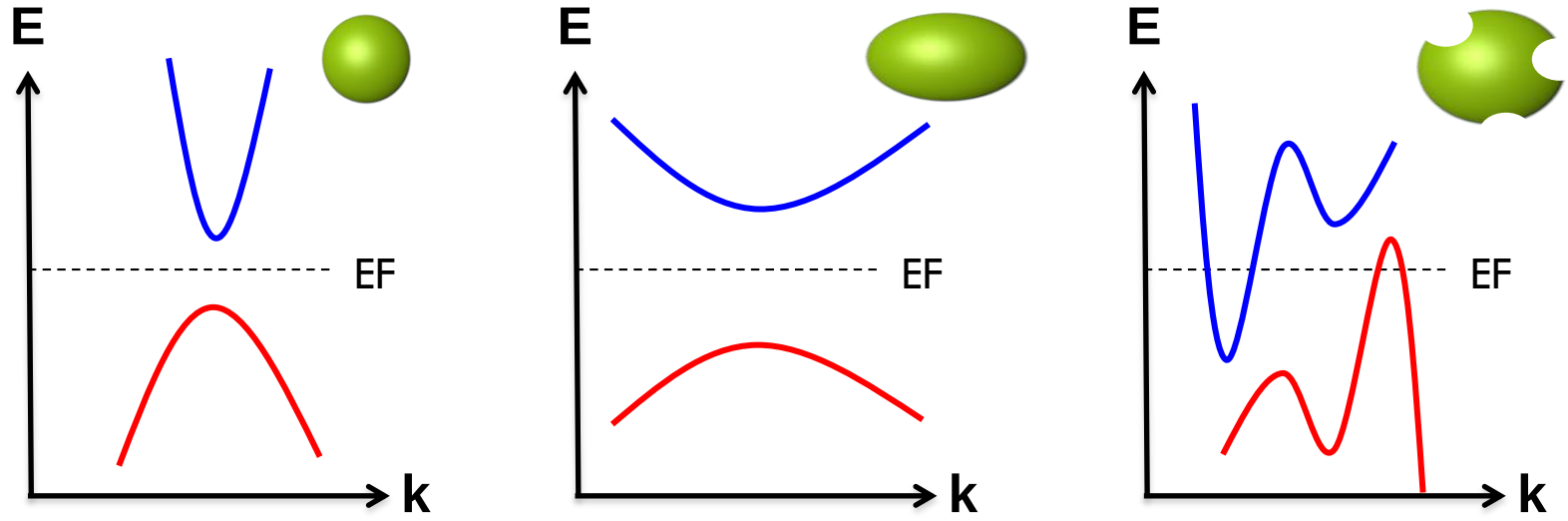
Thouless, Kohmoto, Nightingale, and den Nijs,
Phy. Rev. Lett. **49**, 405 (1982).

Berry curvature(flux)

BZ

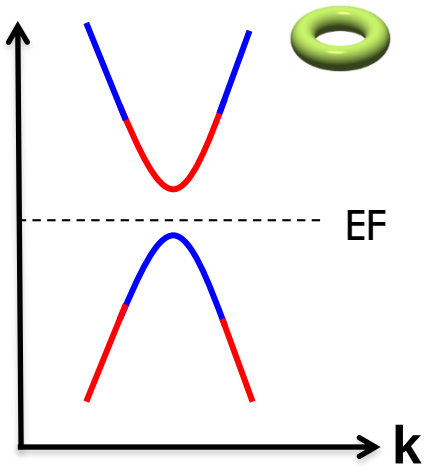


Topology in condensed matter physics



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 Z2.



Topology in condensed matter physics

Math => real space

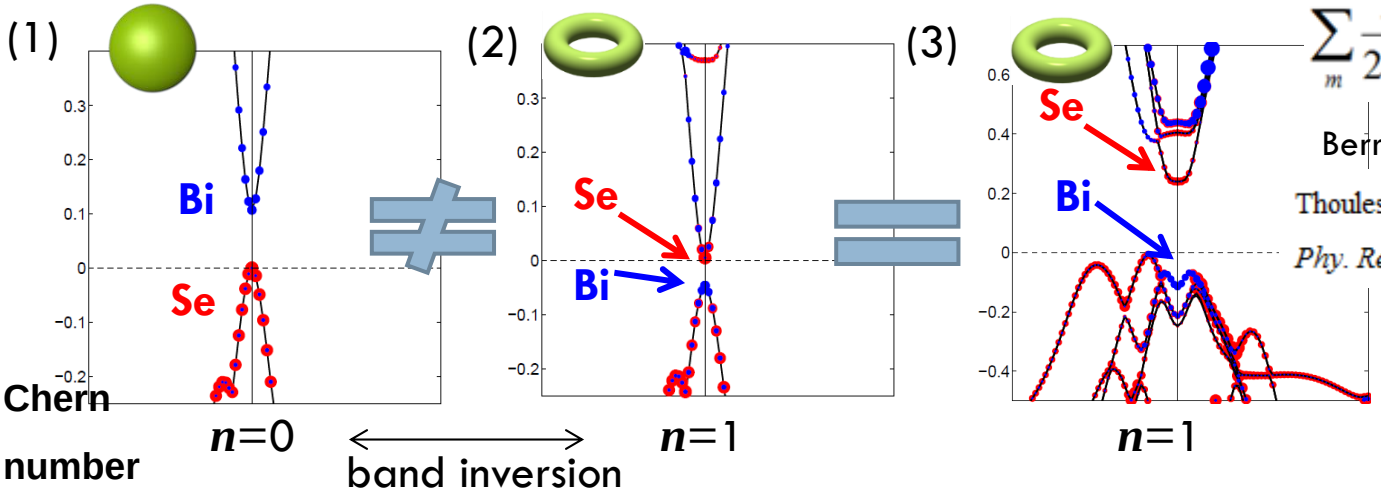
genus $g=0$ $g=1$ $g=1$

Gauss-Bonnet Theorem:

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

Gauss curvature — genus

Phys => momentum space

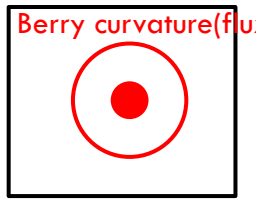


TKNN theory:

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

Berry curvature — Chern number

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



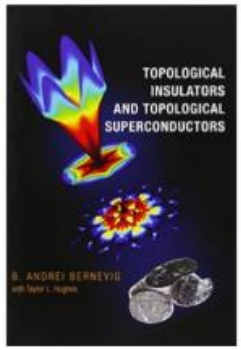
Topological phase transition

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

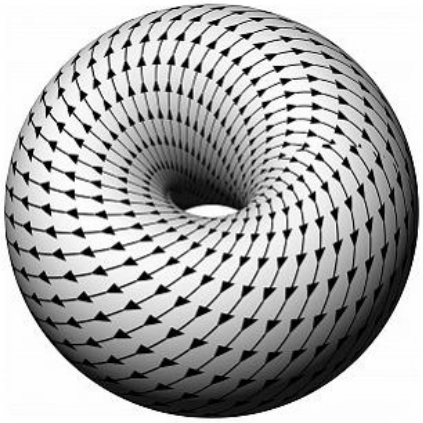
Berry curvature $\mathbf{\Omega}_n(\mathbf{k}) = \nabla_{\mathbf{k}} \times \mathbf{A}_n(\mathbf{k})$

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

Topological Insulators and Topological Superconductors
B. Andrei Bernevig & Taylor L. Hughes
p.30

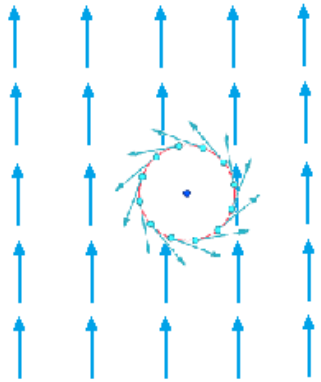


把BZ捲成甜甜圈(no boundary)



波函數平滑: $\gamma_n = 0$

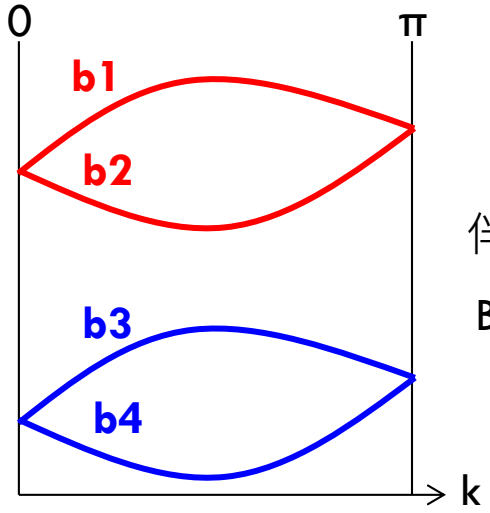
波函數有singularity



$\gamma_n \neq 0$

Topological phase transition

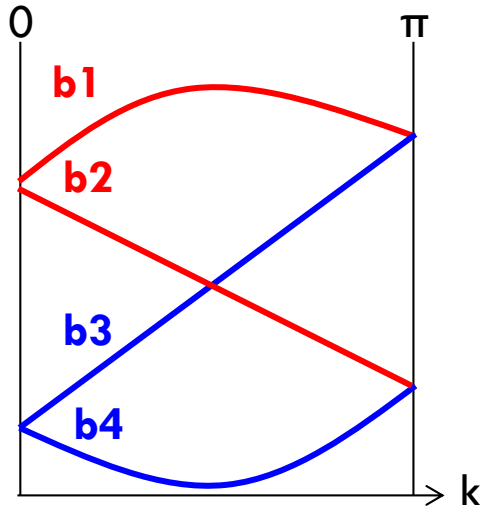
case 1

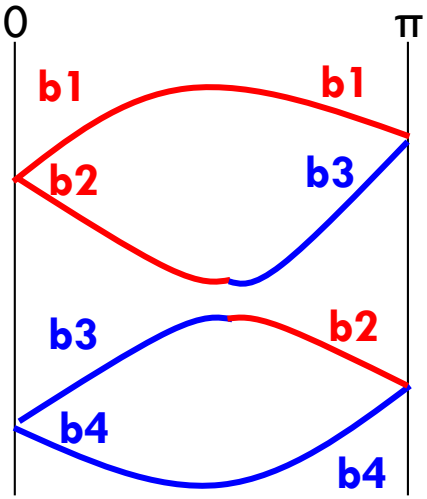


伴侶相同

Band insulator

case 2

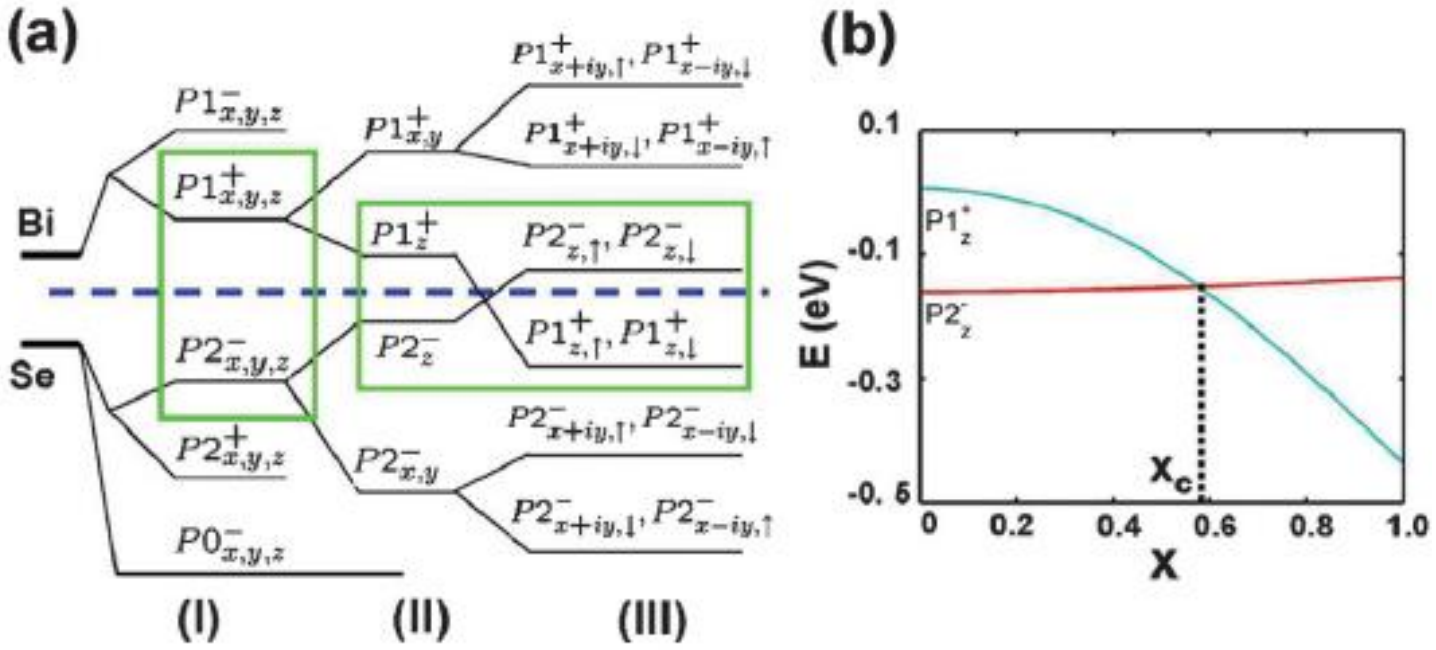




交換伴侶

Topological insulator

Topological phase transition

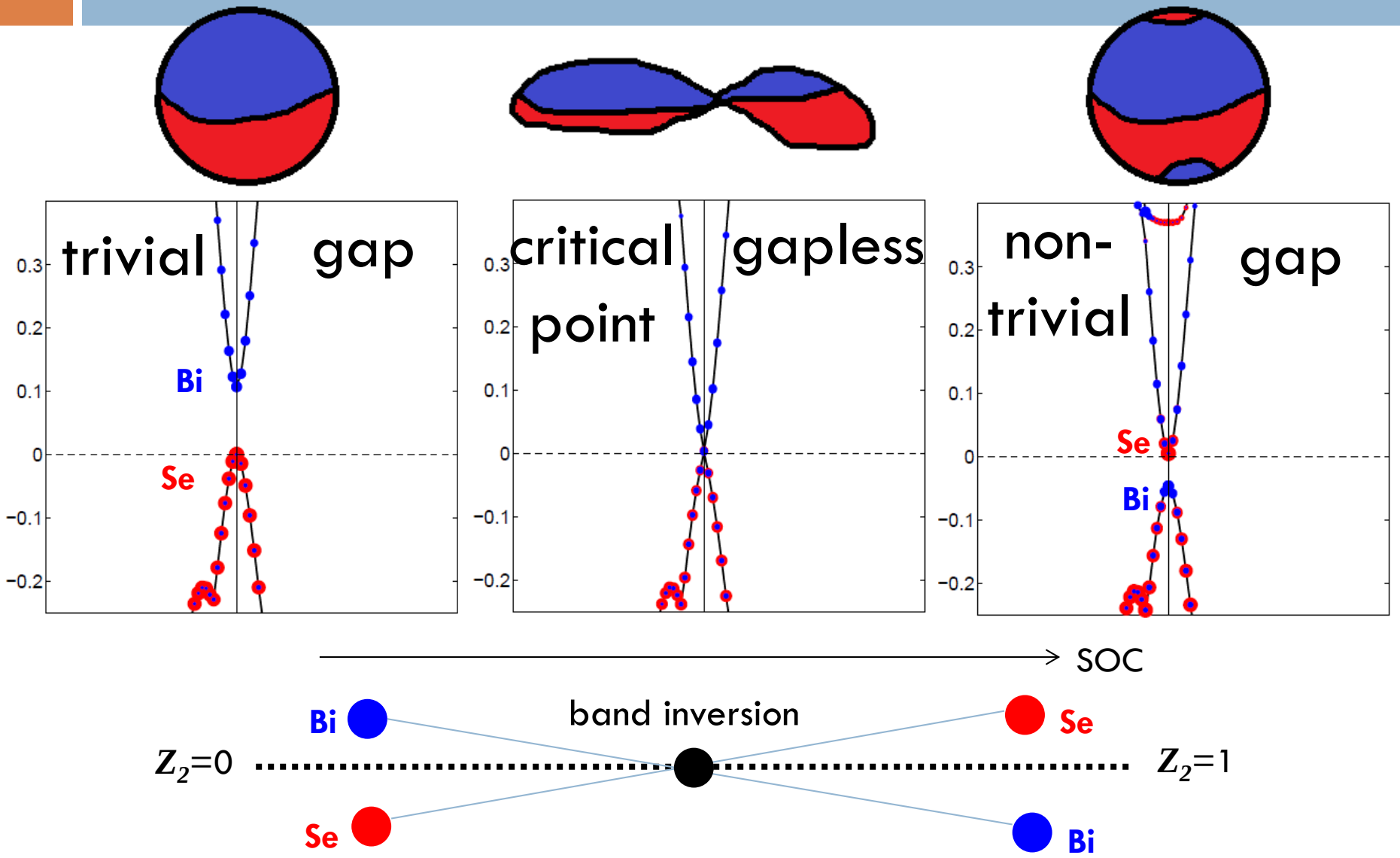


Bond splitting

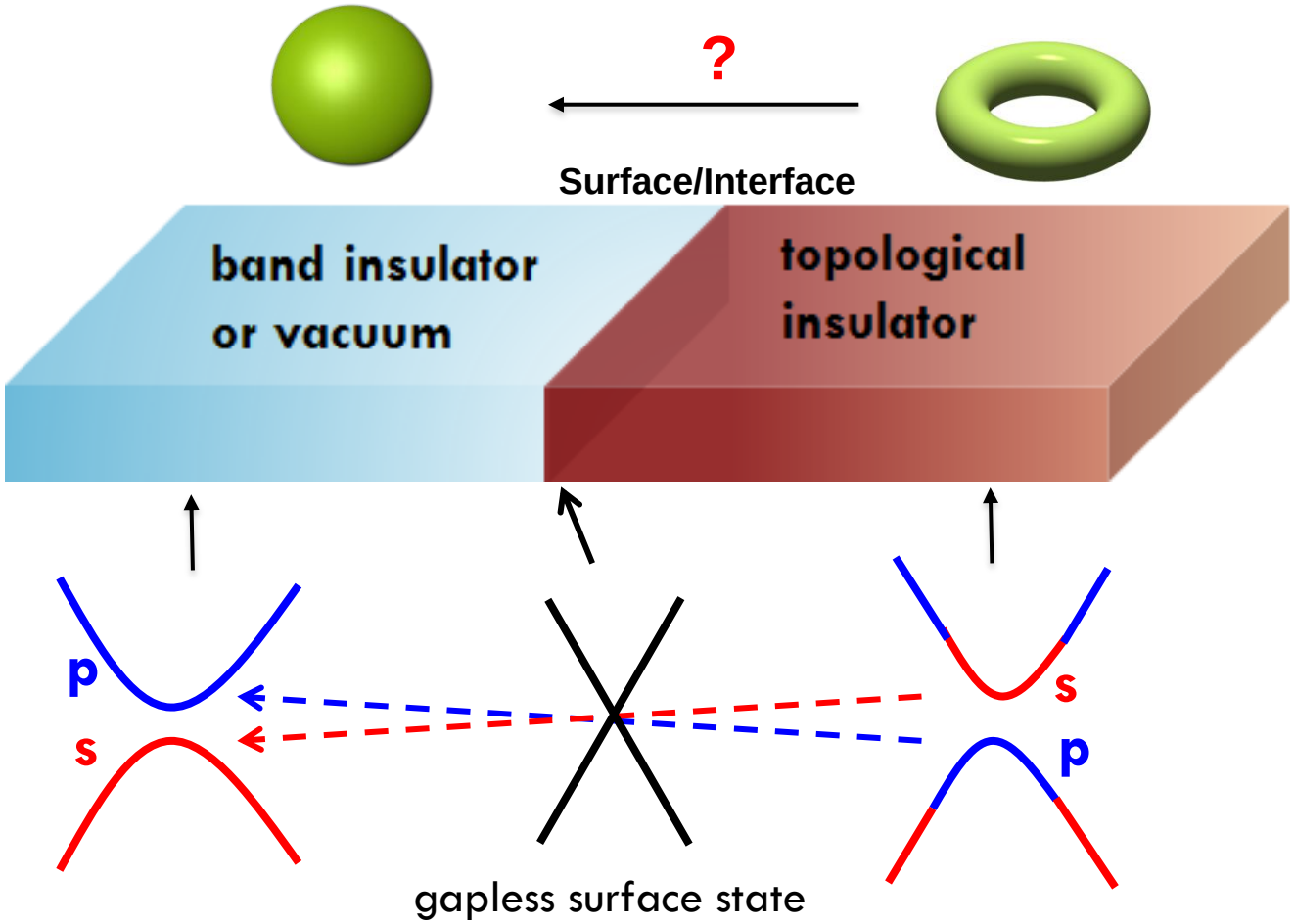
Crystal field splitting

SOC

Topological phase transition

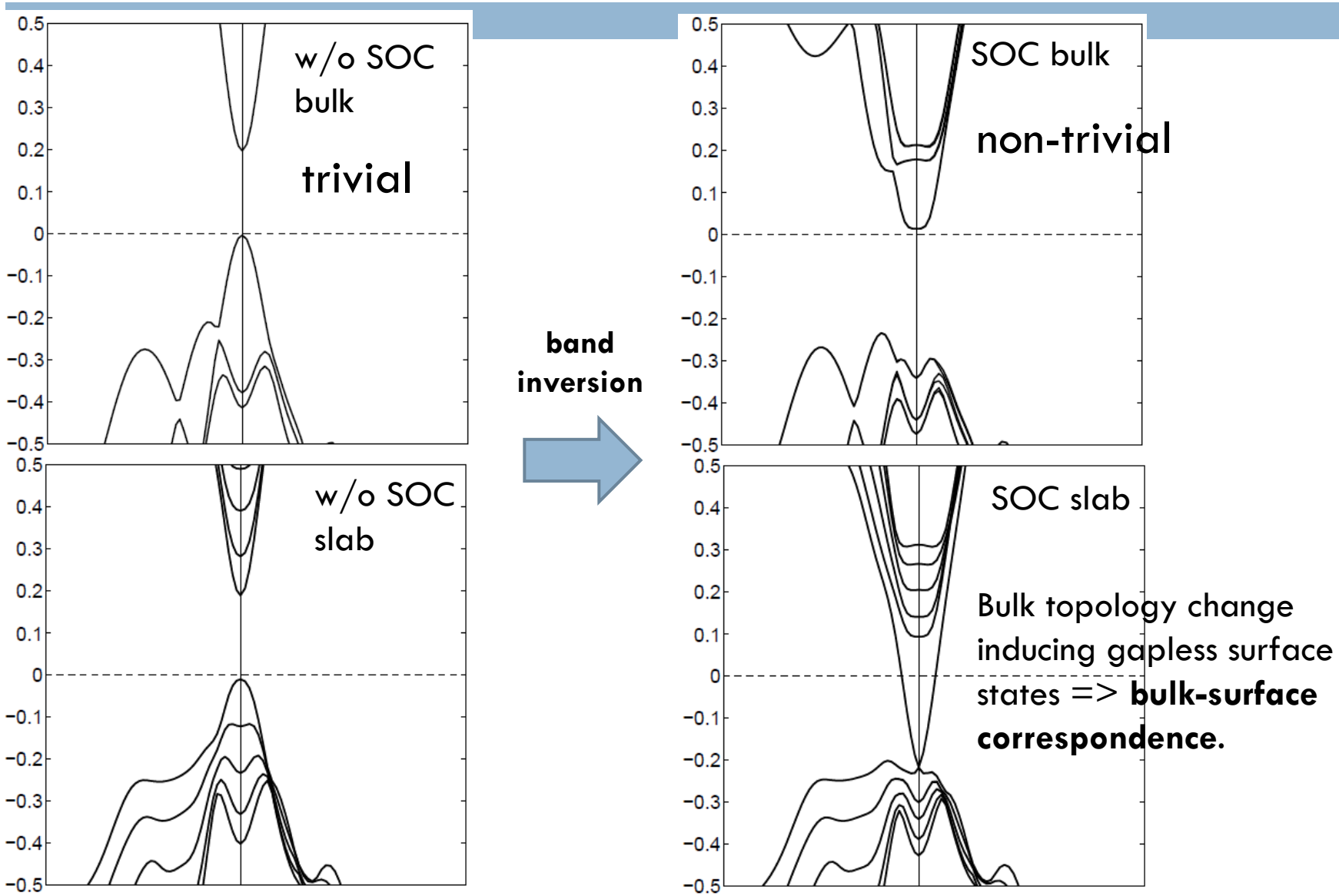


Topology in condensed matter physics (bulk-edge correspondence)

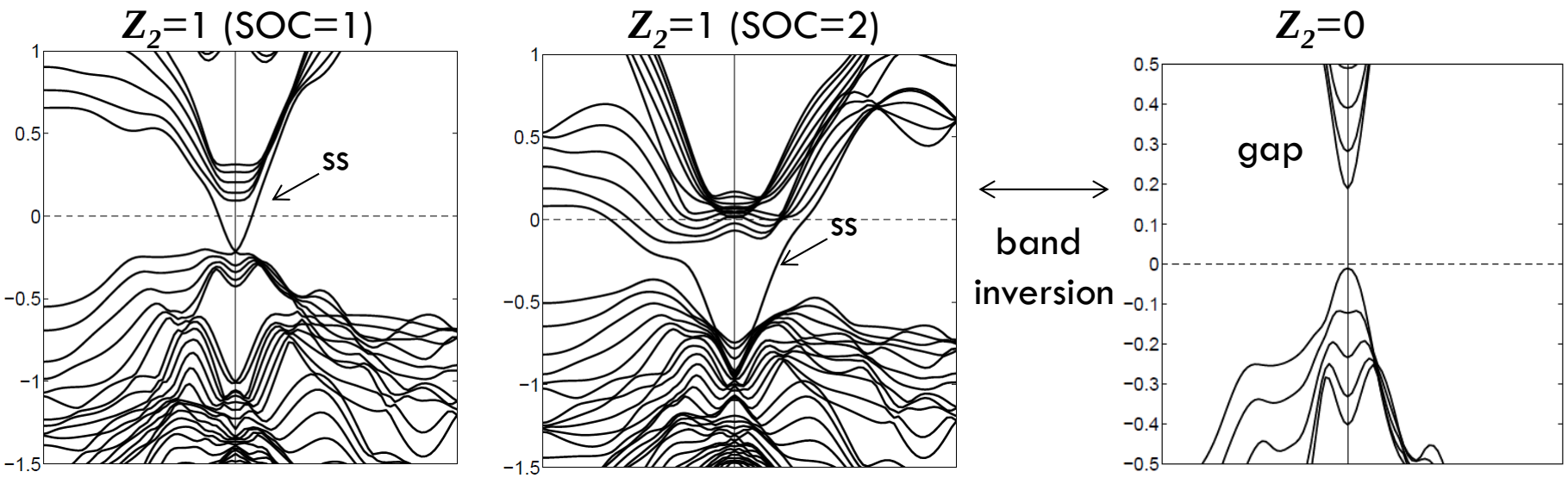


The gapless surface state is the hallmark of topological phase.

Topology in condensed matter physics (bulk-edge correspondence)

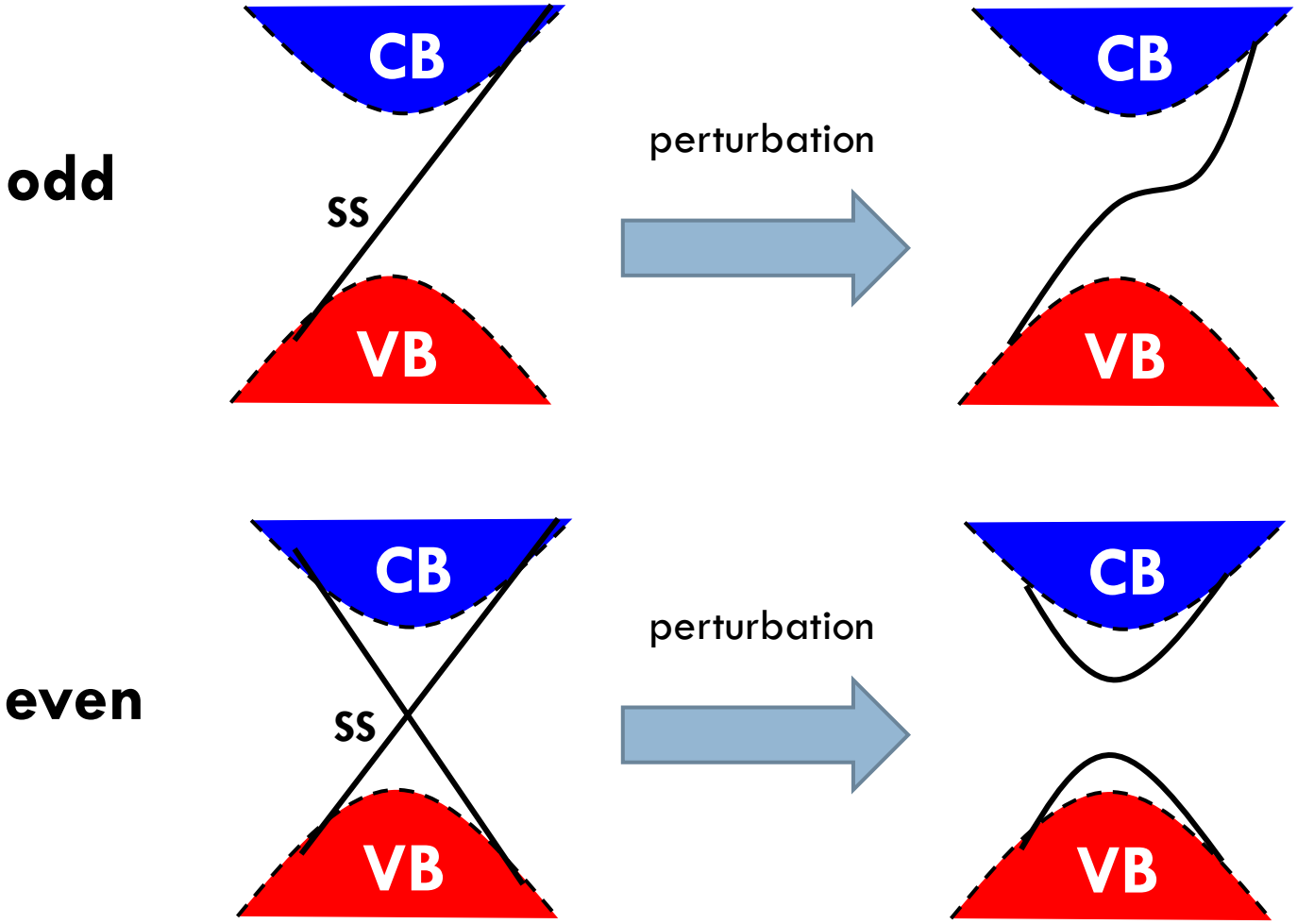


Topology in condensed matter physics (bulk-edge correspondence)



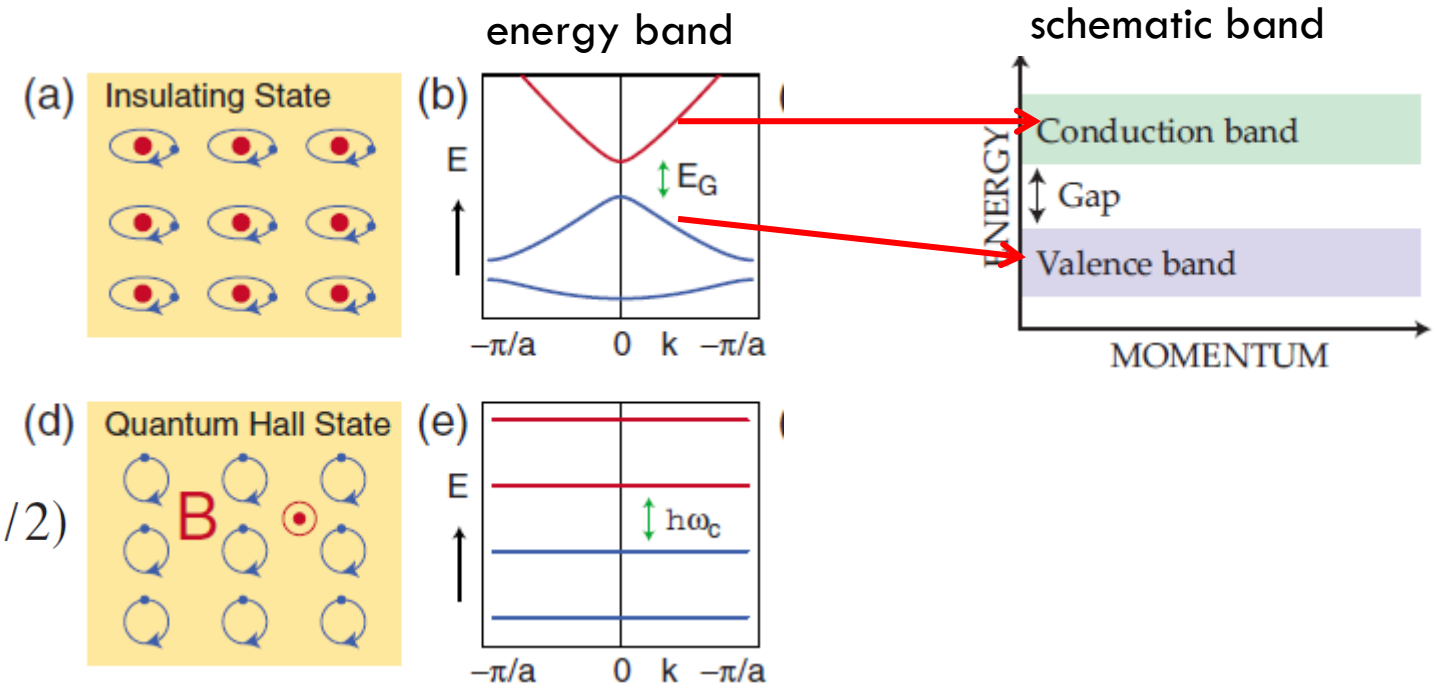
Small perturbation cannot destroy the topological surface states.

Topology in condensed matter physics (bulk-edge correspondence)

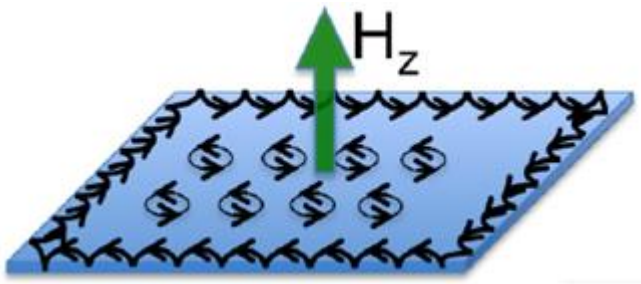


Integer quantum Hall effect (QHE)

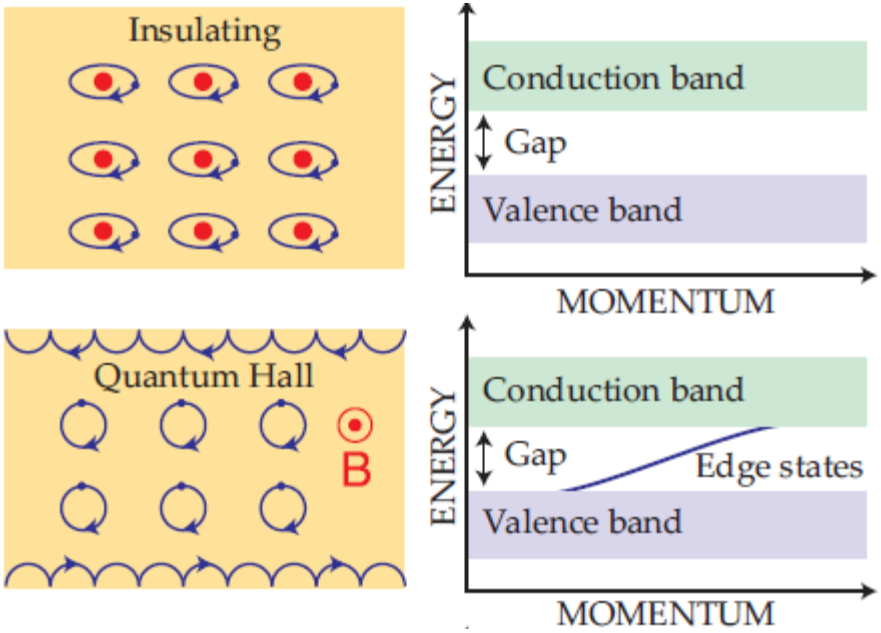
$E_n(\vec{k})$



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



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

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

Chern number

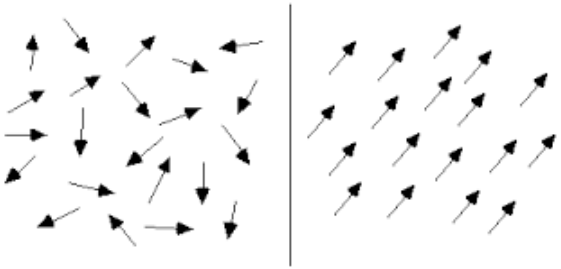
D. J. Thouless ,Phys. Rev. Lett. **49**, 405 (1982)

Landau's approach (order parameter)

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

Magnet

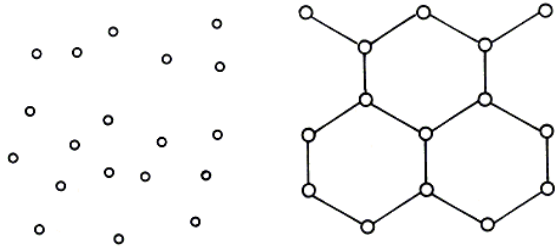
$\langle M\rangle=0$ $\langle M\rangle\neq 0$



broken rotational symmetry

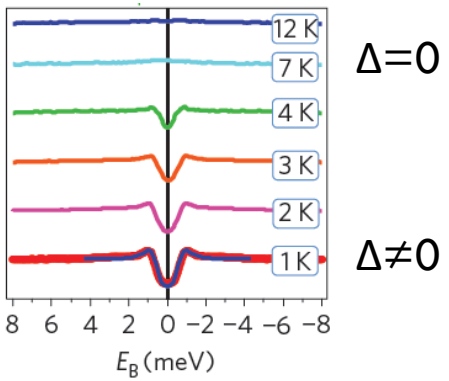
Crystal

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



broken translational symmetry

Superconductor



$\Delta=0$

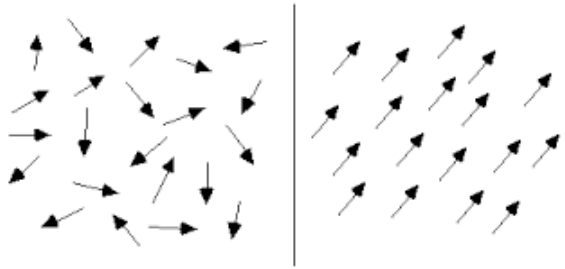
$\Delta\neq 0$

broken U(1) gauge symmetry

Topology in condensed matter physics

Landau approach: order parameter (symmetry breaking)

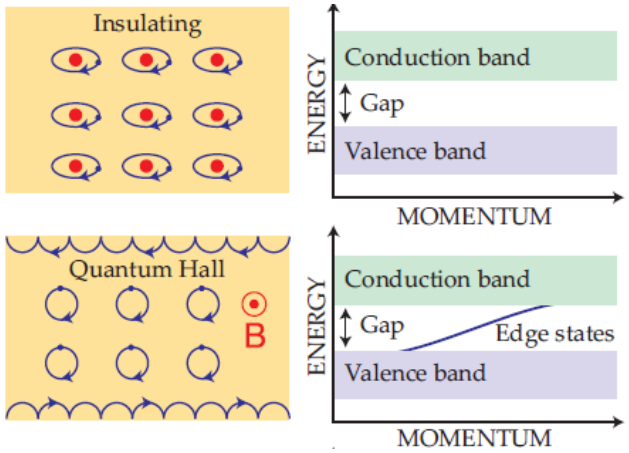
High-T $\langle M \rangle = 0$ $\langle M \rangle \neq 0$ Low-T



measurable properties

Bulk

Topology : topological invariant number



$\nu = 0$

$\nu =$ 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**)

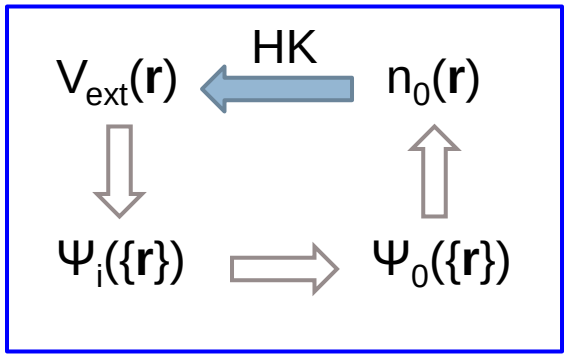
R. Martin
Electronic Structure (CAMBRIDGE 2004)

Density functional theory (DFT)

Hohenberg-Kohn Theorem

(1) For any system of interacting particles in an external potential $V_{ext}(\mathbf{r})$, the potential $V_{ext}(\mathbf{r})$ 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(**r**) can be defined, valid for any external potential $V_{ext}(\mathbf{r})$. For any particular $V_{ext}(\mathbf{r})$, the exact ground state energy of the system is the global minimum value of this functional, and the density n(**r**) that minimizes the functional is the exact ground state density $n_0(\mathbf{r})$.



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

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

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

$T[n]$ 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.

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

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

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

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

Density functional theory (DFT)

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

where $E_{xc}[n] = F_{HK}[n] - (T_0[n] + V_H[n])$ ← approximation

LDA, GGA …etc

functional derivative to minimize E_{KS}

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

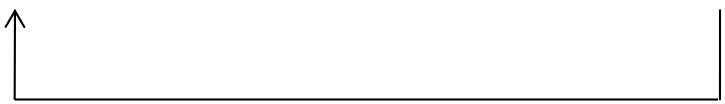
which is the **single-particle Kohn-Sham equation**

Local density approximation (LDA)

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

Self-consistent scheme

$n_{in}(\mathbf{r}) \rightarrow v_{eff} \rightarrow \varepsilon_i\ ;\ \psi_i \rightarrow n_{out}(\mathbf{r})$



Method

Step 1 **Density functional theory (DFT)**

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

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

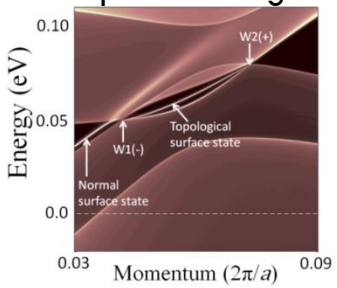
$$w_{n\mathbf{R}}(\mathbf{r}) = \frac{V}{(2\pi)^3}\int_{\mathrm{BZ}}\left[\sum_m U_{mn}^{(\mathbf{k})}\psi_{m\mathbf{k}}(\mathbf{r})\right]e^{-i\mathbf{k}.\mathbf{R}}\,\mathrm{d}\mathbf{k}$$

Wannier Bloch

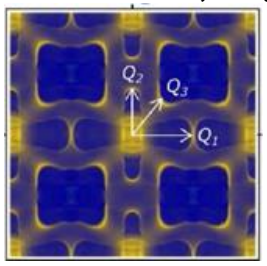
hopping parameters from first-principles

Step 3 **Electronic structures**

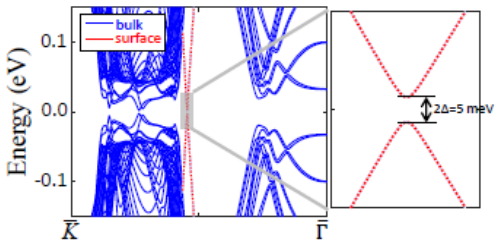
surface spectral weight



quasiparticle interference (QPI)



superconducting gap function



Density functional theory (DFT)

Total Energy and magnetic moment of Fe

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

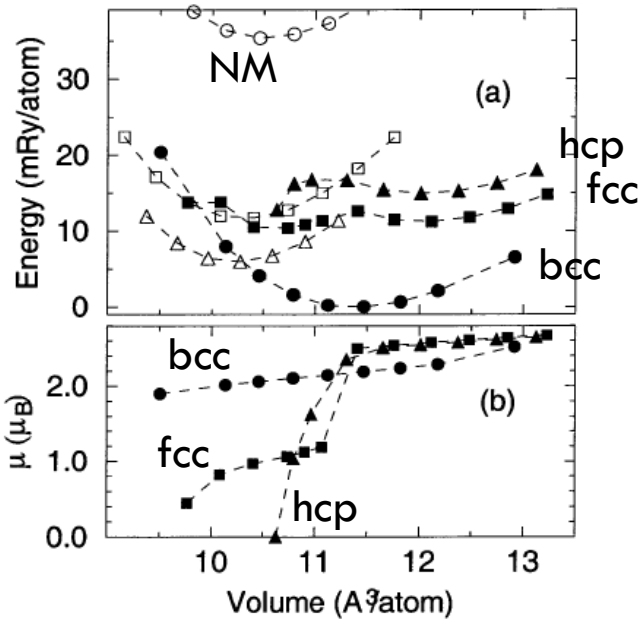
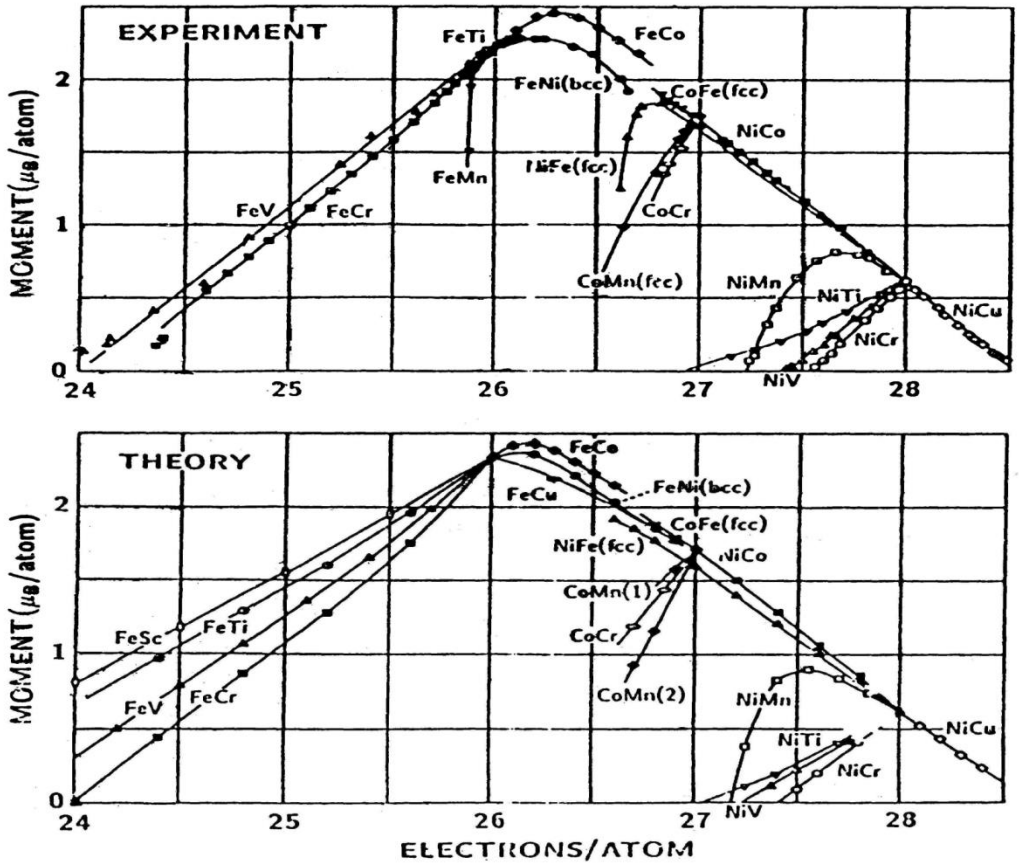


FIG. 1. (a) Total energy (relative to -2545.611 Ry/atom) of Fe as a function of volume per atom for bcc (circles), fcc (squares) and hcp (triangles). The curves are a polynomial fit to the total energies. Solid symbols denote the ferromagnetic states and open symbols, the nonmagnetic states. (b) Magnetic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

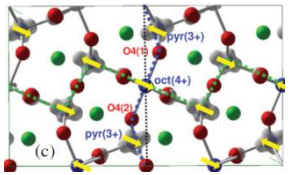


Density functional theory (DFT)

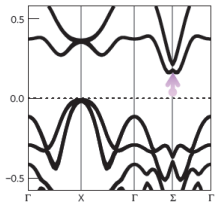
Density functional theory (DFT) + ab-initio tight-binding model:

Transition metal oxides

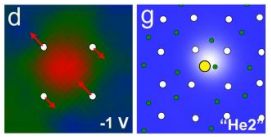
multiferroic: $TbMn_2O_5$
PRB



Iridate: $Sr_3Ir_2O_7$
Nat. Mat.

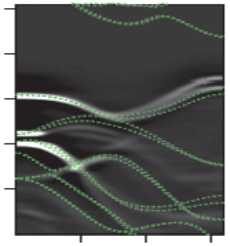


Cuprate: Bi2212
Nano Lett.

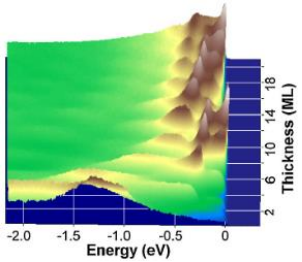


2D materials (TMDC and thin-film)

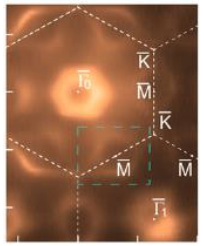
TMDC: $MoSe_2$
Nat. Nano.



Pb/Ge
PRL

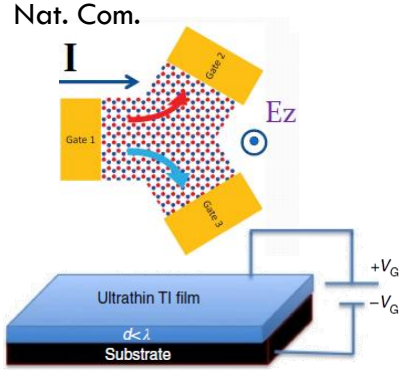


PbAu/Pb
NJP

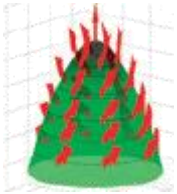


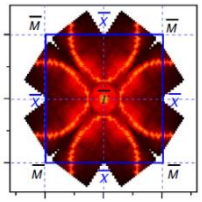
Topological insulator

2D Topological insulator
Nat. Com.



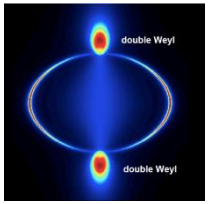
3D Topological insulator
Nat. Phys.
Nat. Com.
PRL



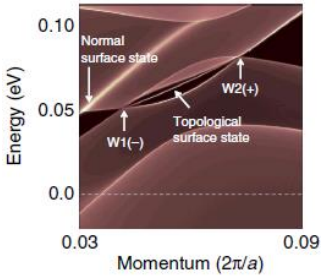


Topological semimetals

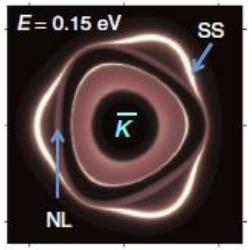
3D Dirac
Science
Nat. Com.



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}	$E_{\mathrm{LSD}+U}$	E_{expt}	m_{LSD}	$m_{\mathrm{LSD}+U}$	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,[g]4.58[i]

[a]Y. Tokura, T. Arima, S. Koshihara, T. Ido, S. Ishibasi, H. Takagi, and S. Uchida, *Proceedings of the Second International Symposium on Superconductivty*, Tsukuba (Springer, New York, in press).
[b]D. Vaknin, E. Couignol, P. K. Devies,
39, 9122 (1989).
[c]F. P. Koffyberg and F. A. Benko, J. Ap
[d]J. B. Forsyth, P. J. Brown, and B. M. W
[e]G. A. Sawatzky and J. W. Allen, Phys.
[f]S. Hüfner, J. Osterwalder, T. Riesterer,
[g]B. E. F. Fender, A. J. Jacobson, and F.
[h]H. A. Alperin, J. Phys. Soc. Jpn. Suppl.
[i]A. K. Cheetham and D. A. O. Hope, Ph
[j]J. van Elp *et al.* (unpublished).
[k]R. J. Powell and W. E. Spicer, Phys. Rev. B **2**, 2182 (1970).
[l]D. C. Kahn and R. A. Ericson, Phys. Rev. B **1**, 2243 (1970).
[m]W. L. Roth, Phys. Rev. **110**, 1333 (1958); D. Hermann-Ronzaud, P. Burlet, and J. Rossat Mignod, J. Phys. C **11**, 2123 (1978).
[n]H. K. Bowen, D. Adler, and B. H. Auker, J. Solid State Chem. **12**, 355 (1975).
[o]R. 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

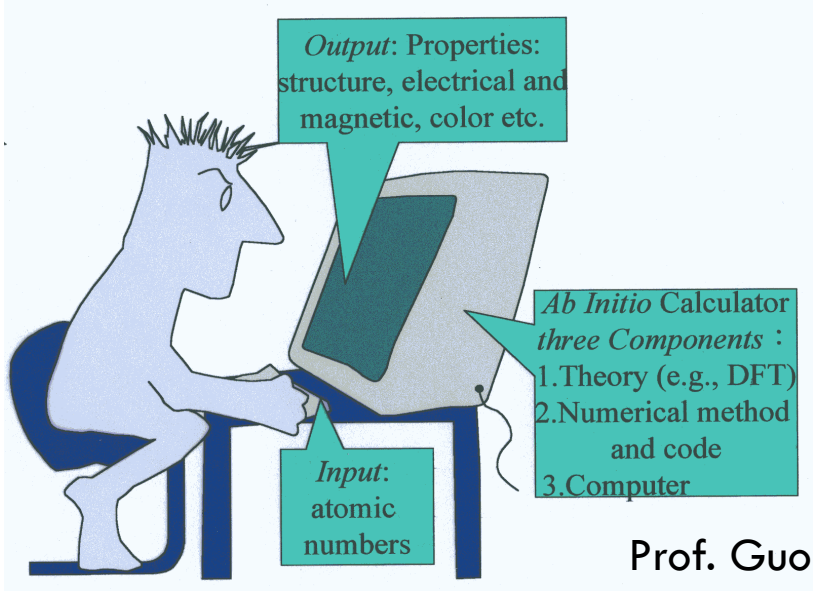
Spin and orbital moment too small

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)

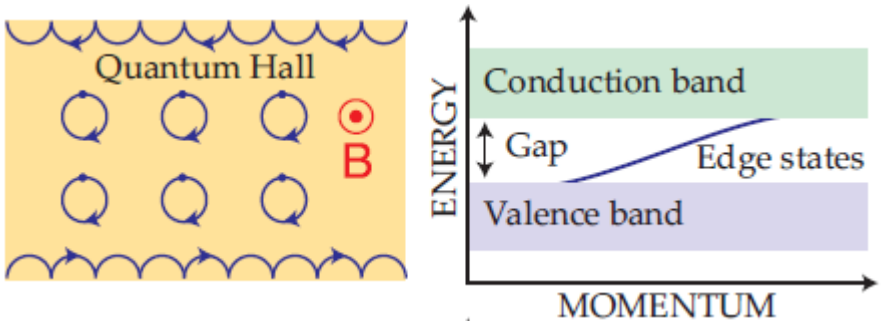
(5) Chao-Xing Liu, Shou-Cheng Zhang and Xiao-Liang Qi, arXiv:1508.07106 (2015)

(6) M. Z. Hasan, S.-Y. Xu, G. Bian, *Phys. Scr.* **T164**, 014001 (2015)

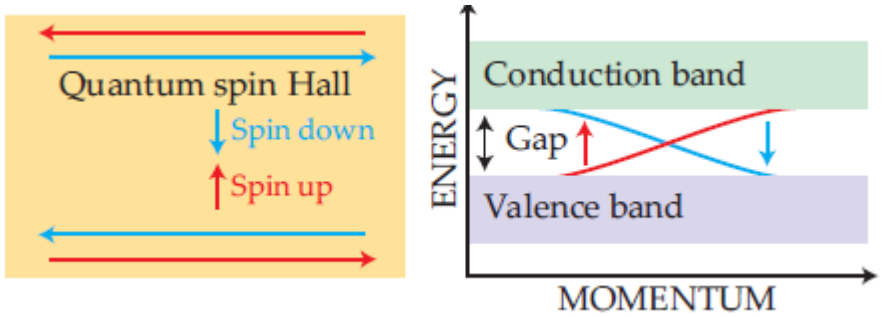
(7) Hongming Weng et al., arXiv:1603.04744 (2016)

Quantum spin Hall (QSH)

External magnetic field



Spin-orbit coupling (SOC)



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

TRS : E(k, ↑) = E(-k, ↓)

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

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

$\mathbb{Z}_2$ invariant is

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

$\upsilon_0 = 0$: *normal insulator*

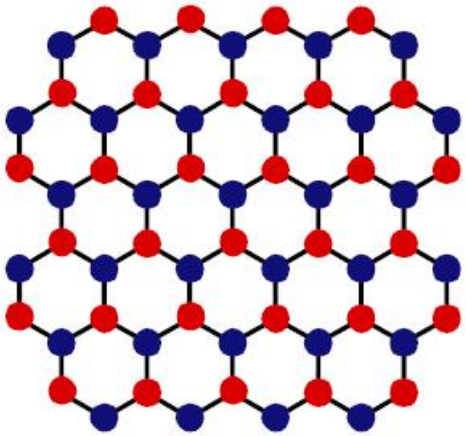
$\upsilon_0 = 1$: *QSH insulator*

T-breaking : Chern number

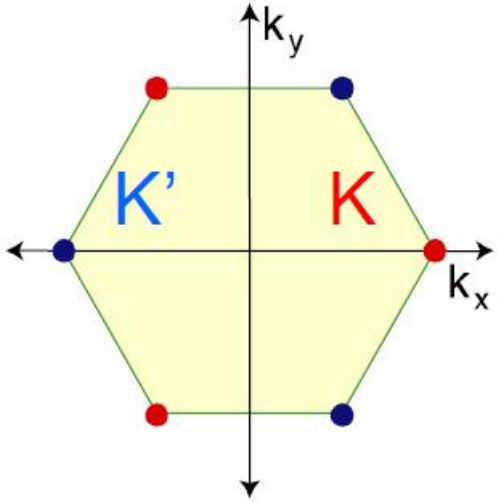
T-preserve : Z_2 number (spin Chern number)

Quantum spin Hall (QSH)

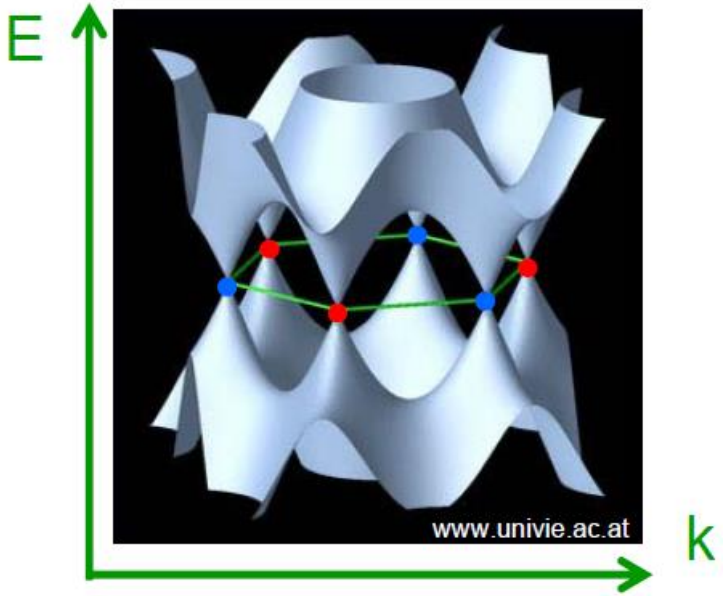
$$H = t \sum_{<i,j>} c_i^{\dagger} c_j$$



Honeycomb Lattice

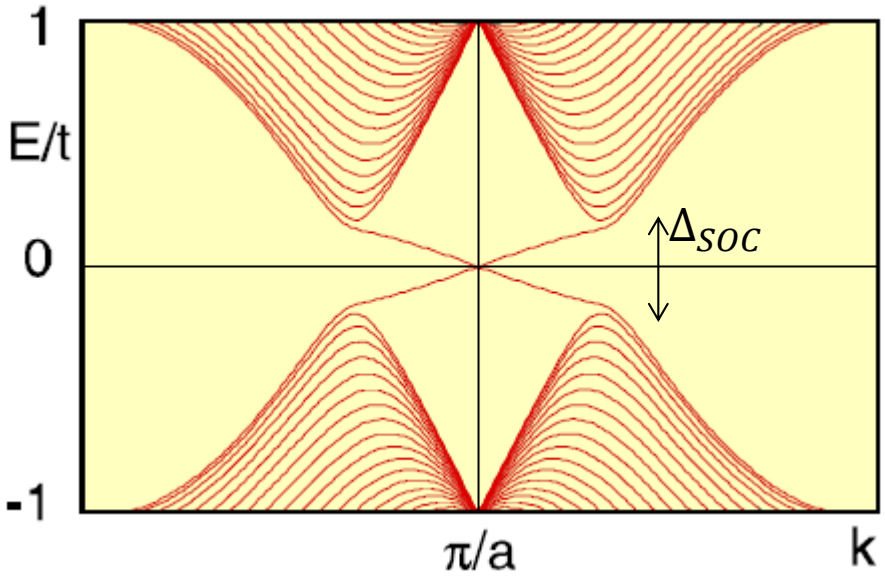


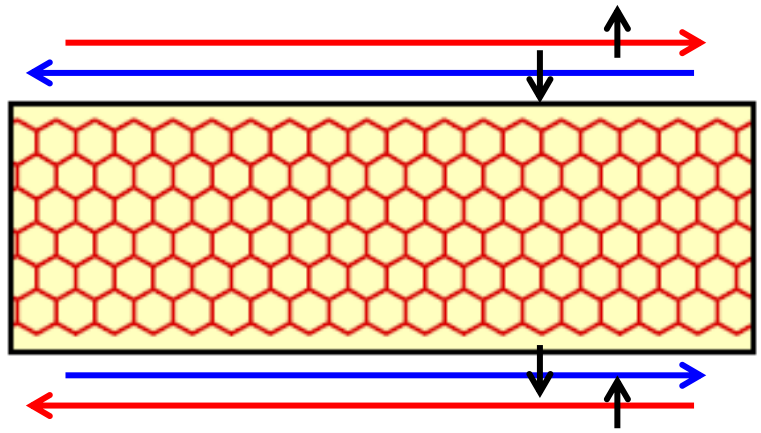
Brillouin Zone



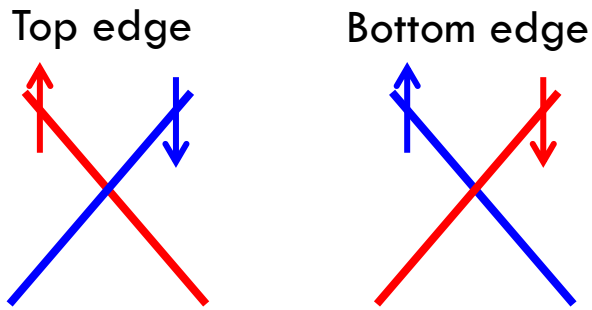
Quantum spin Hall (QSH)

$$H = t\sum_{<i,j>} c_i^{\dagger} c_j + i\lambda_{SO} \sum_{\ll i,j \gg} \nu_{ij} c_i^{\dagger} s^z c_j$$





helical spin texture



gap ~ 10^{-3} meV

C. L. Kane, Phys. Rev. Lett. **95**, 226801 (2005)

Topological invariant and parity

method 1: berry phase

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

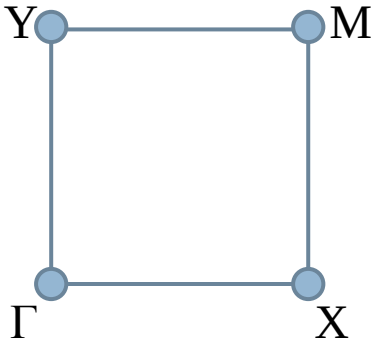
Berry curvature $\mathbf{\Omega}_n(\mathbf{R}) = \nabla_{\mathbf{R}} \times \mathcal{A}_n(\mathbf{R})$

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

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

$$n_\uparrow + n_\downarrow = 0,$$
$$n_\sigma = (n_\uparrow - n_\downarrow)/2$$
$$\mathbb{Z}_2 \text{ invariant is}$$
$$\nu = n_\sigma \bmod 2$$

method 2: parity

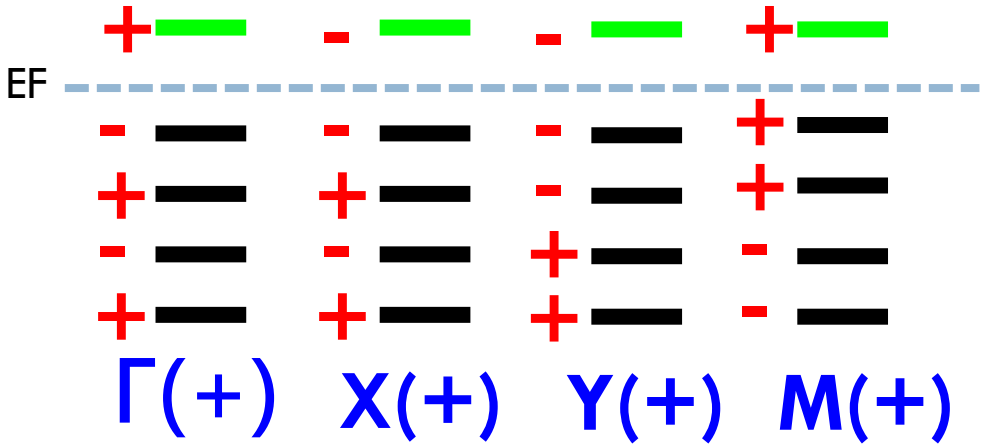


If the system preserves time-reversal and inversion symmetry

$$Z_2 = \delta_\Gamma \delta_X \delta_M \delta_Y = (-1)^v$$

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

Topological invariant and parity



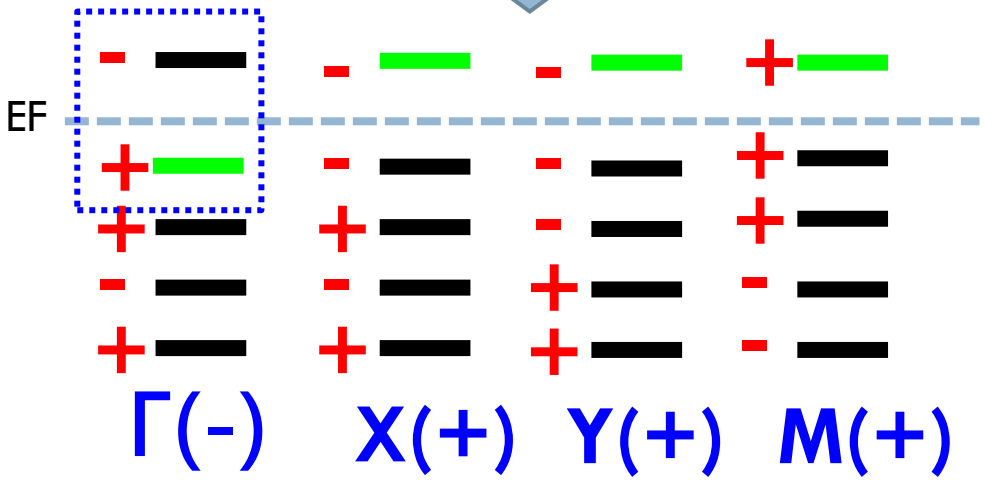
L. Fu, Phys. Rev. B **76**, 045302 (2007)

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

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

$$Z_2 = 0$$

band inversion at Γ point



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

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

$$Z_2 = 1$$

Topological insulator

$2D$: υ_0 — *Quantum spin Hall insulator*

$3D$: $(\upsilon_0; \upsilon_1, \upsilon_2, \upsilon_3)$ — *Topological insulator*

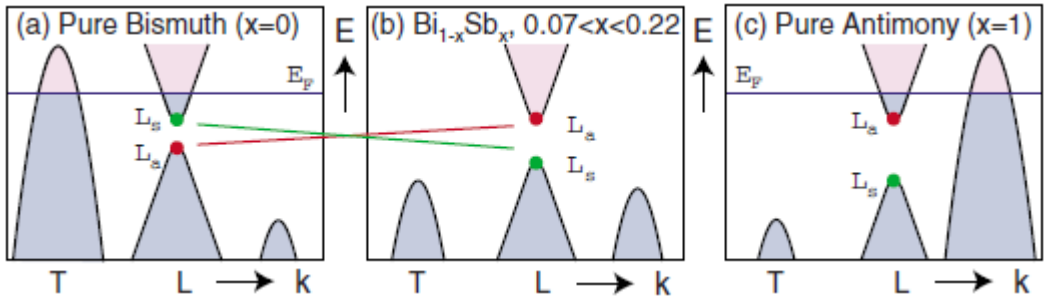
strong index — weak index

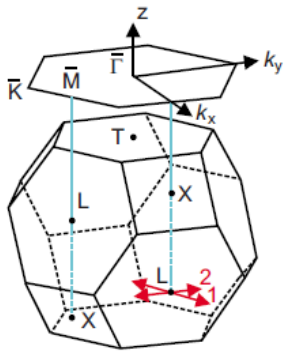
$\upsilon_0 \neq 0$: *strong topological insulator*

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

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

Topological insulator ($Bi_{1-x}Sb_x$)

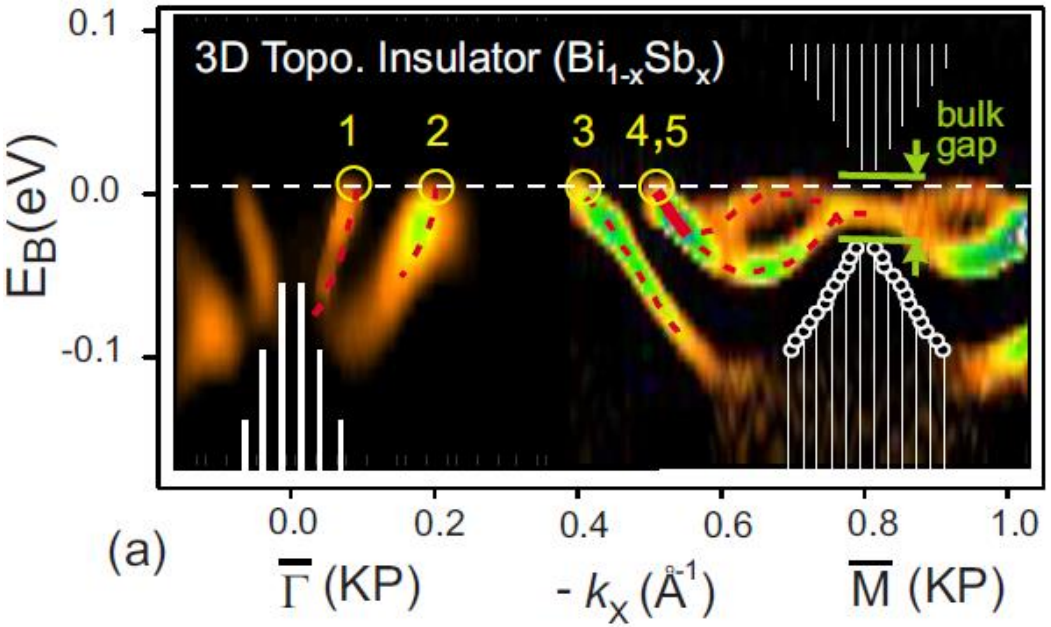


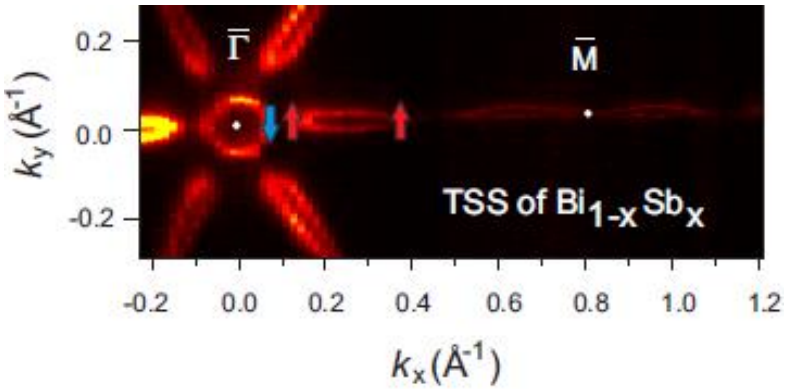


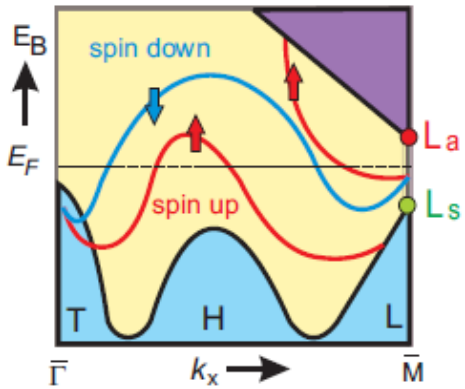
Bi: Class (0;000)							Sb: Class (1;111)						
Λ_a	Symmetry label					δ_a	Λ_a	Symmetry label					δ_a
1Γ	Γ_6^+	Γ_6^-	Γ_6^+	Γ_6^+	Γ_{45}^+	−1	1Γ	Γ_6^+	Γ_6^-	Γ_6^+	Γ_6^+	Γ_{45}^+	−1
$3L$	L_s	L_a	L_s	L_a	L_a	−1	$3L$	L_s	L_a	L_s	L_a	L_s	+1
$3X$	X_a	X_s	X_s	X_a	X_a	−1	$3X$	X_a	X_s	X_s	X_a	X_a	−1
$1T$	T_6^-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

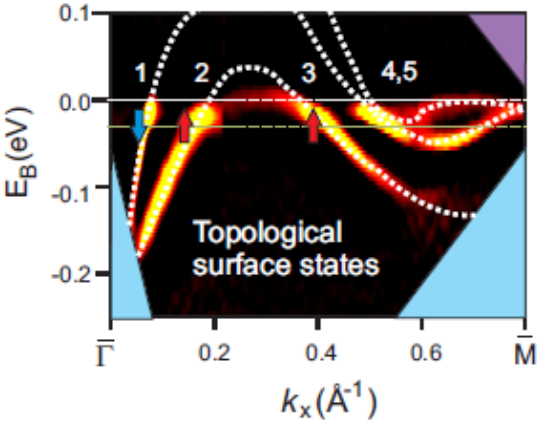
D. Hsieh et al., Nature **452**, 970 (2008)

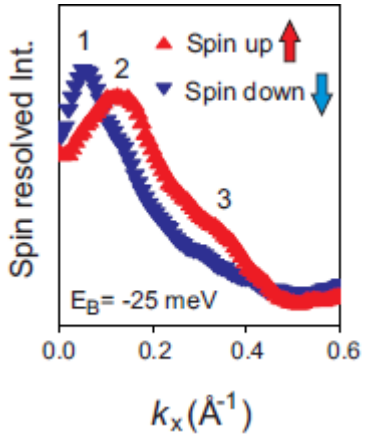
Topological insulator ($Bi_{1-x}Sb_x$)

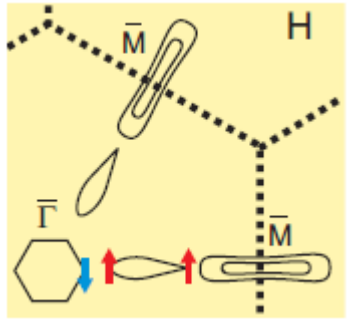










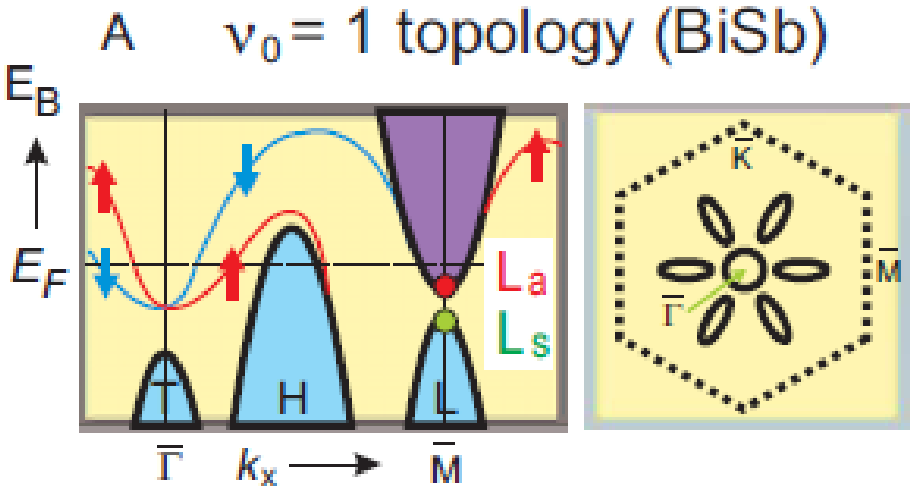


D. Hsieh et al., Nature **452**, 970 (2008)

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

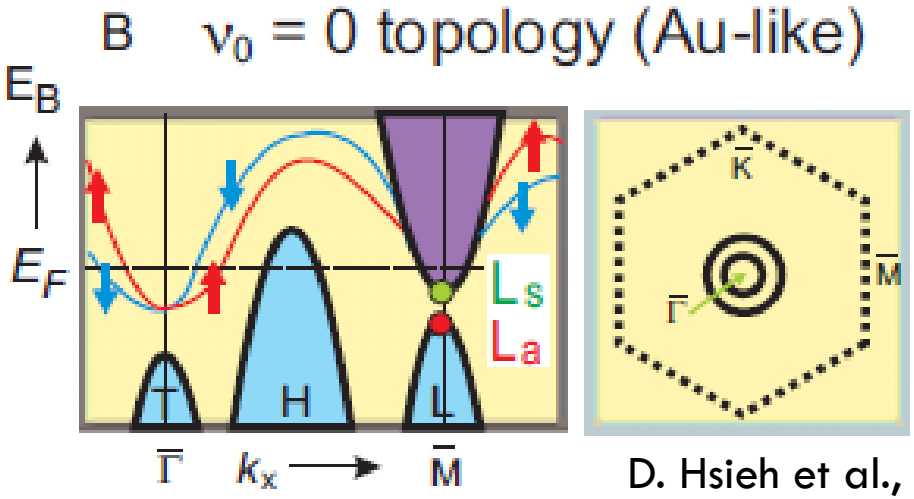
Topological insulator ($Bi_{1-x}Sb_x$)

Conduction to valence



Odd number of FS

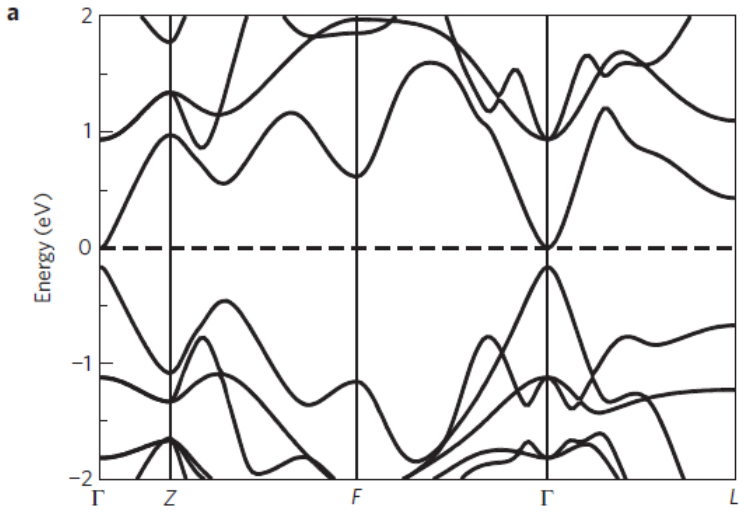
Conduction to conduction

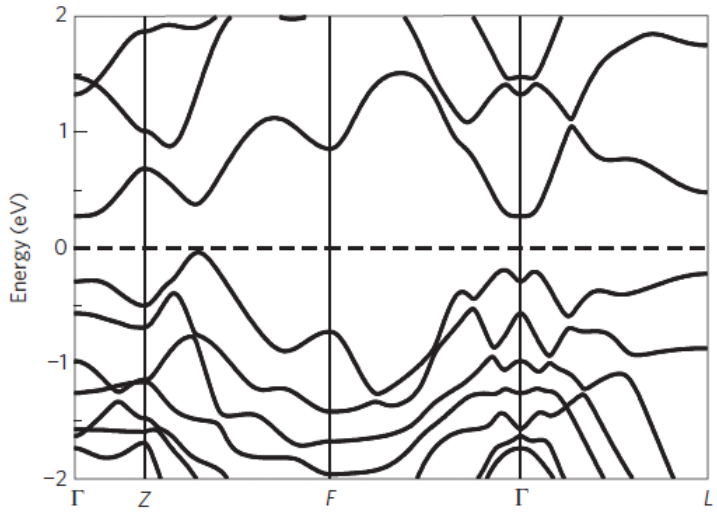


Even number of FS

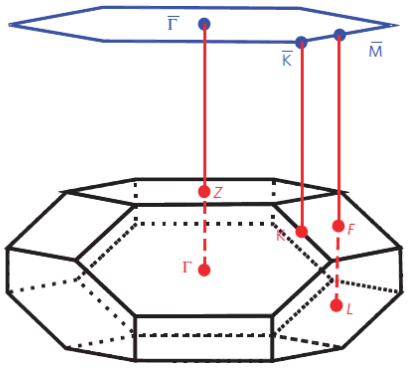
D. Hsieh et al., Science **323**, 919 (2009)

Topological insulator (Bi_2Se_3)

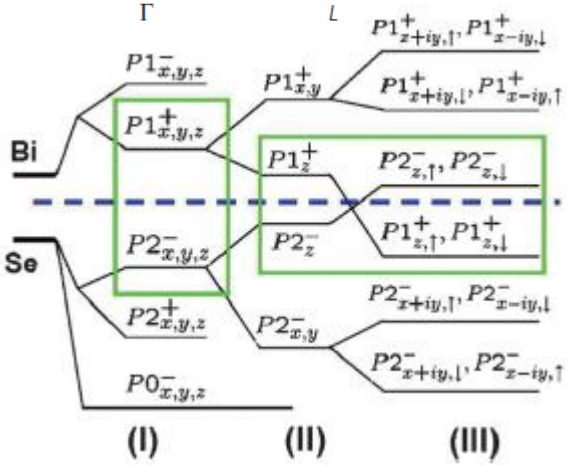




c

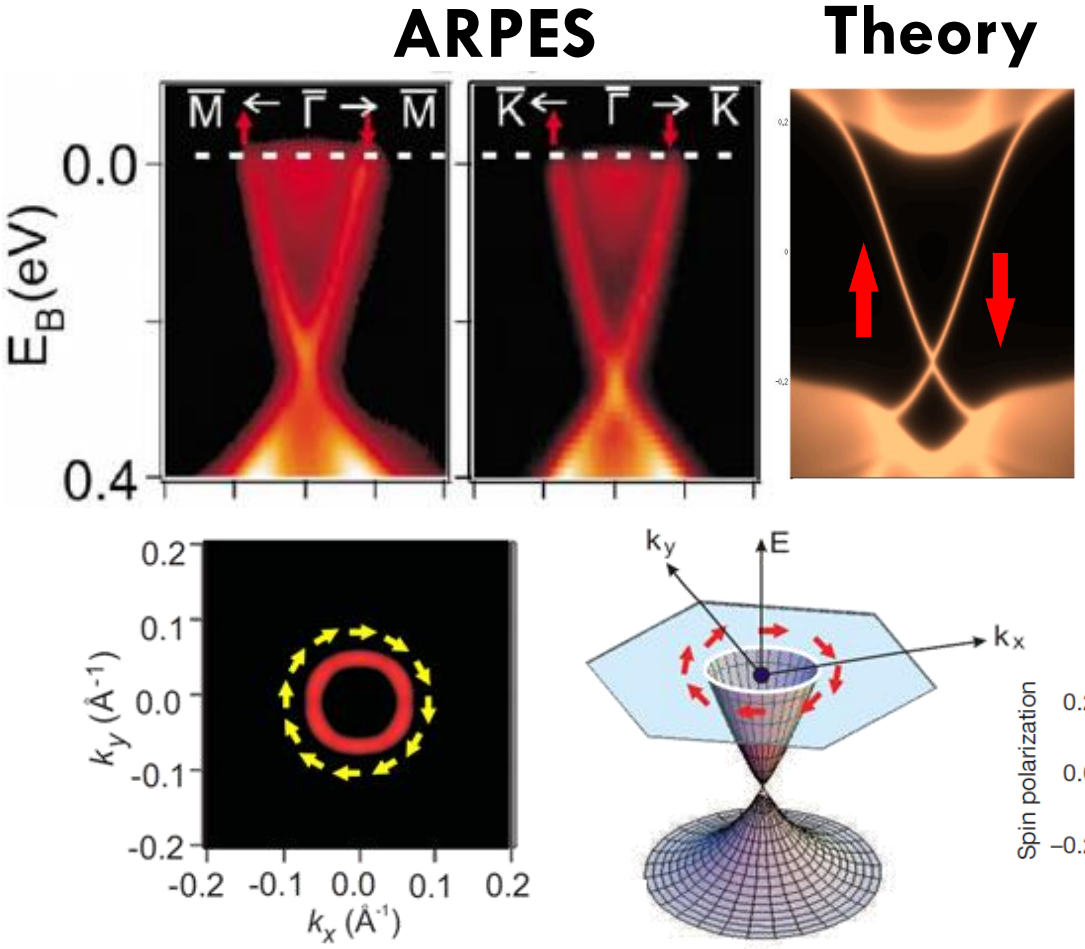


Sb_2Se_3	+ − + − + − + − + − + − −; +	(+)
Sb_2Te_3	+ − + − + + − + − + − − −+; −	(−)
Bi_2Se_3	+ − + − + − + − + − + − −+; −	(−)
Bi_2Te_3	+ − + − + − + + − + − − −+; −	(−)



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

Topological insulator (Bi_2Se_3)



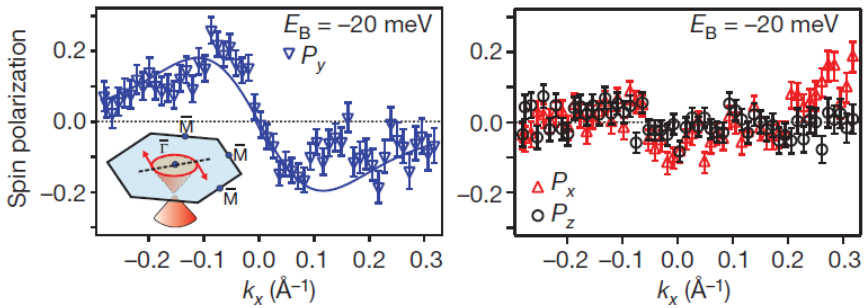
Bulk: insulating gap

topological Z_2 invariant

odd/even number surface states

Surface: gapless surface states

spin-momentum locked

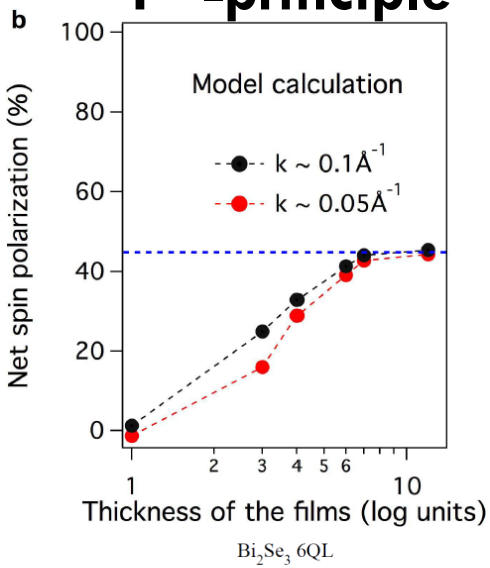


Y. Xia et al. Nature Physics **5**, 398 (2009)

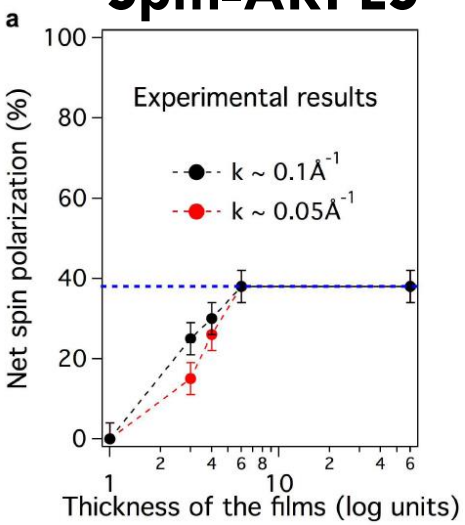
D. Hsieh et al. Nature **460**, 1101 (2009)

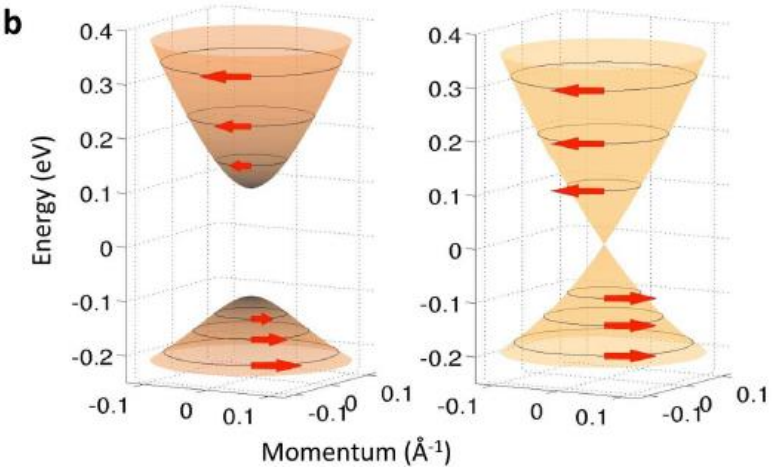
Topological insulator (Bi_2Se_3)

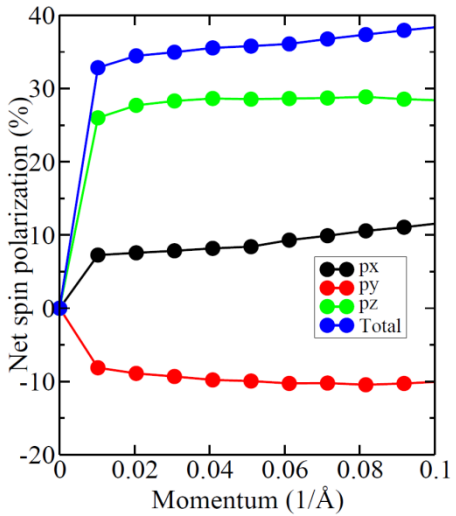
1st -principle

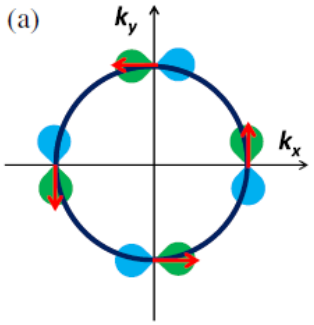


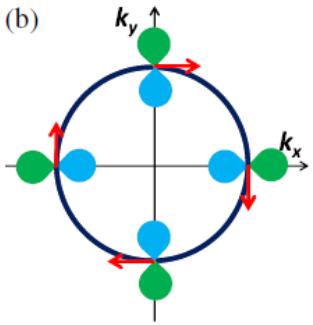
Spin-ARPES





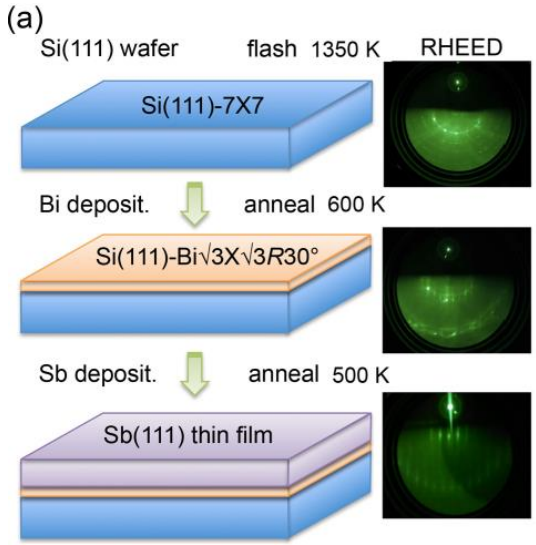


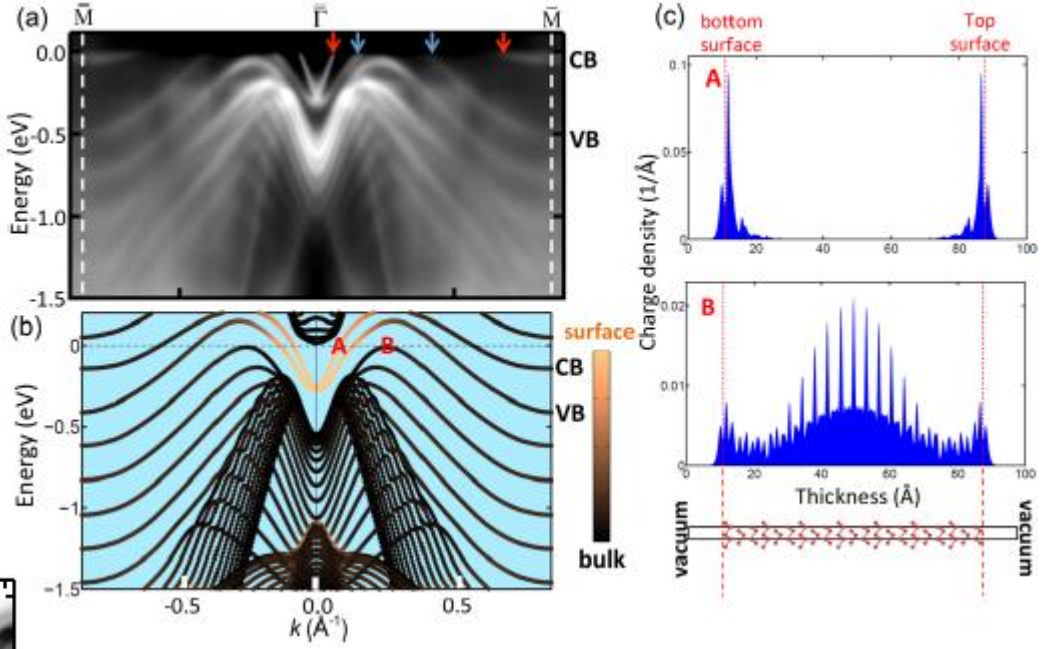


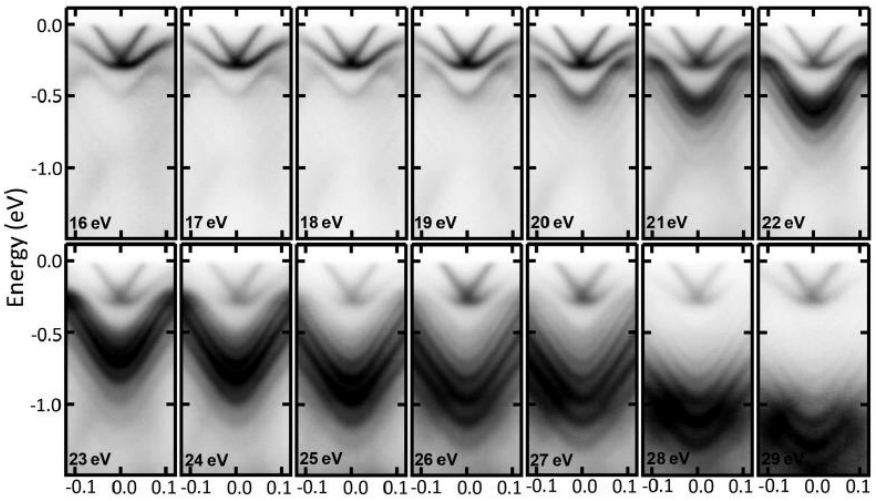


M. Neupane… **T.-R. Chang** et al., Nat. comm. **5**, 3841 (2014)

Topological insulator

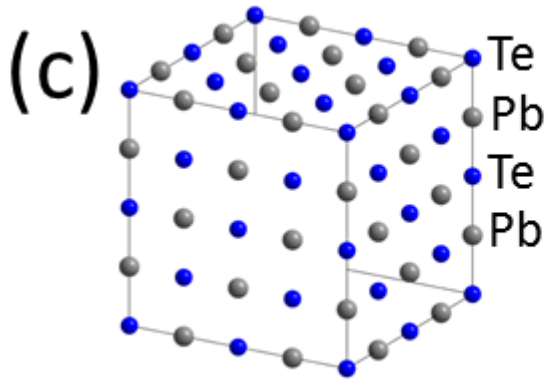


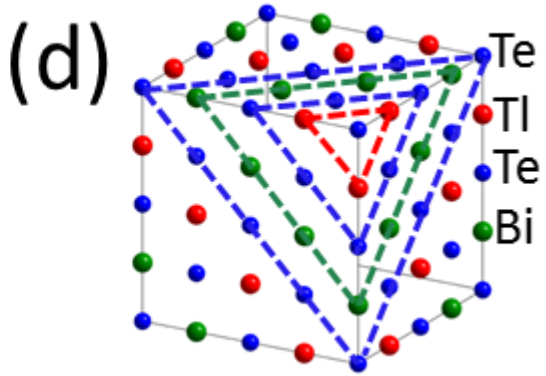


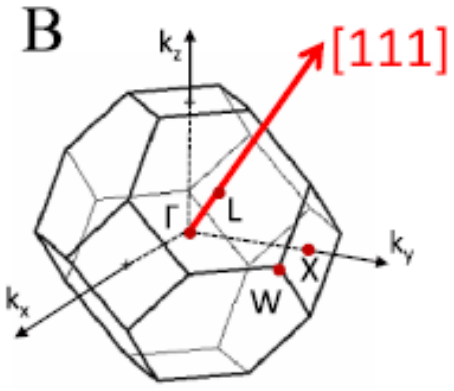


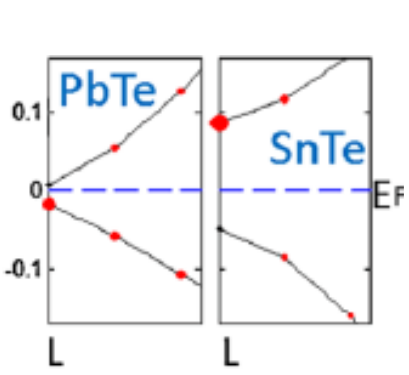
G. Bian, G. Xu, **T.-R. Chang** et al PRB **92,** 241401 (R) (2015)

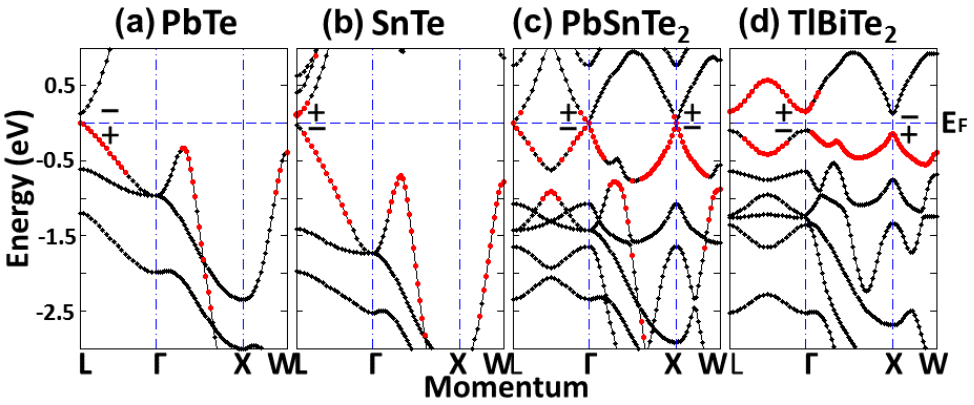
Topological phase transition

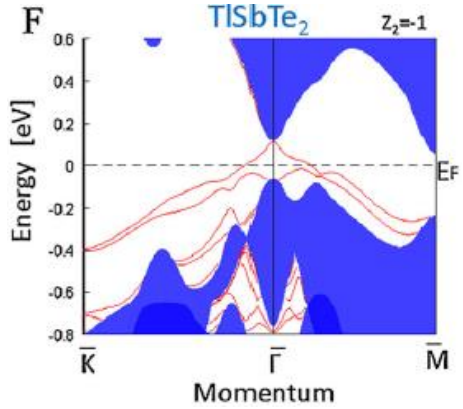








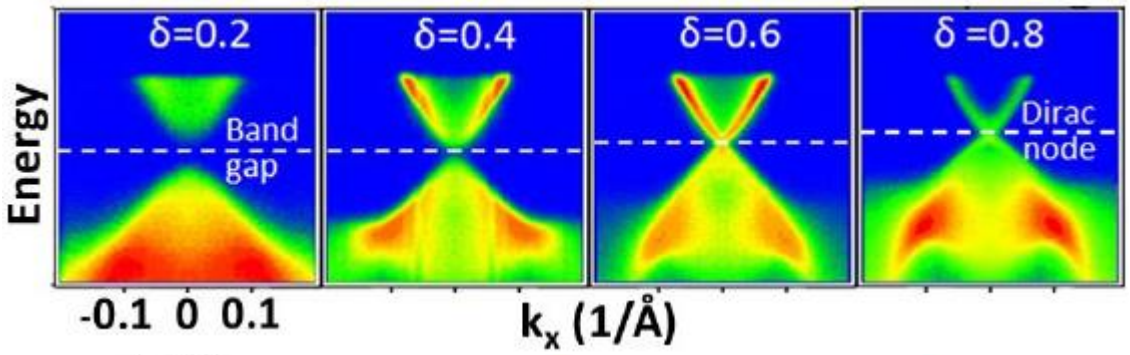


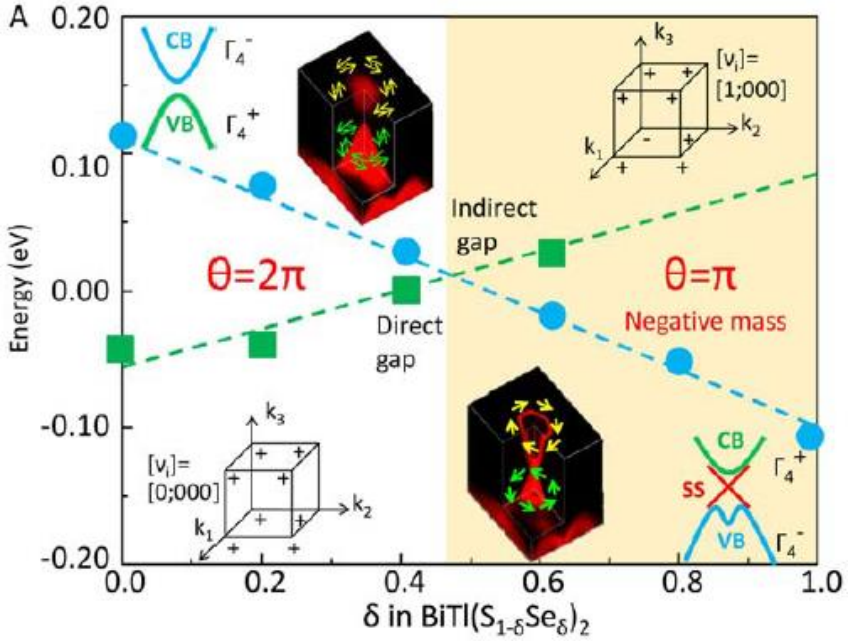


H. Lin et al., PRL **105**, 036404 (2010)

Topological phase transition

$TlBi(S_xSe_{1-x})_2$





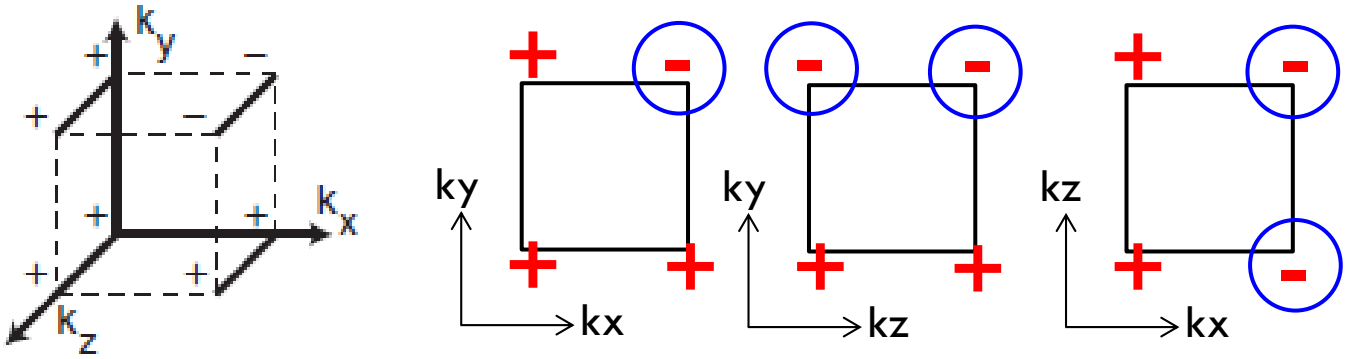
Su-Yang Xu et al., Science **332**, 560 (2011)

Weak topological insulator

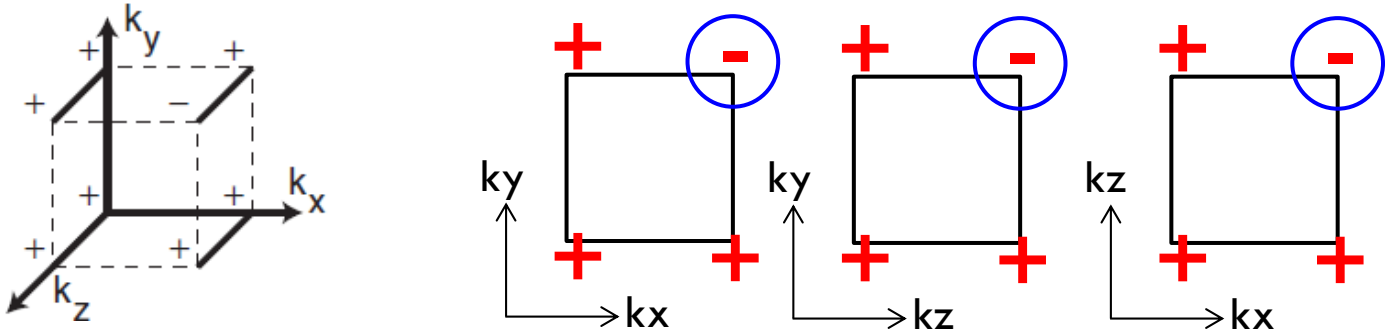
$$3D: (\upsilon_0; \underbrace{\upsilon_1, \upsilon_2, \upsilon_3}_{\text{weak index}})$$

strong index

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

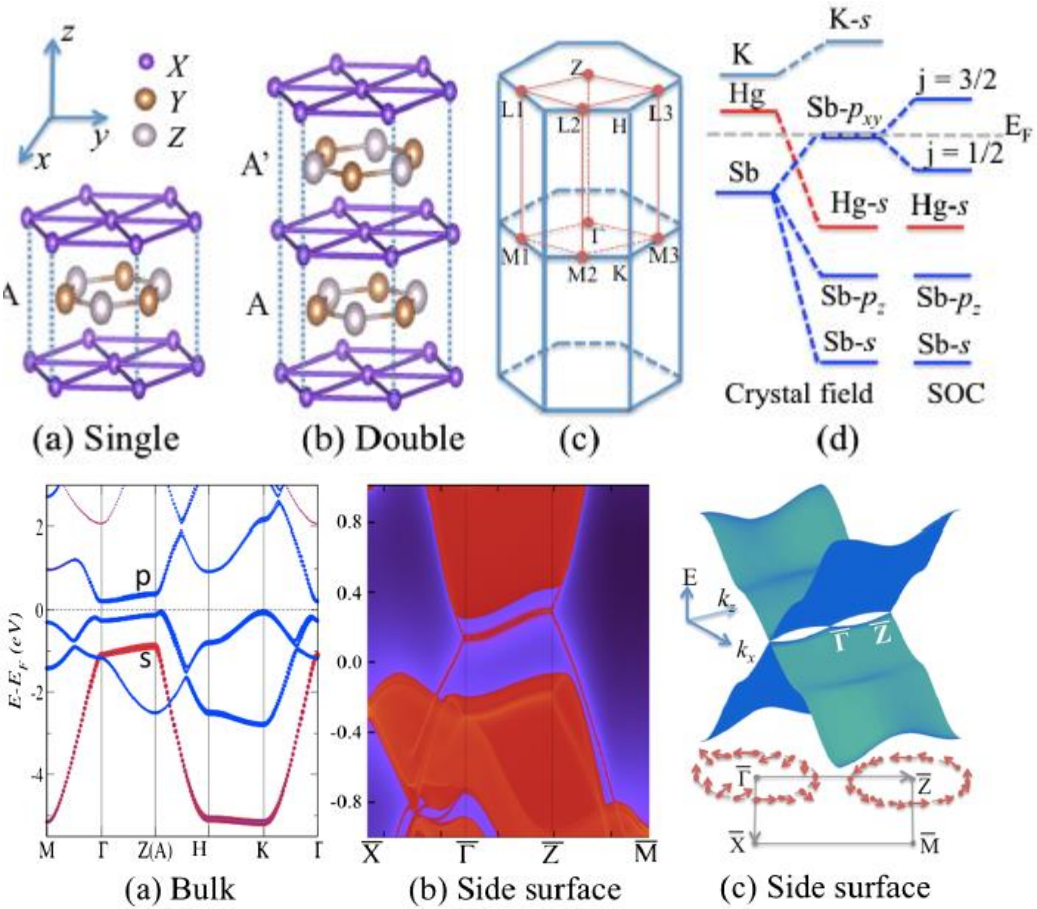


Strong topological insulator $Z_2 = (1; 1,1,1)$

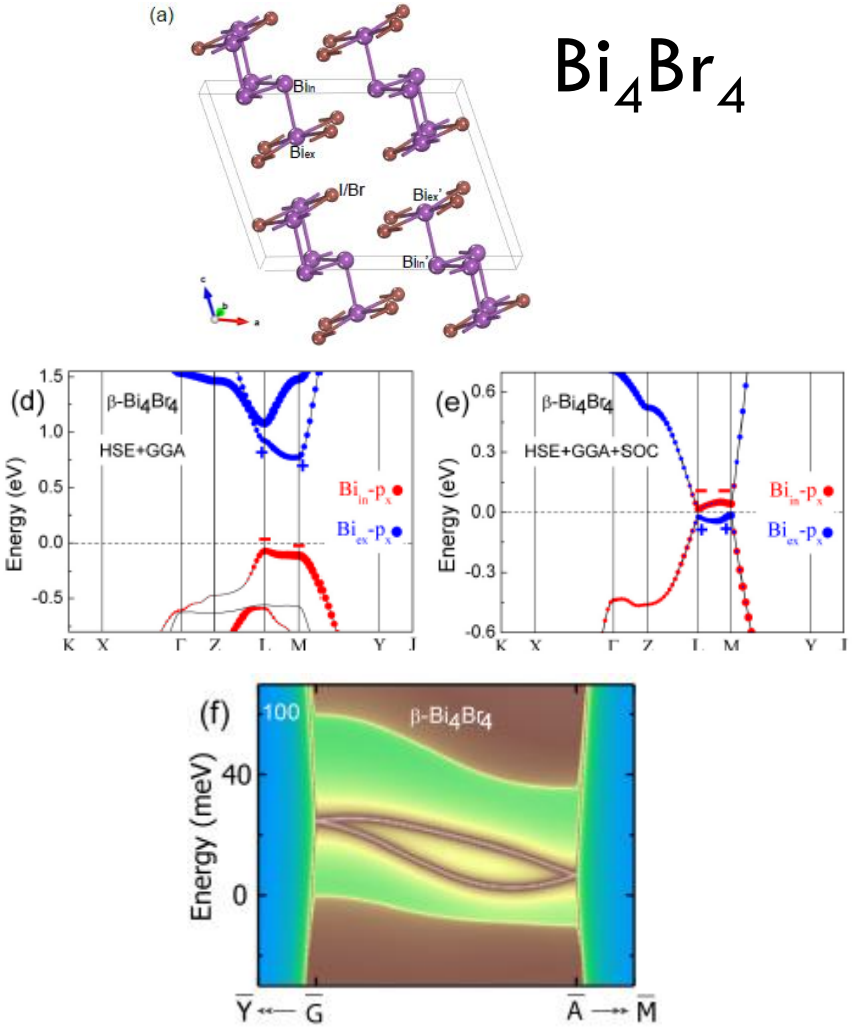


Weak topological insulator

KHgSb



Bi_4Br_4



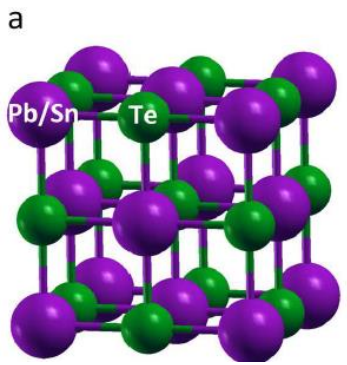
B. Yan, PRL **109**, 116406 (2012)

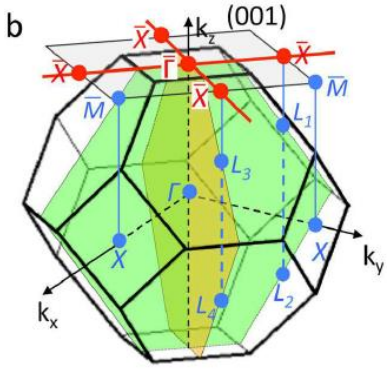
C.-C. Liu et al., PRL **116**, 066801 (2016)

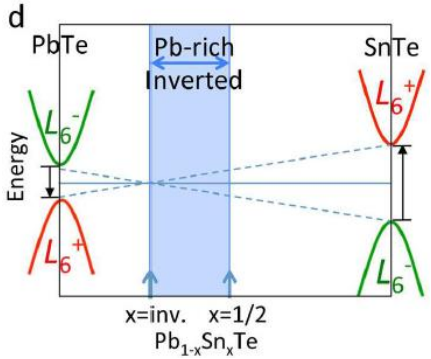
Topological crystalline insulator

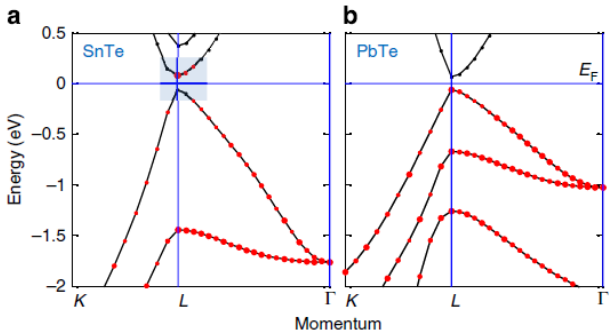
SnTe and PbTe

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







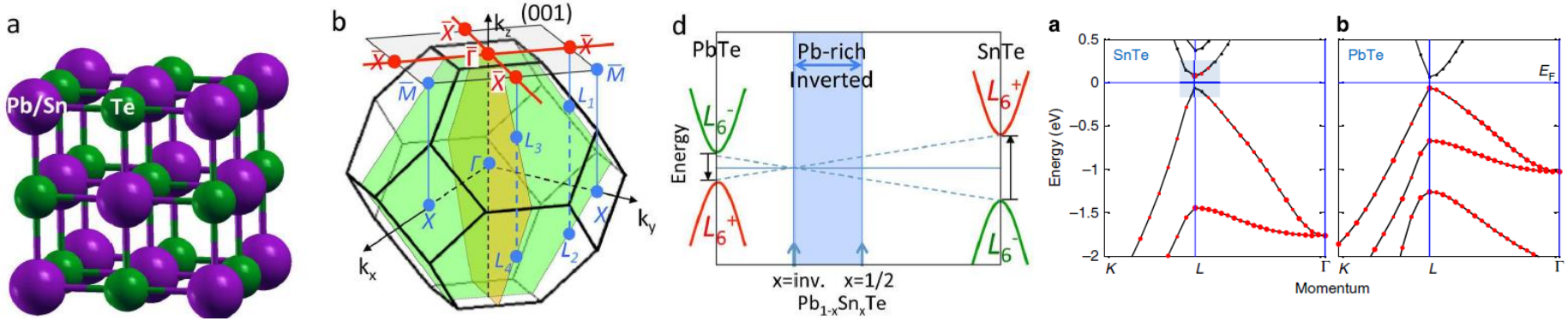


$Z_2 = (0; 0,0,0)$ Is SnTe (PbTe) a normal band insulator ?

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 => mirror eigenvalue $\mathrm{M} = \pm i$

$\mathrm{M} = \pm i$ => Chern number $n_{\pm i}$

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

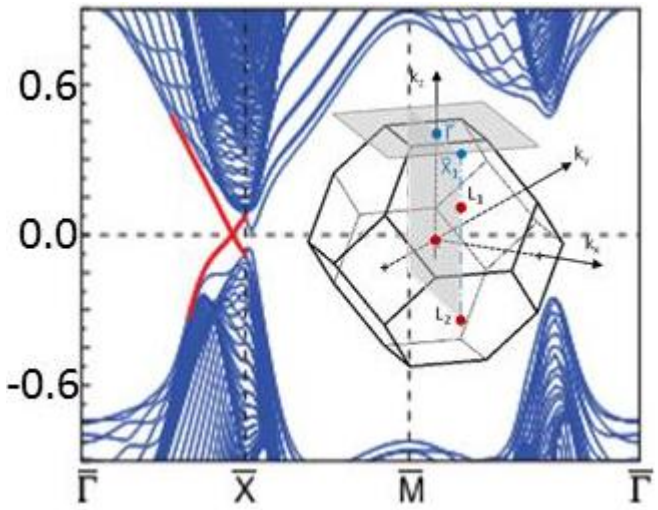
A non-zero mirror Chern number defines a topological crystalline insulator with mirror symmetry.

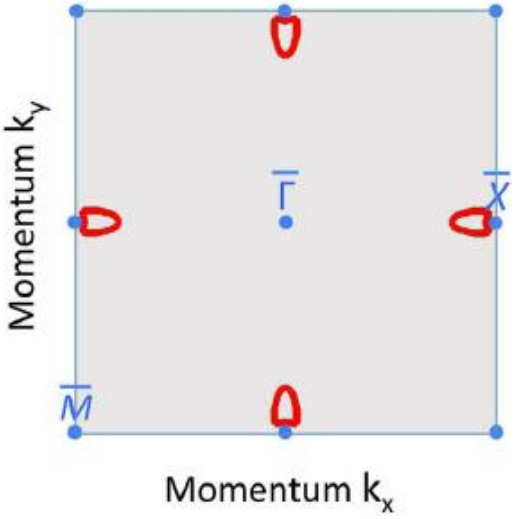
Topological crystalline insulator

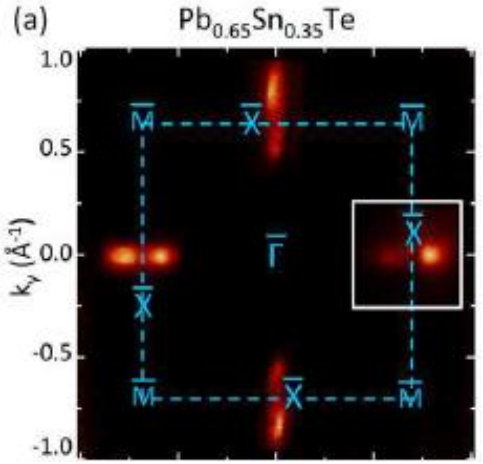
S. Y. Xu, Nat. comm **3**, 1192 (2012)

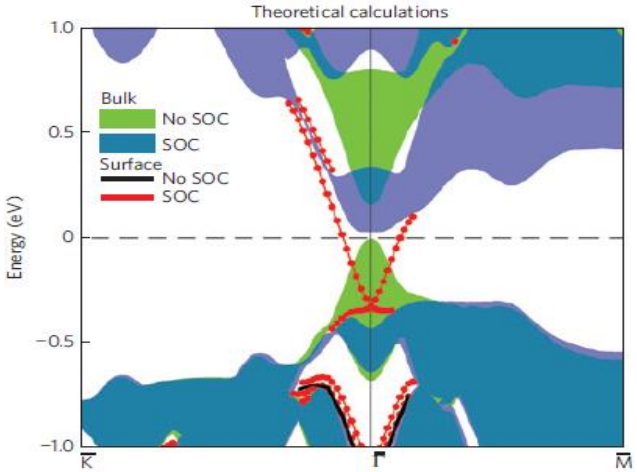
DFT

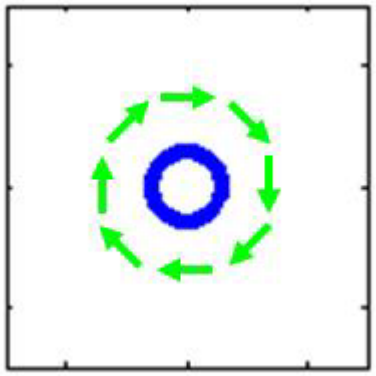
ARPES

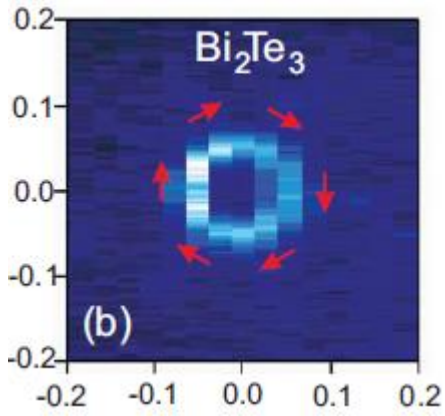








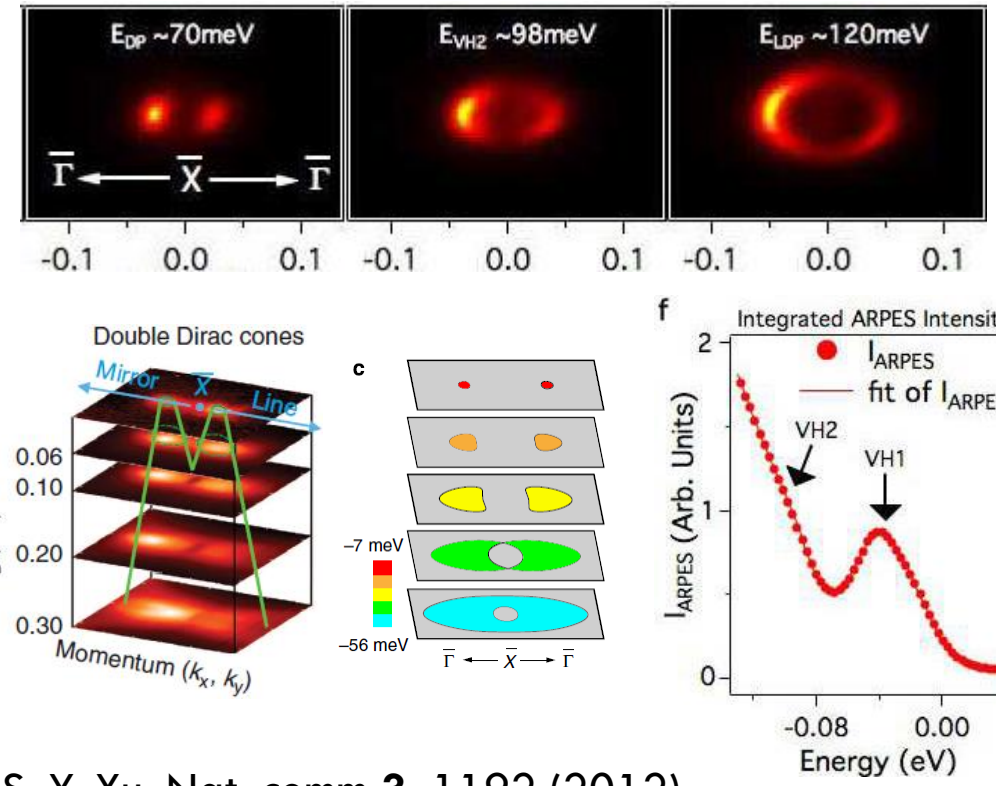




Lifshitz transition

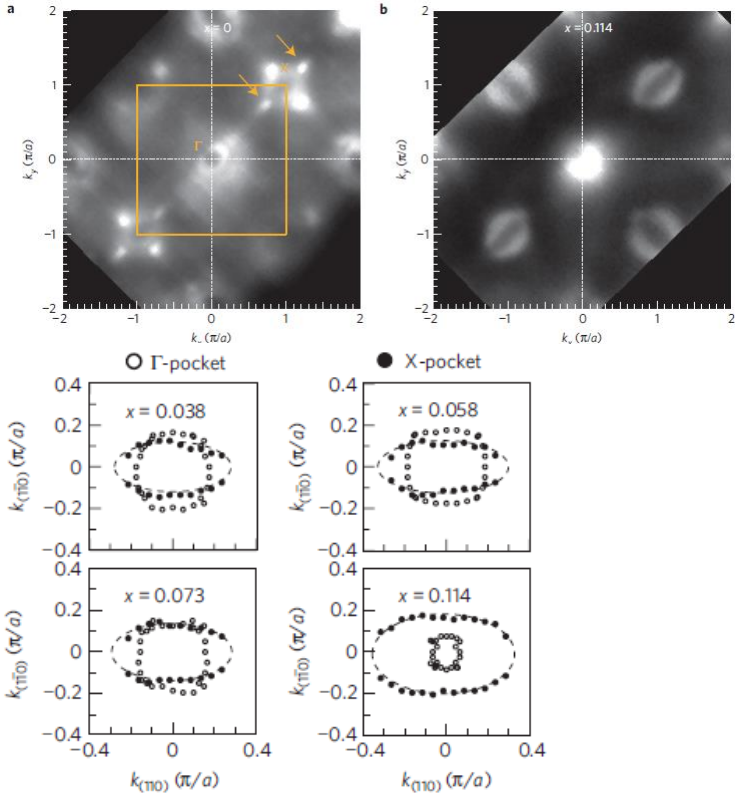
What is Lifshitz transition ?

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



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

$Ba(Fe_{1-x}Co_x)_2As_2$

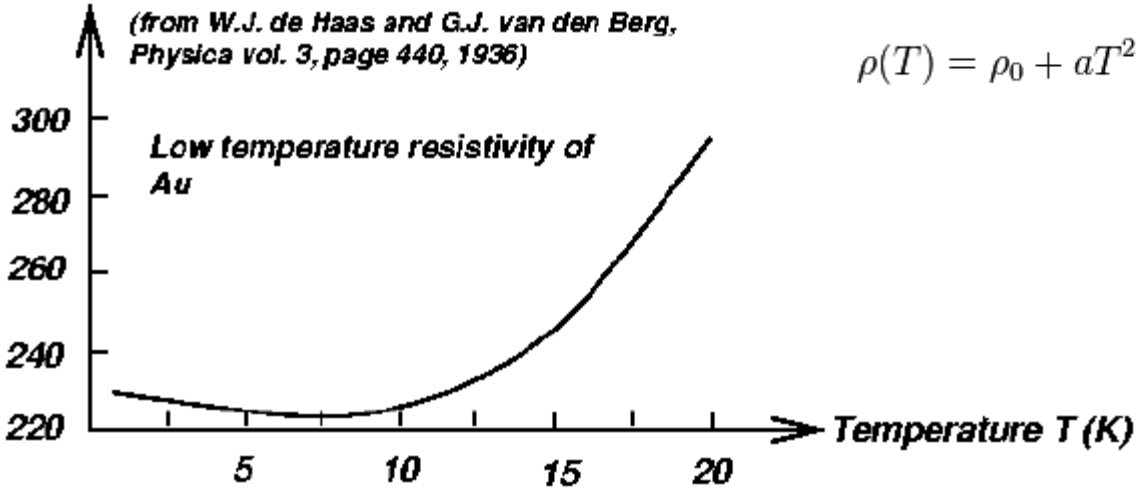


C. Liu, Nat. phys. **6**, 419 (2010)

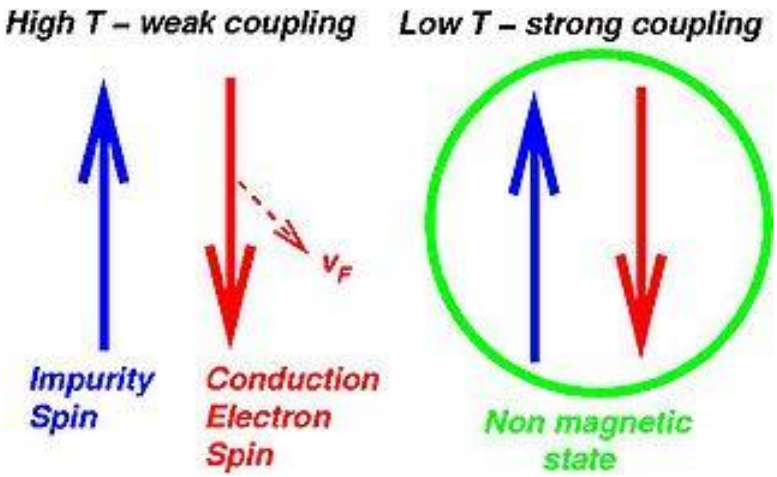
Topological invariant number

	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:	$Z_2 = (0; 0,0,0)$	$n_M \neq 0$	even
Normal band insulator:	$Z_2 = (0; 0,0,0)$	$n_M = 0$	none

Topological Kondo insulator



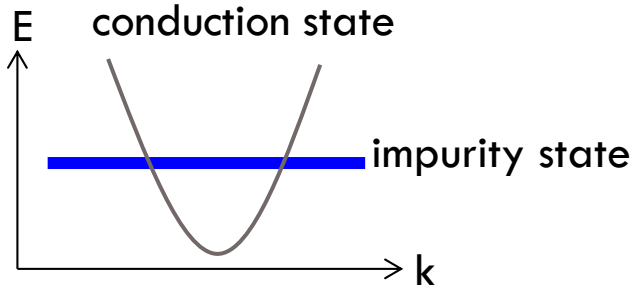
$$\rho(T) = \rho_0 + aT^2 + c_m \ln \frac{\mu}{T} + bT^5,$$

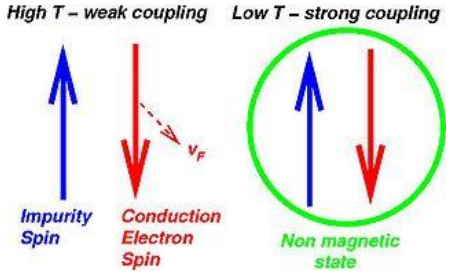


wiki: Kondo effect

Topological Kondo insulator

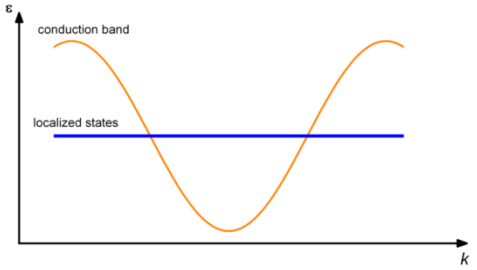
Kondo effect



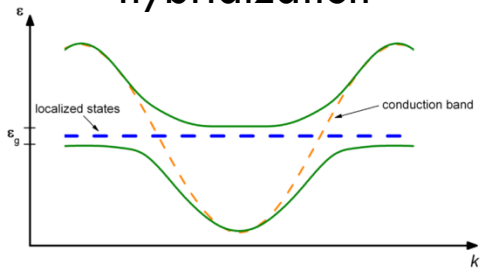


Kondo insulator

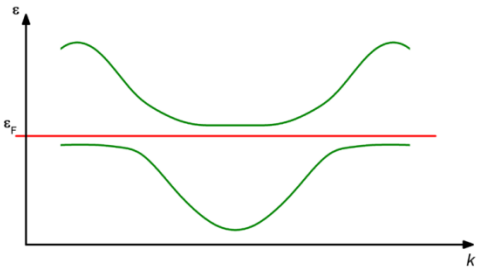
T > Tc



hybridization

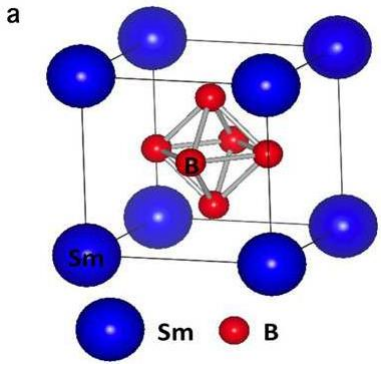


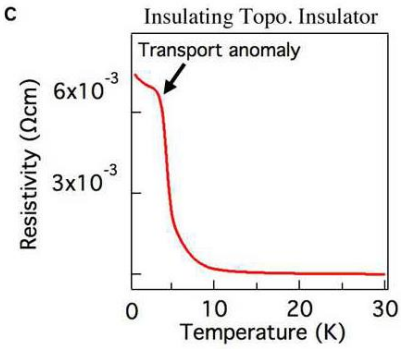
T < Tc

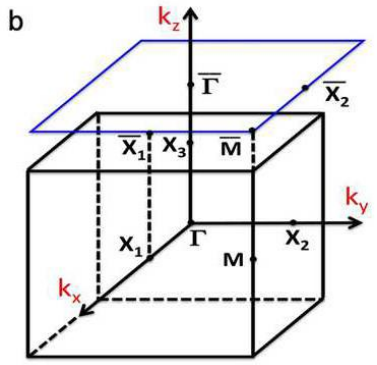


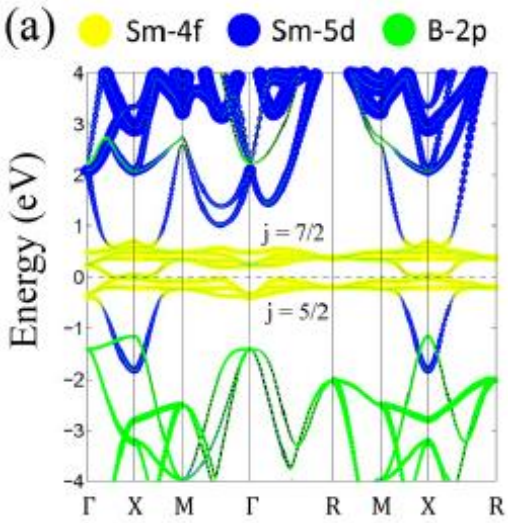
wiki: Kondo insulator

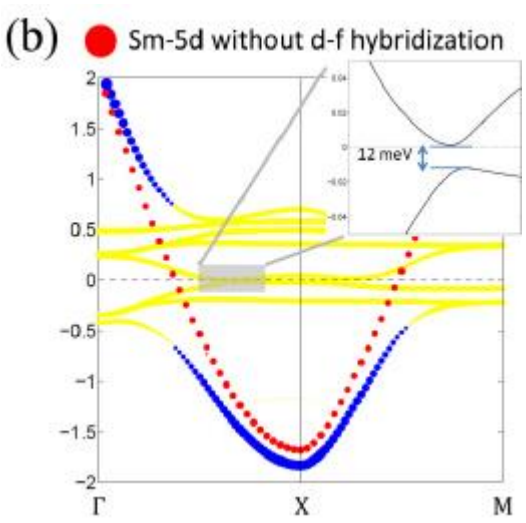
Topological Kondo insulator

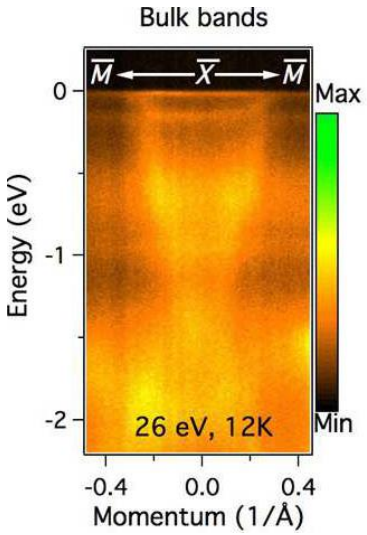


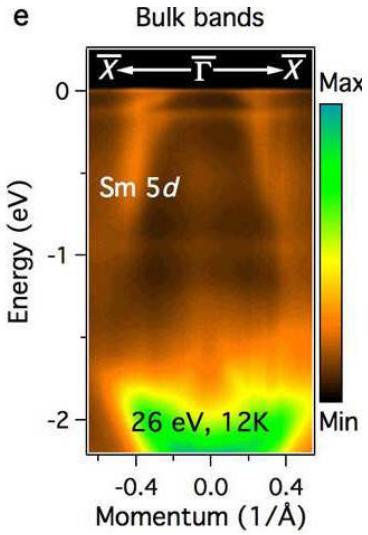








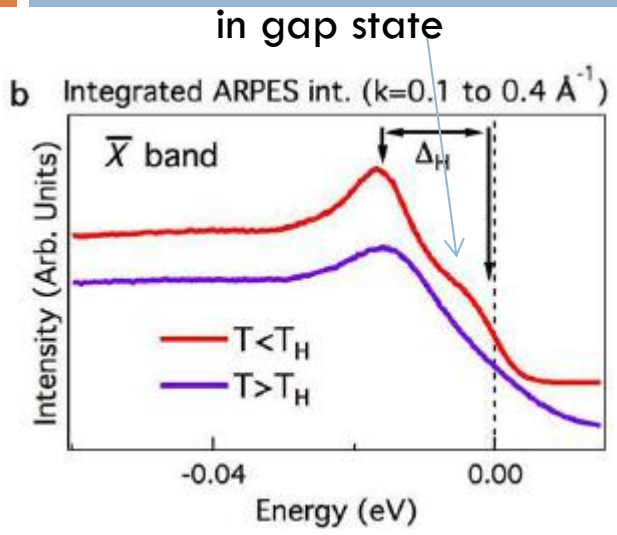


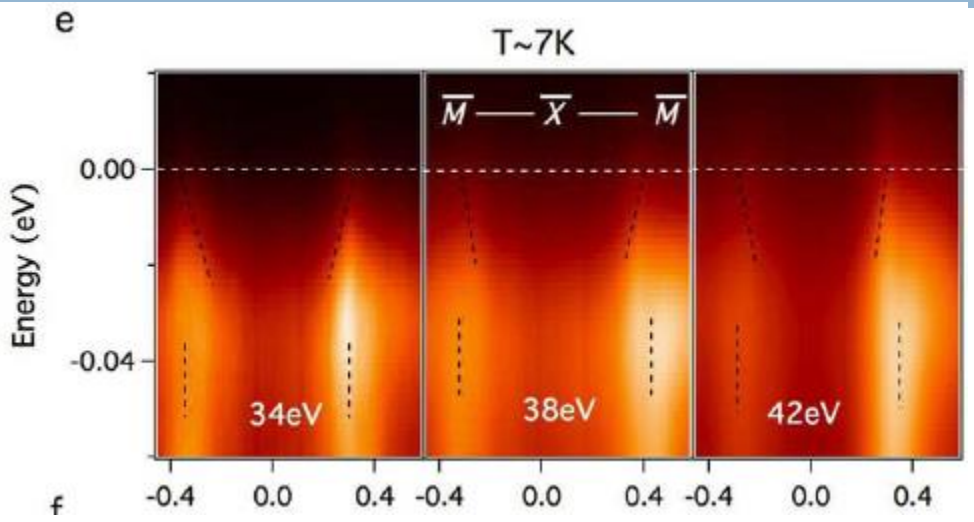


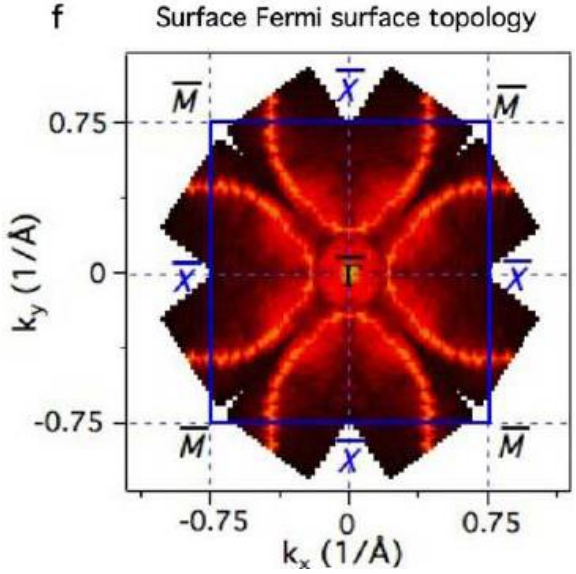
M. Neupane… **T.-R. Chang** et al, Nat. comm. **4**, 2991 (2013)

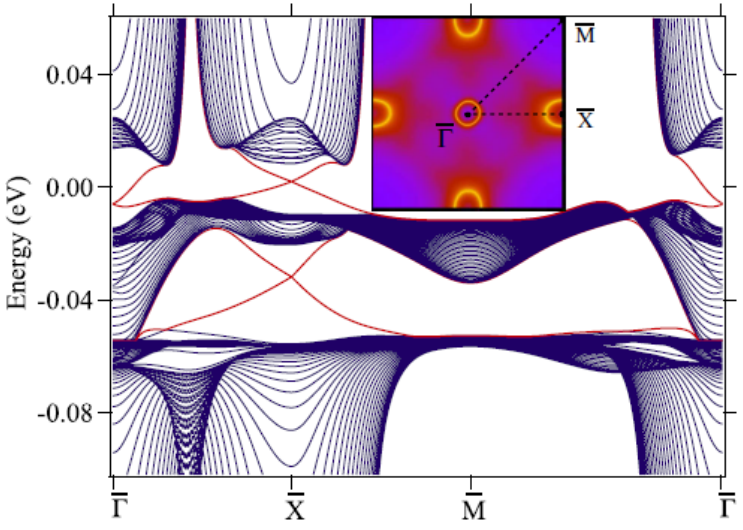
T. R. Chang et al, PRB **91**, 155151 (2015)

Topological Kondo insulator



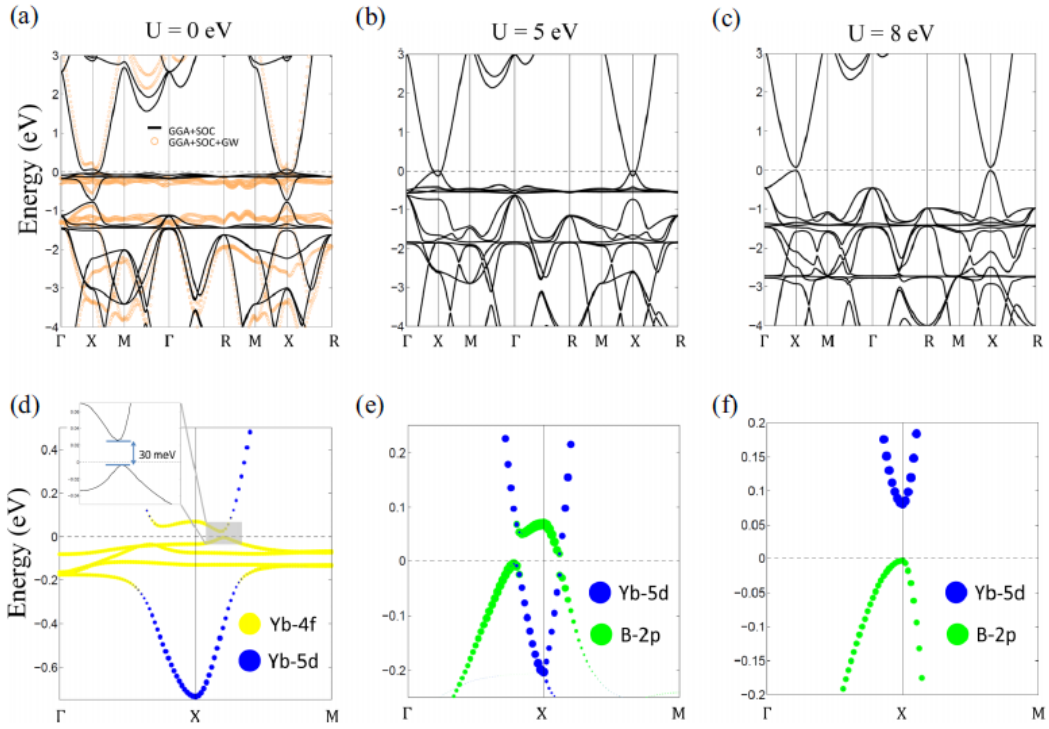


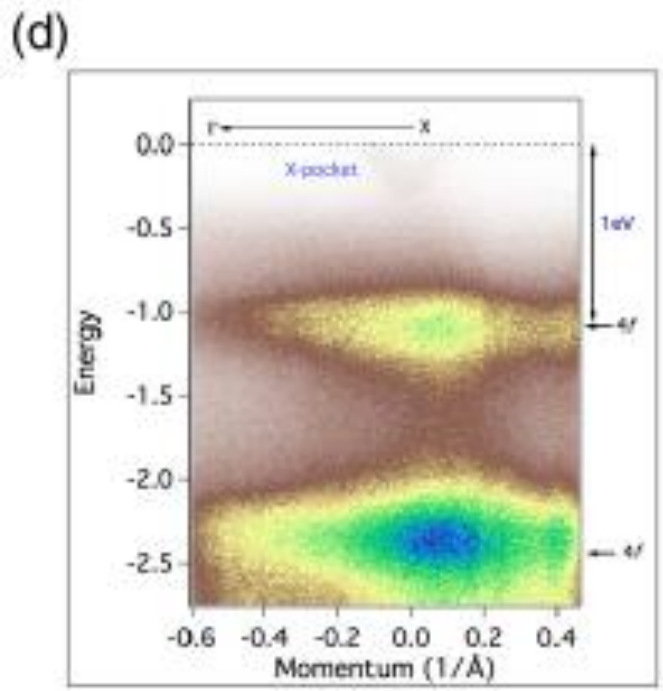




M. Neupane… **T.-R. Chang** et al, Nat. comm. **4**, 2991 (2013)
L. Feng et al, PRL **110**, 096401 (2013)

Topological Kondo insulator





M. Neupane… **T.-R. Chang** et al, PRL **114**, 016403 (2015)
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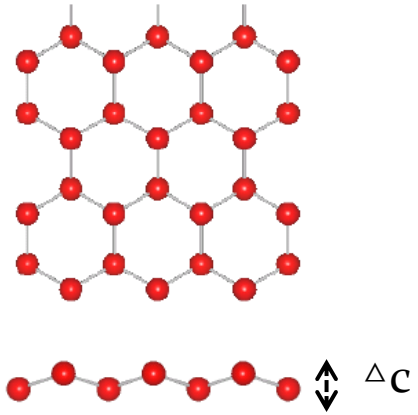
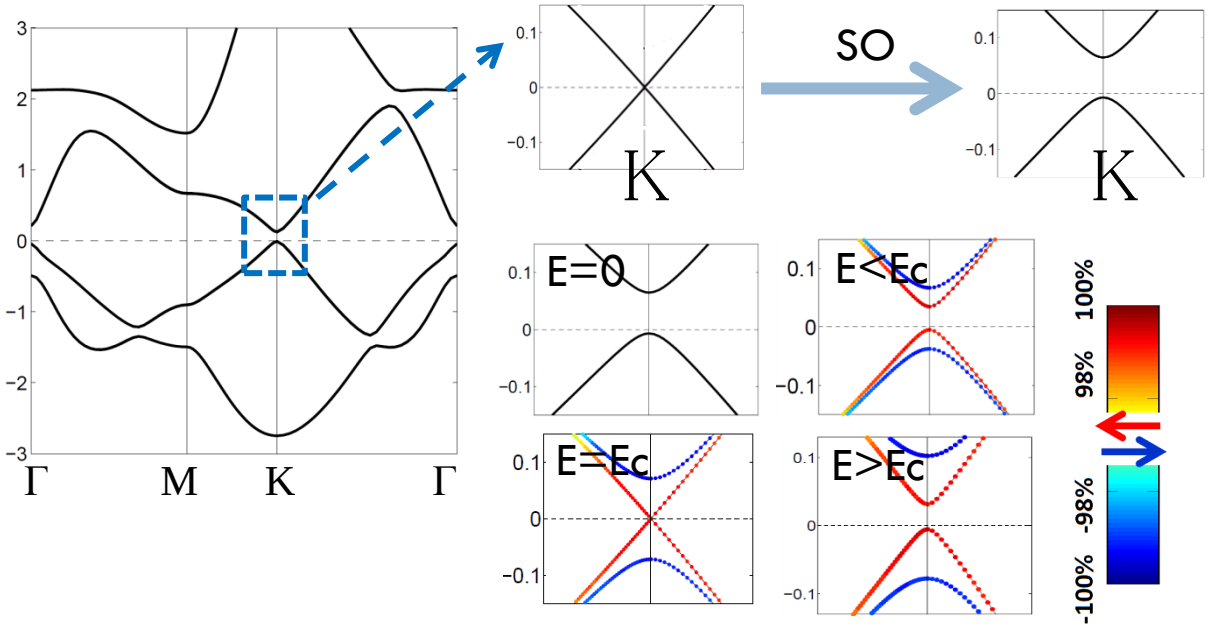
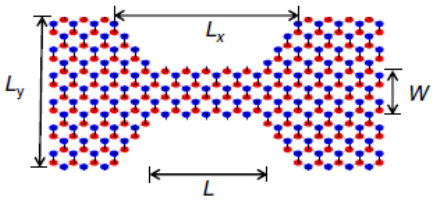
Possible applications

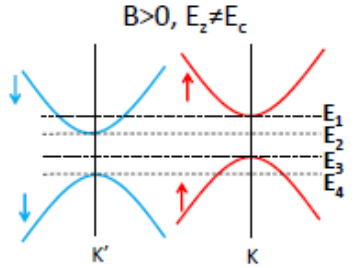
Silicene family

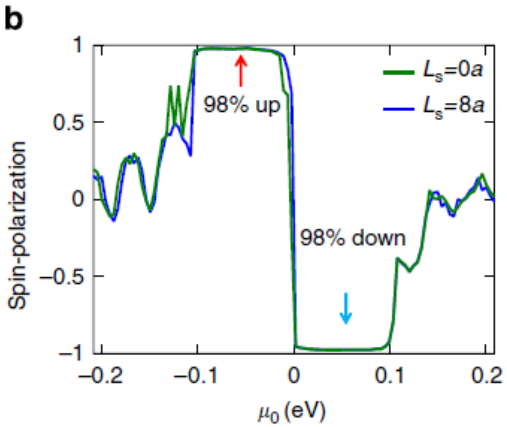


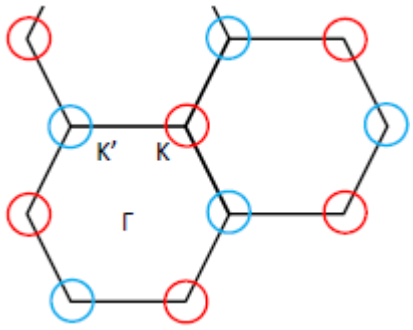


spin filter









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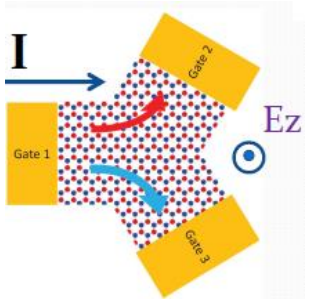
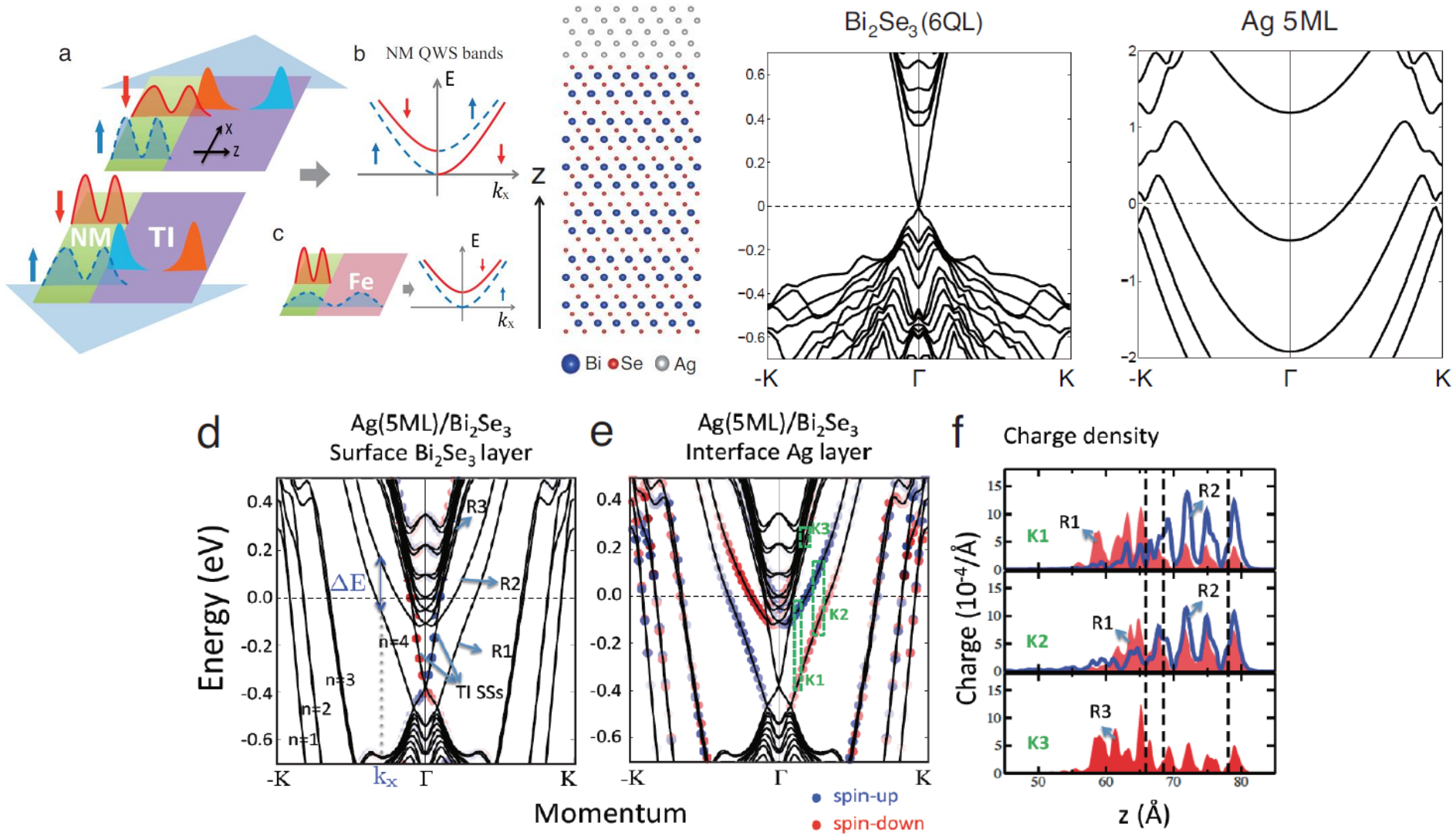
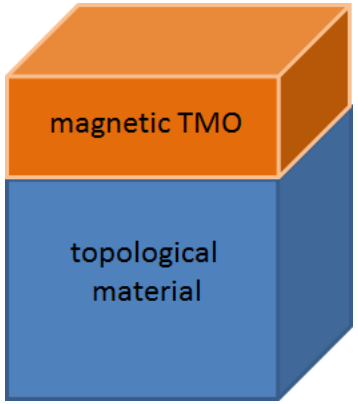


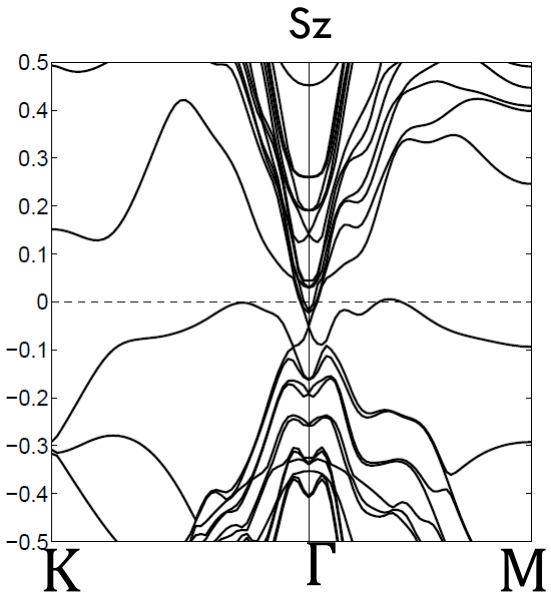
Tsai… **T.-R. Chang** et al. Nature Commun. **4,** 1500 (2013)

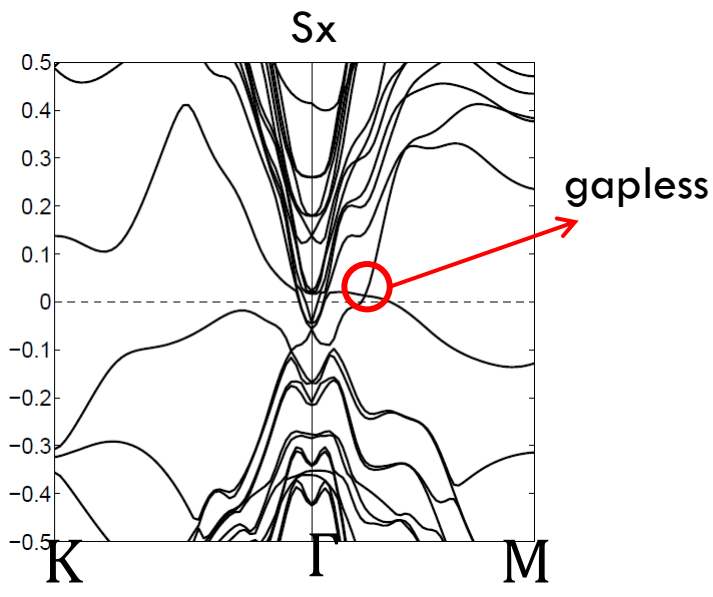
Possible applications

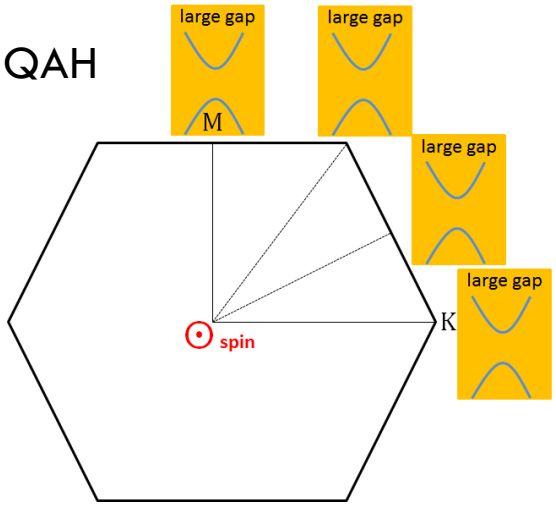


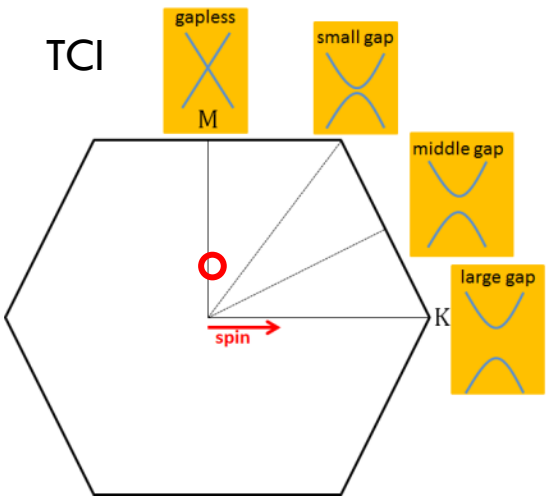
Possible applications



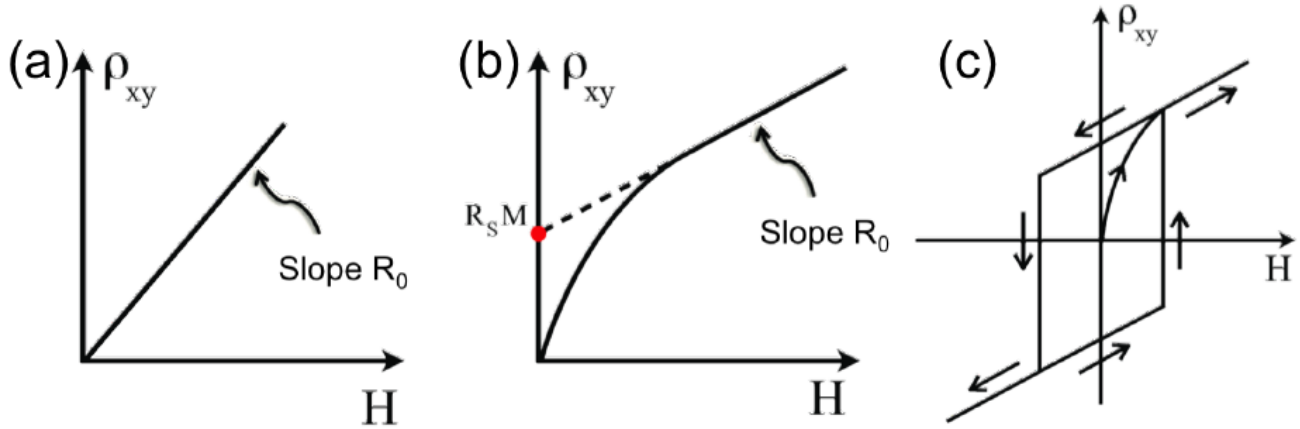








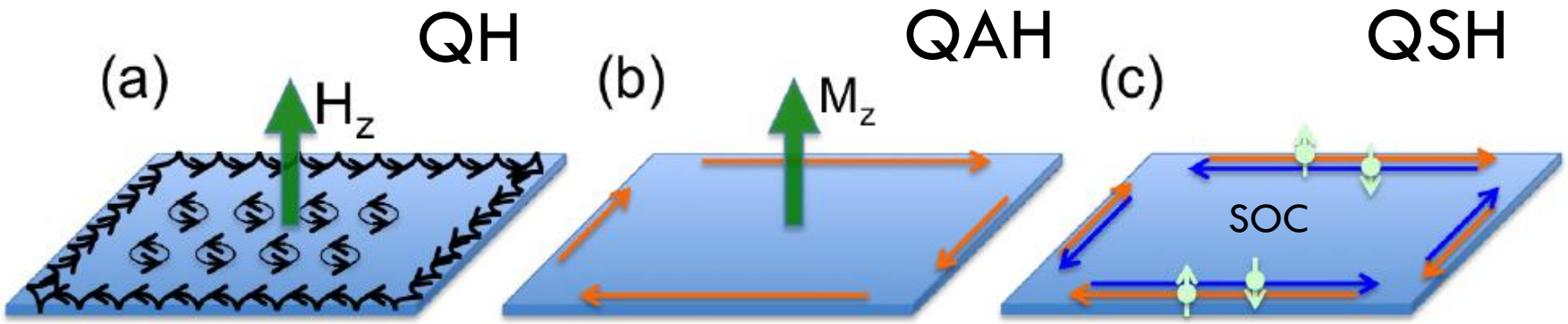
Anomalous Hall effect



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

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

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

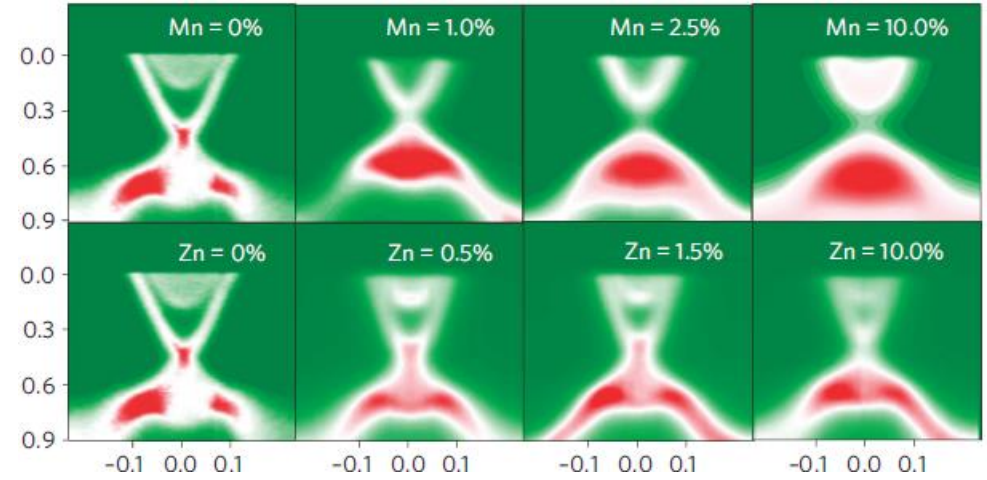
4. The occupied bands must carry a non-zero Chern number

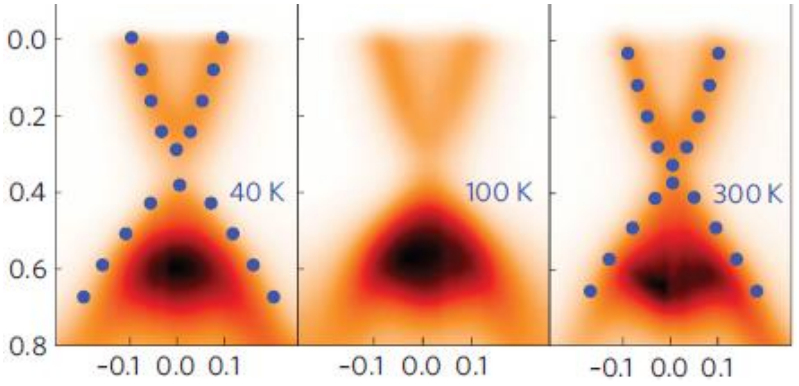
Quantum anomalous Hall effect

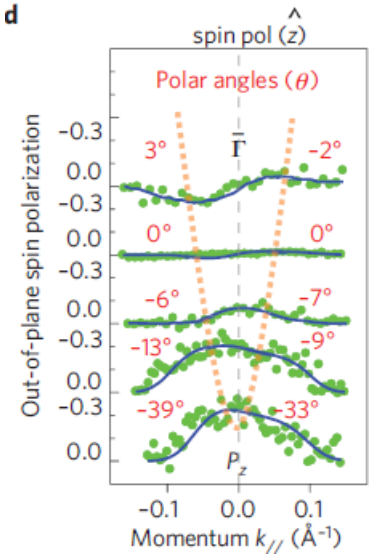
2D topological insulator might be an answer

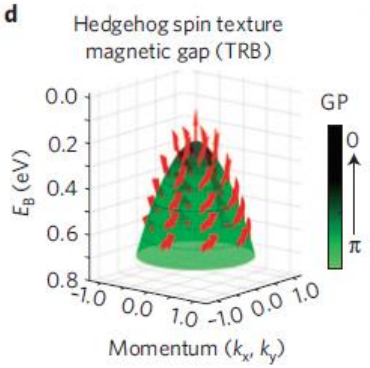
- To sandwich a TI thin lm with FM insulators. The FM proximity effect will open up a gap for the Dirac surface states on both surfaces of the TI, which gives rise to the QAHE.
- To dope the magnetic ions into the TI thin lm and make it a FM semiconductor. The QAHE can be obtained by proper control of 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 lm with interface band inversion in EuO/GdN or CdO/EuO, etc.

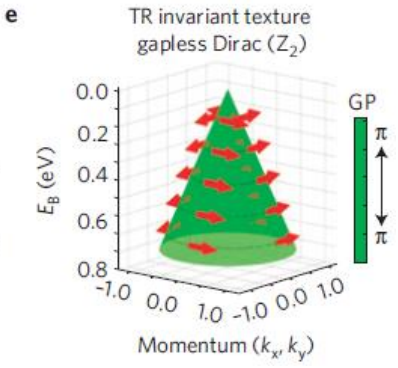
Quantum anomalous Hall effect

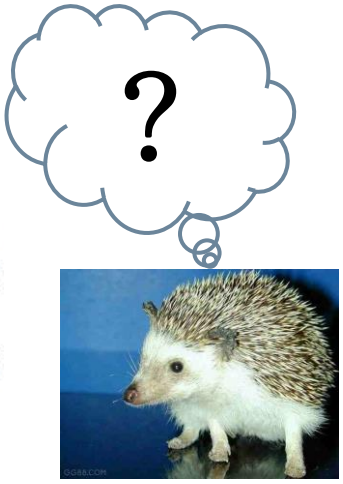








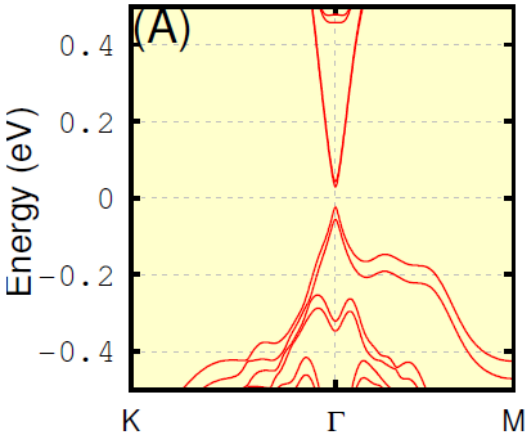


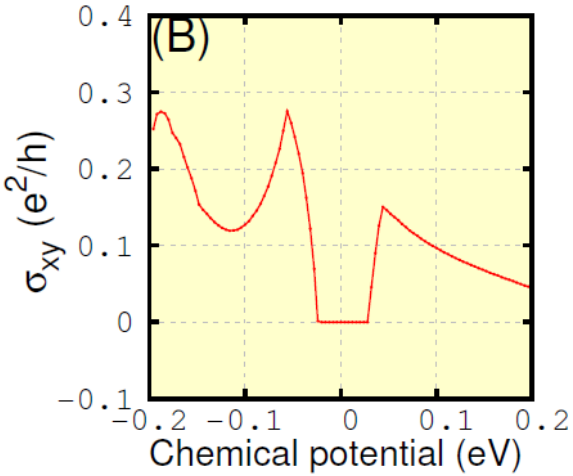


Su-Yang Xu… **T.-R. Chang** et al., Nature phys. **8**, 616 (2012)

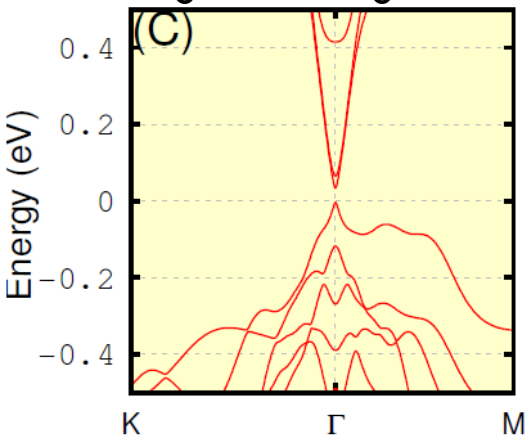
Quantum anomalous Hall effect

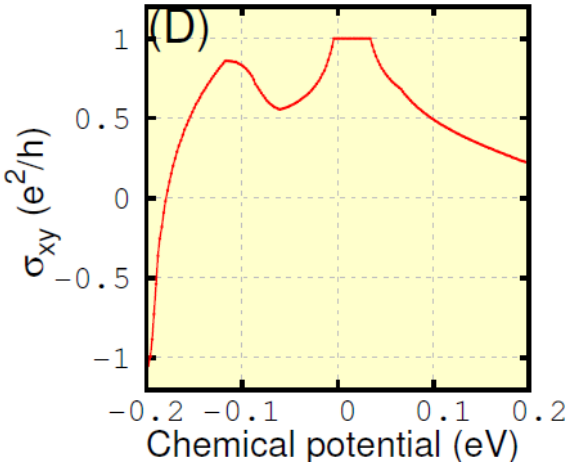
Small exchange field



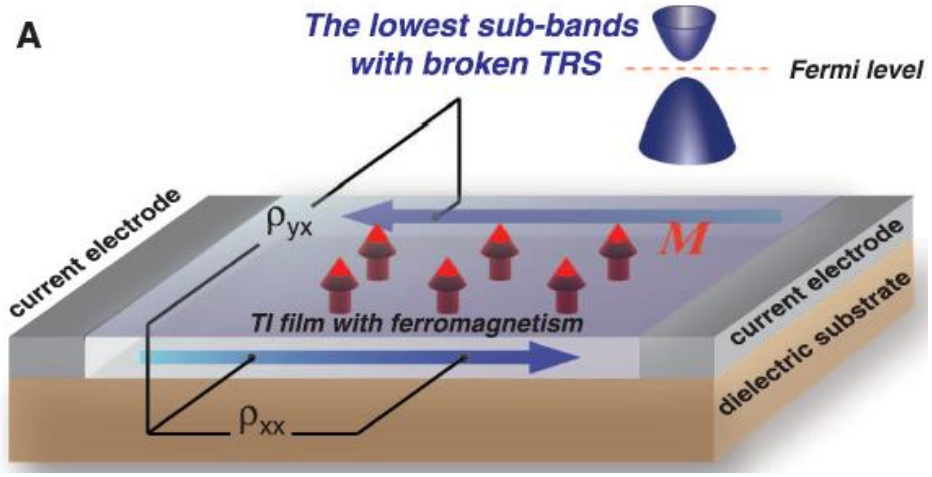


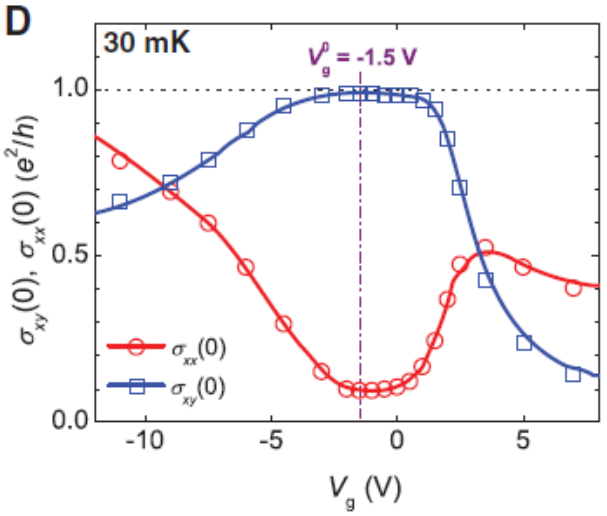
Large exchange field





Quantum anomalous Hall effect





C.-Z. Chang *et al.*, *Science* **340,** 167–170 (2013)

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

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

$$= -\frac{e^2}{2\pi h}\int_{BZ} d^2\mathbf{k}\Omega_z(\mathbf{k}),$$

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

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