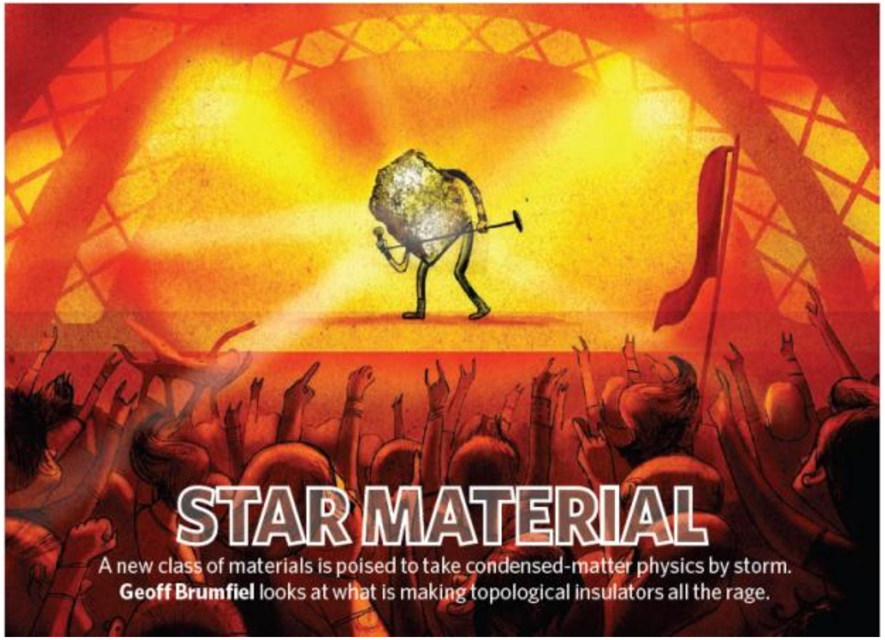
2010 7/22-24
Matsuda Lab. Seminar

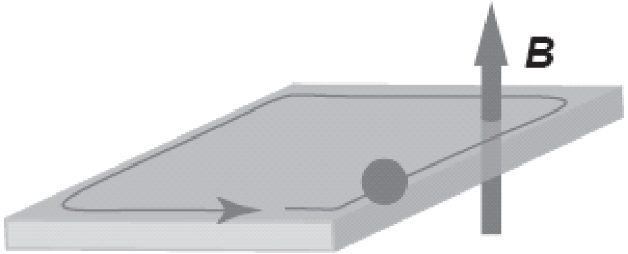
Introduction of topological insulators



Kyoto University   Sho Tonegawa

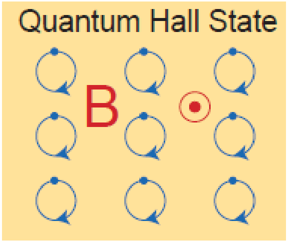
Quantum Hall effect(QHE)

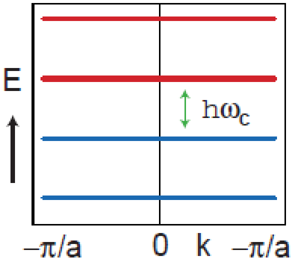
- Integer Quantum Hall effect (IQHE)



Strong magnetic field

⇒ Landau Quantization

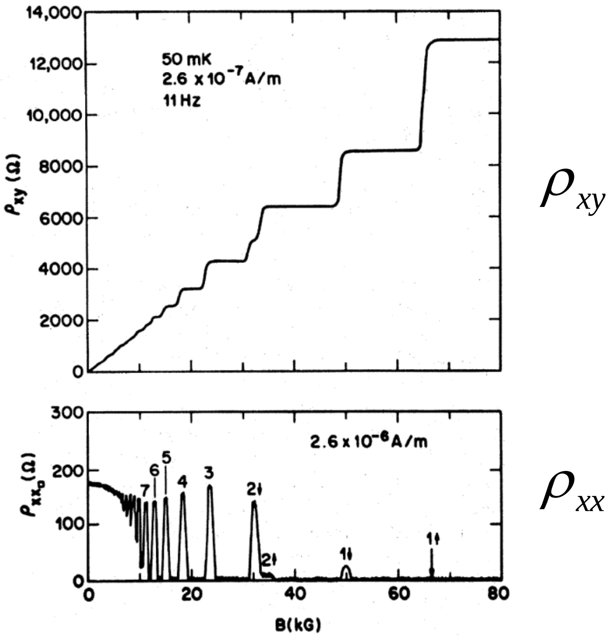




Quantization of Hall conductance

$$\sigma_{xy} = n\frac{e^2}{h} \qquad n: \text{integer}$$

GaAs-AlGaAs ヘテロ接合



M.A.Paalanen *et al.*, PRB **25**,5566(1982)

Quantization is incredibly precise.(～10^{-8} order)

$$R_K = \frac{h}{e^2} = 25812.807\Omega$$

Protected by **topological number** (Chern number)

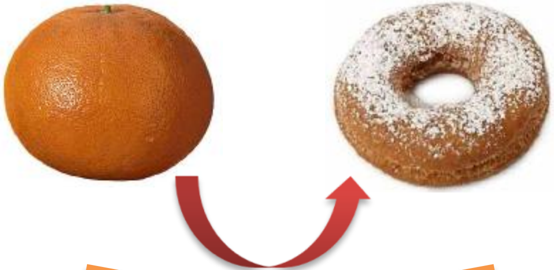
$$n = \cdots -2, -1, 0, 1, 2, \cdots$$

Discrete invariant can't be changed continuously.

Strong against non-magnetic impurity.

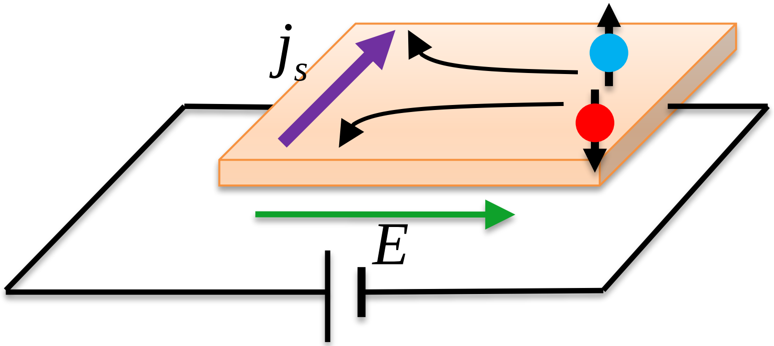
Topologically protected

$n_{\text{hole}} = 0$ $n_{\text{hole}} = 1$



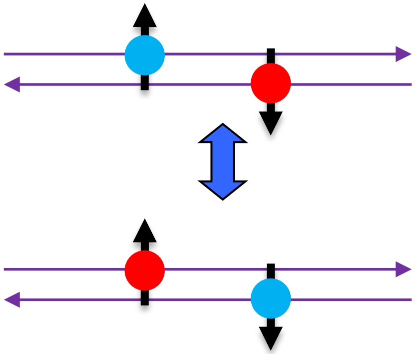
~~Change continuously~~

Spin Hall effect(SHE)



$j_s \propto s \times E \qquad s: \text{spin}$

Spin current ***j$_s$*** is induced by spin-orbit interaction.



j$_s$: even under time-reversal

Nonzero in nonmagnetic materials
Magnetic field is not needed.

- **Spin-orbit coupling**
  (spin-dependent) effective magnetic field
- **Spin current** ***j$_s$***

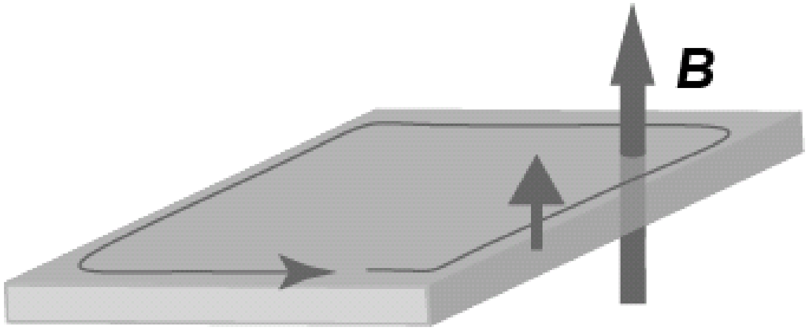
$$\sigma_{xy}^{\text{charge}} = \sigma_{xy,\uparrow} + \sigma_{xy,\downarrow} = 0 \Rightarrow \text{Net charge current} = 0$$

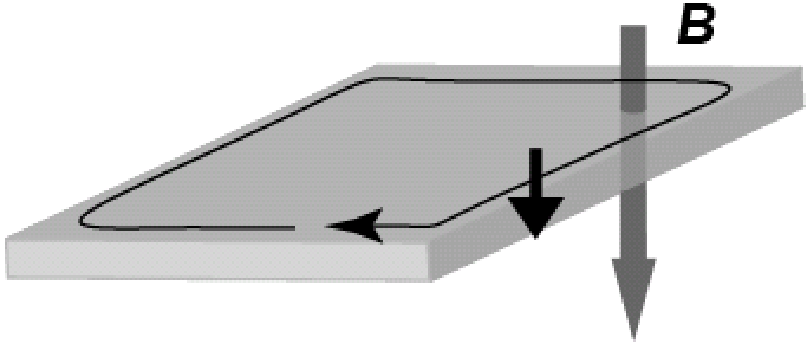
$$\sigma_{xy}^{\text{spin}} = \sigma_{xy,\uparrow} - \sigma_{xy,\downarrow} = 2\sigma_{xy,\uparrow}$$

Quantum Spin Hall effect (QSH)

- **bulk = gapped (insulator)**
- **gapless edge states -- carry spin current**

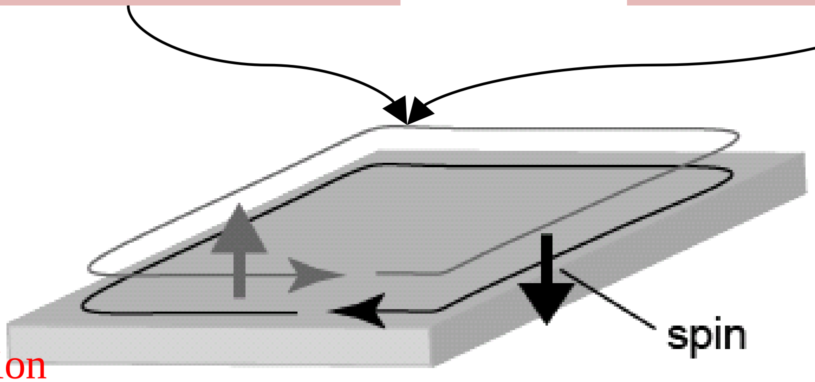
Quantum spin Hall state ≈ Quantum Hall state × 2





$\sigma_{xy} = \dfrac{e^2}{h}$ for up spin

$\sigma_{xy} = -\dfrac{e^2}{h}$ for down spin



When S_z is conerved

$$\sigma_{xy}^{\text{charge}} = \sigma_{xy,\uparrow} + \sigma_{xy,\downarrow} = 0$$

$$\sigma_{xy}^{\text{spin}} = \sigma_{xy,\uparrow} - \sigma_{xy,\downarrow} = \underline{\underline{2\sigma_{xy,\uparrow}}}$$

Quantization

Zero magnetic field

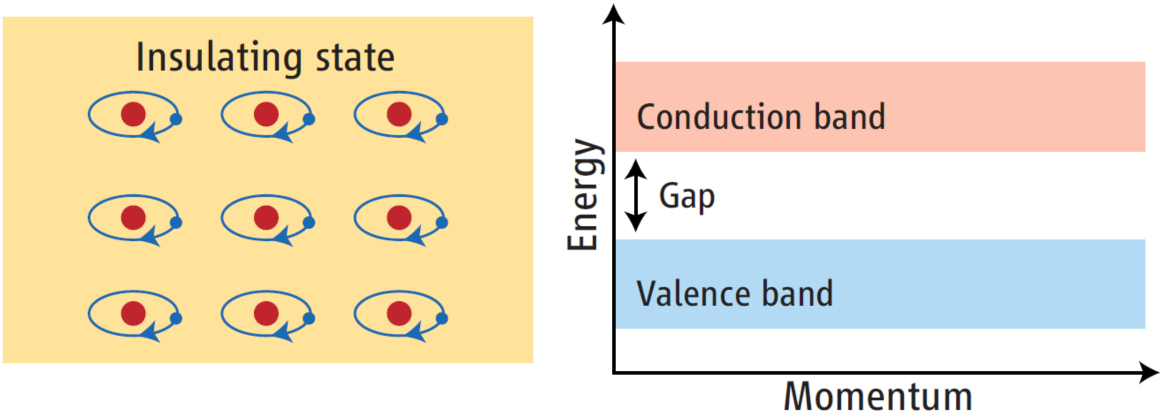
Spin-orbit coupling
→ (spin-dependent) effective
magnetic field

Various Bulk insulator

Kane,Mele Science 314,1692(2009)

Band insulator

- Localized orbitals

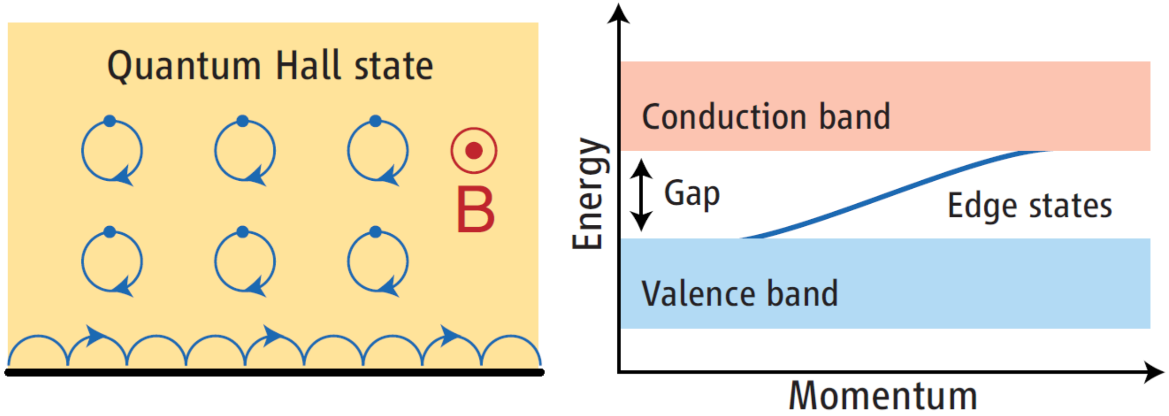


Quantum Hall state

- bulk energy gap
- **Chiral edge mode**

  “one way” edge states
  along the sample boundary

- Classified by **Chern number**

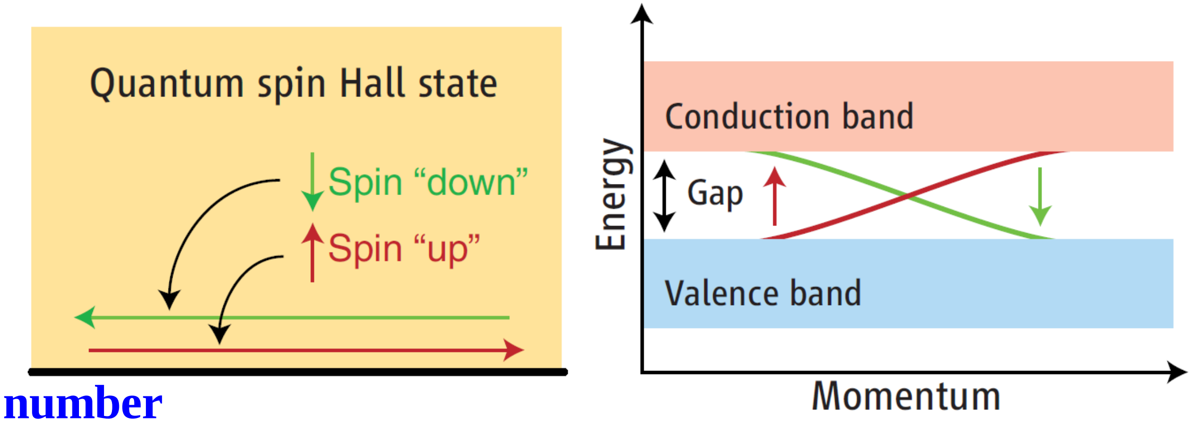


Quantum Spin Hall state

- bulk energy gap
- **Helical edge mode**

  Spin filterd edge states

- Classified by **Z_2 topological number**

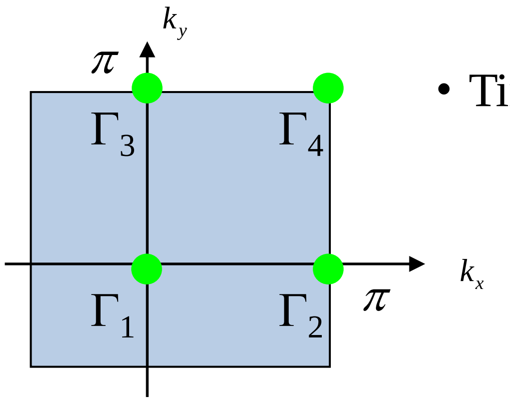


Z_2 topological number

Fu,Kane, PRB **76**,045302(2007)

2D system with inversion symmetry

Time-reversal and inversion symmetry ⇒ All bands is degenerate. (Kramers pair)

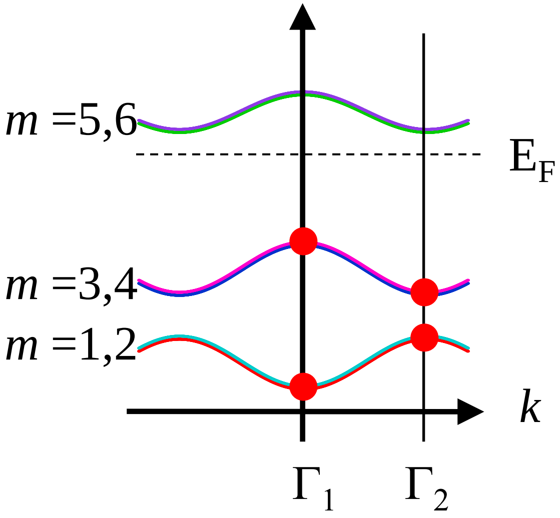


- Time Reversal Invariant Momentum (TRIM)

$$k \equiv -k \ (\mathrm{mod}\ G)$$

Four TRIM in 2D system

$\Gamma_1, \Gamma_2, \Gamma_3, \Gamma_4$



- Time Reversal Polarization(TRP)

$$P(\Gamma_i) \equiv \prod_{m=1}^{N} \xi_{2m}(\Gamma_i)$$

$\xi_{2m}(\Gamma_i)$: the parity eigenvalue of the 2*m*th occupied energy band at Γ_i

N : the number of Kramers pair under $\mathrm{E_F}$

Parity eigenvalue

$$\hat{P}\psi(r) = \pm\psi(-r) \quad \begin{cases} +1\text{: symmetric} \\ -1\text{: asymmetric} \end{cases}$$

Kramers degenerate partner

$$\xi_{2m-1}(\Gamma_i) = \xi_{2m}(\Gamma_i) = \pm 1$$

- Z_2 topological number

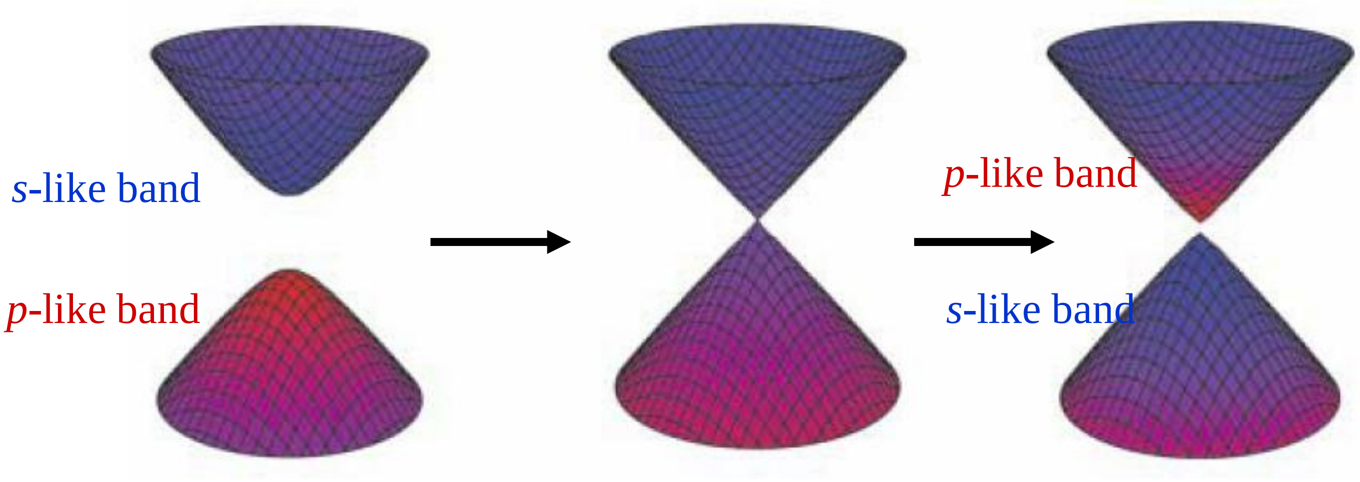
$$\boxed{(-1)^{\nu} = \prod_{i=1}^{4}\prod_{m=1}^{N} \xi_{2m}(\Gamma_i) = P(\Gamma_1)P(\Gamma_2)P(\Gamma_3)P(\Gamma_4)}$$

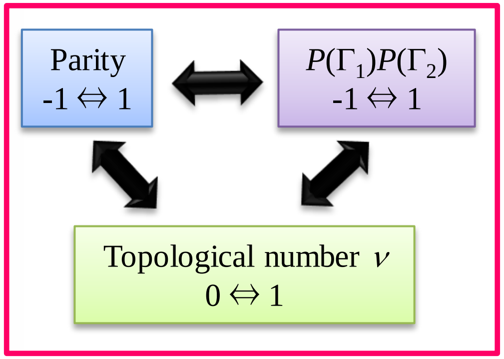
$\nu = 0$: trivial insulator
$\nu = 1$: QSH

What material is topological insulator ?

Ex. Insulator with band-inversion

Bernevig, Hughes & Zhang, Science (2006)





Parity
-1 ⇔ 1

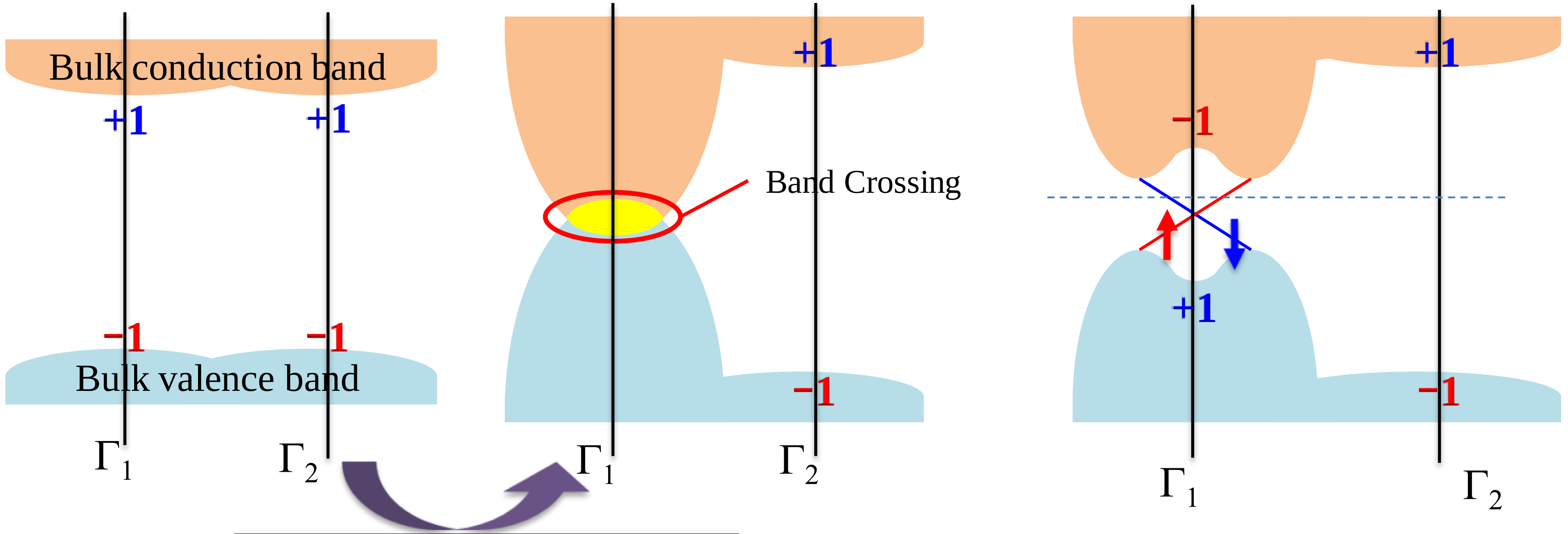
$P(\Gamma_1)P(\Gamma_2)$
-1 ⇔ 1

Topological number ν
0 ⇔ 1

Ordinary Insulator

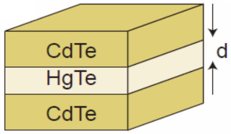
Band Crossing

Quantum Spin Hall Insulator

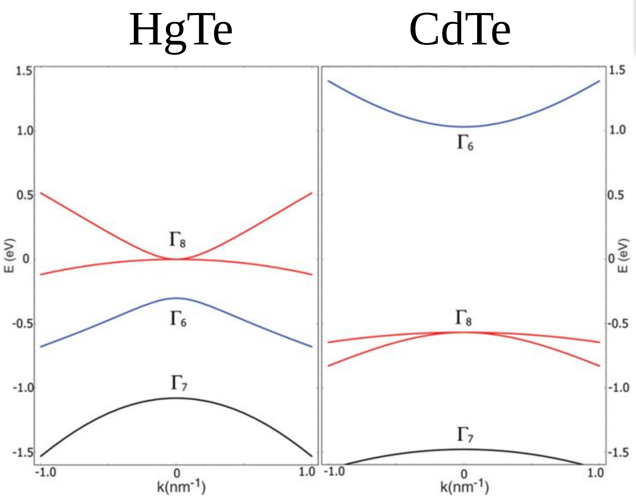


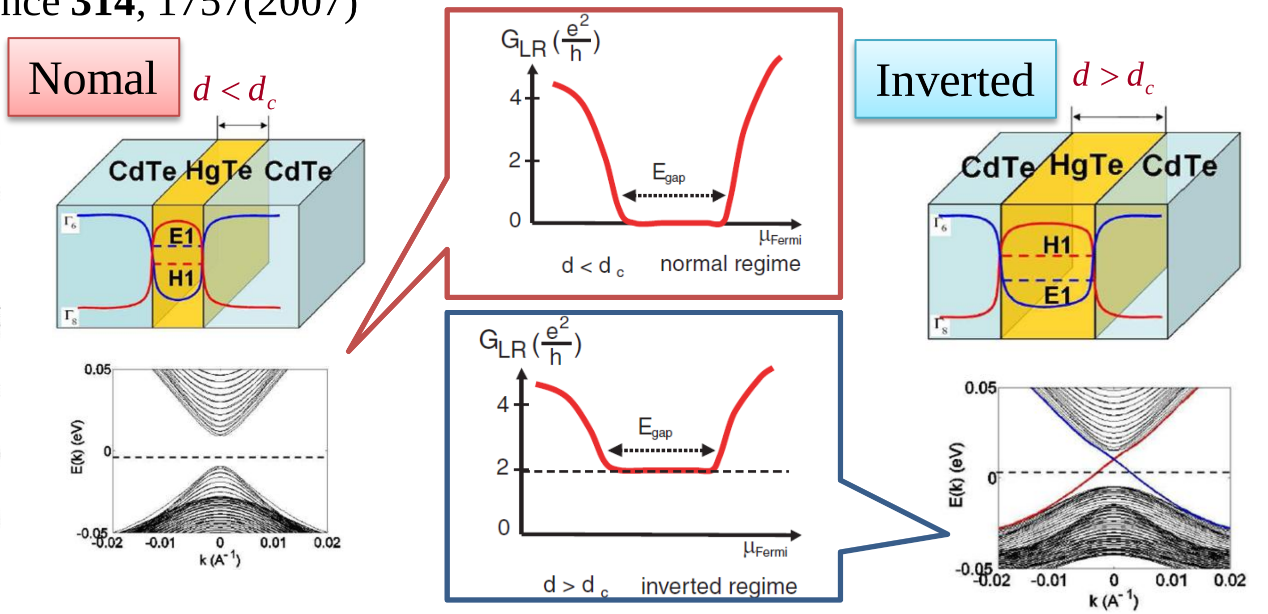
Tuning by S-O interaction *etc.*

2D QSH state in CdTe/HgTe/CdTe quantum well

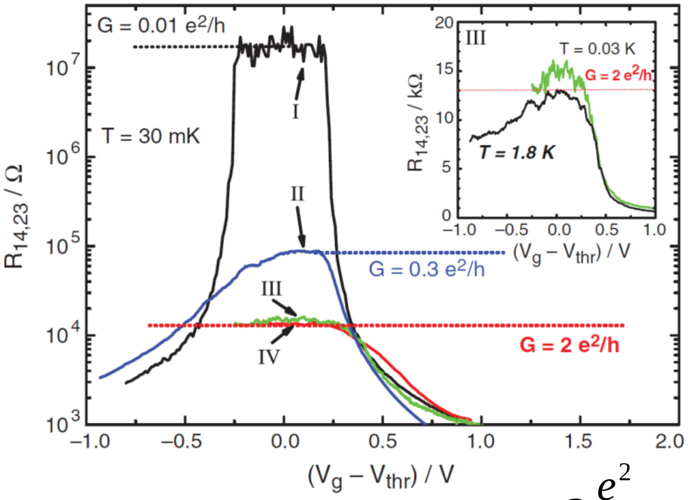


Theory: B. A. Bernevig *et al.*, Science **314**, 1757(2007)

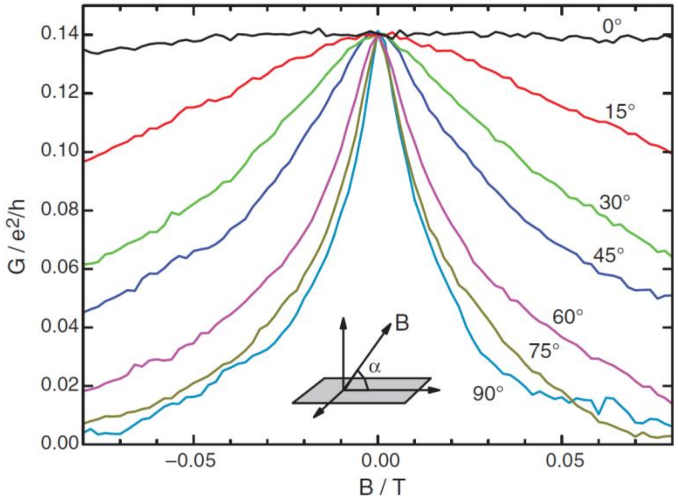




Experiment: Markus König, *et al.*, Science **318**, 766 (2007);



Quantized conductance= $2\frac{e^2}{h}$



Magnetic field breaks the QSH phase

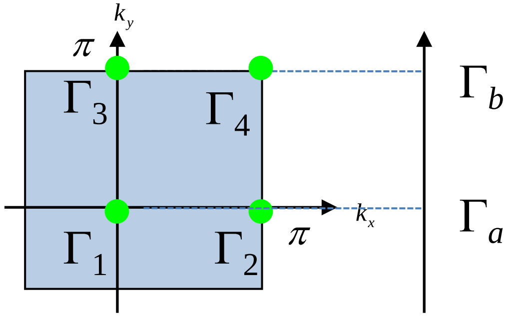
Surface States

Fu,Kane, PRB **76**,045302(2007)

$$(-1)^{\nu} = \prod_{i=1}^{4}\prod_{m=1}^{N}\xi_{2m}(\Gamma_i) = P(\Gamma_a)P(\Gamma_b)$$

$$P(\Gamma_a) \equiv P(\Gamma_1)P(\Gamma_2)$$

$$P(\Gamma_b) \equiv P(\Gamma_3)P(\Gamma_4)$$



$$P(\Gamma_a)P(\Gamma_b) = \pm 1$$

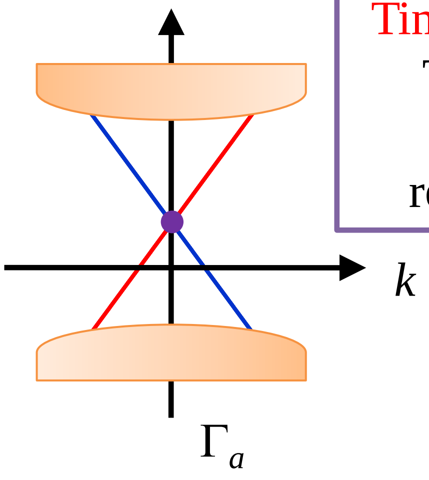
The product of TRP ⇔ Direct relation ⇔ The topology of surface state intersecting E_F

$P(\Gamma_a)P(\Gamma_b) = -1$ ⇔ An **odd** number of surface bands intersects E_F between Γ_a and Γ_b

$P(\Gamma_a)P(\Gamma_b) = 1$ ⇔ An **even** number of surface bands intersects E_F between Γ_a and Γ_b

We can briefly determine topological or trivial insulator by the surface states.

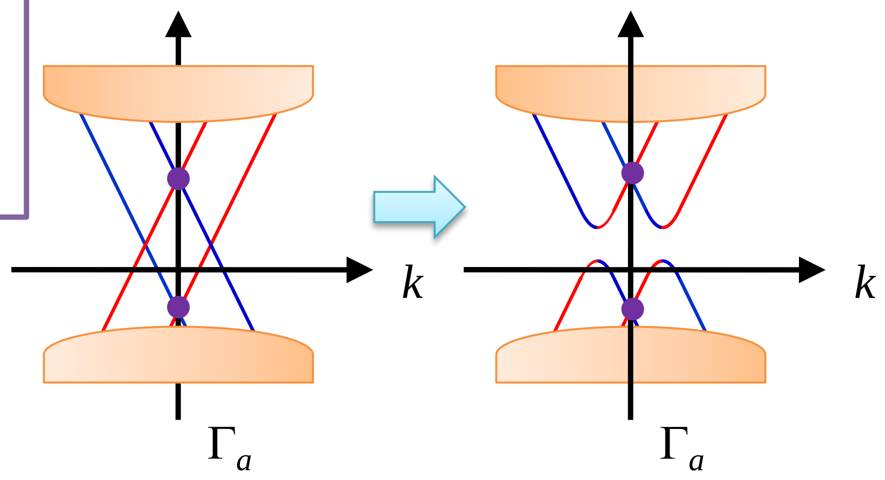
- $n = 1$ (odd)



At least, one of the edge states survive.
(Topological insulator)

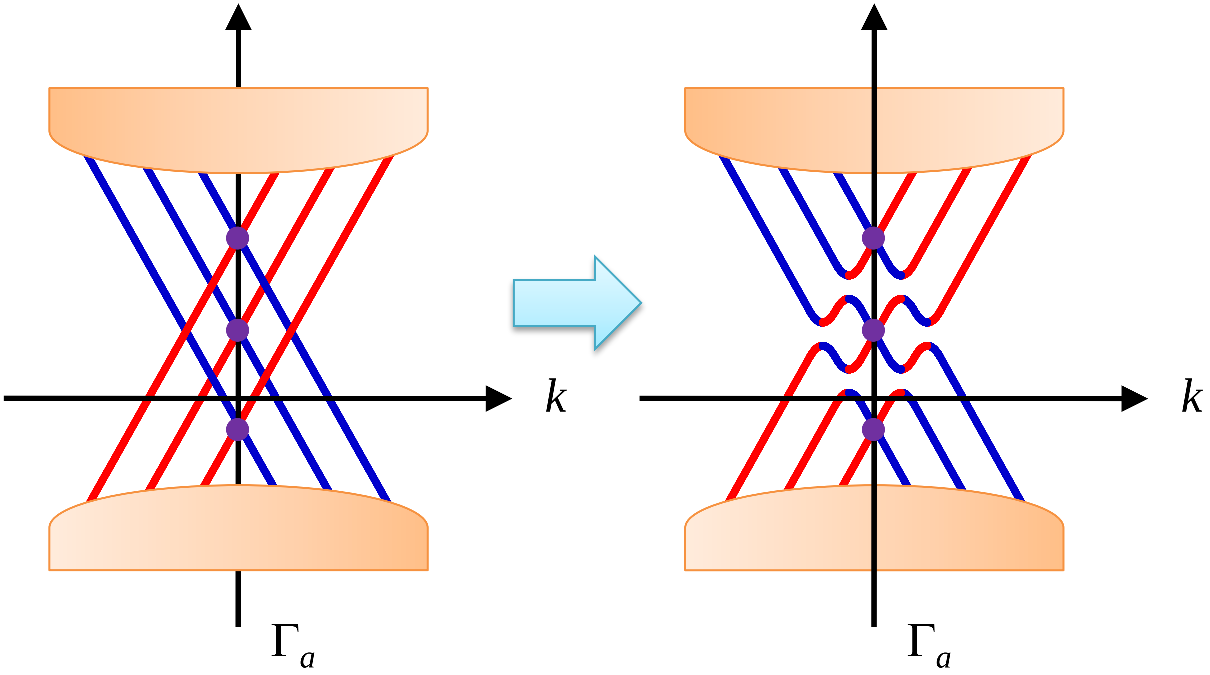
Time reversal invariant
The surface states
on TRIM
remains degenerate

- $n = 2$ (even)



Surface states open gap.
(Trivial insulator)

- $n = 3$ (odd)



At least, one of the edge states survive.

Appendix

Time-reversal symmetry

$E(\boldsymbol{k},\uparrow) = E(-\boldsymbol{k},\downarrow)$

Inversion symmetry

$E(\boldsymbol{k},\uparrow) = E(-\boldsymbol{k},\uparrow)$

Time-reversal + Inversion

$E(\boldsymbol{k},\uparrow) = E(\boldsymbol{k},\downarrow)$

All bands is degenerate.
(Kramers pair)

~~Contradiction~~ ?

Surface state

Inversion symmetry is broken.

Time-reversal symmetry

$E(\boldsymbol{k},\uparrow) = E(-\boldsymbol{k},\downarrow)$

The topology of surface state intersecting E_F

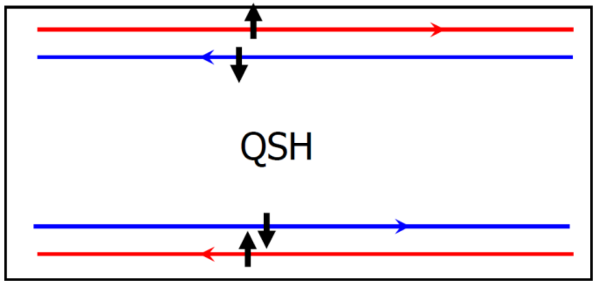
Topological insulator ⇔ An **odd** number of surface bands intersects E_F between Γ_a and Γ_b

Trivial insulator ⇔ An **even** number of surface bands intersect E_F between Γ_a and Γ_b

We can briefly determine topological or trivial insulator by the surface states.

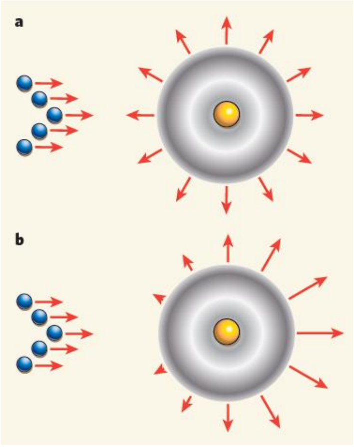
Suppression of the backscattering by nonmagnetic impurities

Quantum Spin Hall phase



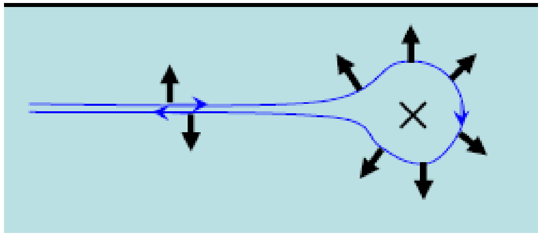
Forward mover with up spin
Backforward mover with down spin

Conversely for the other edge

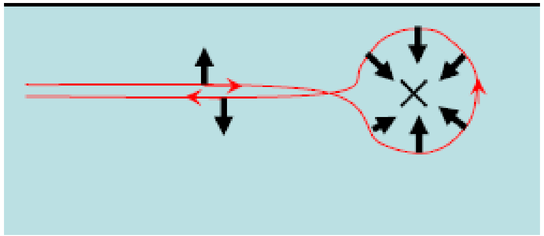


Joel Moore, Nature **460**,1090

backscattering by nonmagnetic impurities



Clockwise
spin rotation
π



Counterclockwise
spin rotation
$-\pi$

Xiao-Liang Qi et al., arXiv:1001.1602

The two paths differ by 2π

Spin ½ rotation

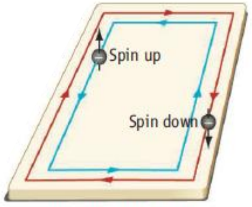
$$\exp(-\frac{i}{2}\phi)$$

The two backscattering paths always interfere destructively.

The backscattering by nonmagnetic impurities is forbidden !

From 2D to 3D topological insulator

2D topological insulator



Quantum spin Hall system

N. Nagaosa *et al.*, Science **318**, 758

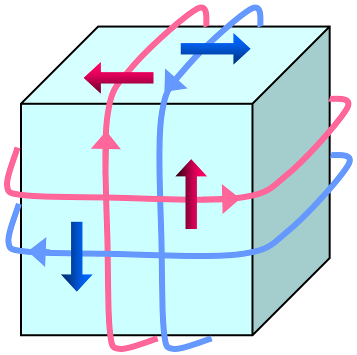
Helical 1D edge state

The dispersion of the state obeys Dirac equation.

1D massless Dirac Fermion

material
- HgTe quantum well

3D topological insulator



Helical 2D surface states
(2D massless Dirac Fermion)

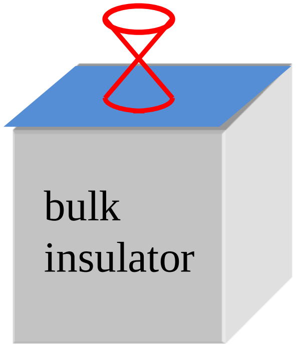
Dirac Cone

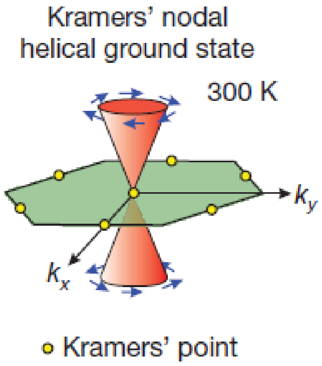
material

first topological insulator
- $Bi_{1-x}Sb_x$

second topological insulator
- Bi_2Te_3
- Bi_2Se_3

surface Dirac fermion





Spin polar surface state

Second topological insulator
- Nearly idealized **single** Dirac cone
- Stoichiometric ⟶ high purity
- Large band gap ∼0.3eV

※ graphene Dirac cone ×4

Topological invariant: 3D system with inversion symmetry

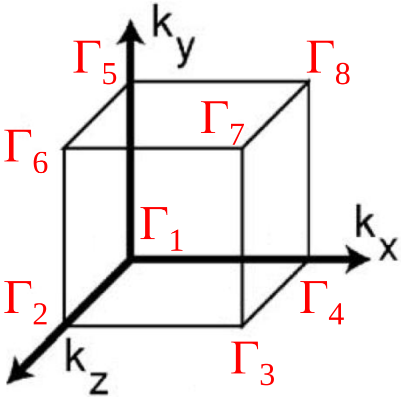
- Time Reversal Invariant Momentum (TRIM)

Eight TRIM in 3D system

$\Gamma_1 \sim \Gamma_8$

$$k \equiv -k \pmod{G}$$

- **Four Z_2 topological invariant** $\nu_0 ;(\nu_x, \nu_y, \nu_z)$



$$\boxed{(-1)^{\nu_0} = \prod_{i=1}^{8} P(\Gamma_i)}$$

$$(-1)^{\nu_x} = P(\Gamma_3)P(\Gamma_4)P(\Gamma_7)P(\Gamma_8)$$

$$(-1)^{\nu_y} = P(\Gamma_5)P(\Gamma_6)P(\Gamma_7)P(\Gamma_8)$$

$$(-1)^{\nu_z} = P(\Gamma_2)P(\Gamma_3)P(\Gamma_6)P(\Gamma_7)$$

$\nu_0 = 1$: strong topological insulator (STI)
$\nu_0 = 0$: weak topological insulator (WTI)

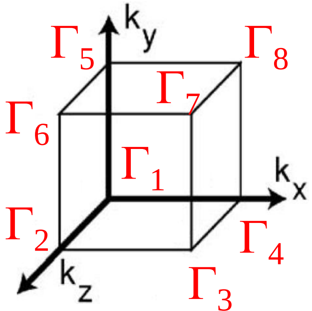
These states can be interpreted
as layered 2D dimensional QSH states.
Literally weak !

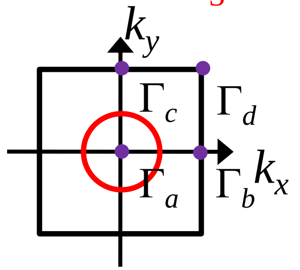
We are interested in only strong topological insulator ($\nu_0 = 1$).

Surface state: 3D system with inversion symmetry

Fermi surface of the surface states on (001) surface

$$(-1)^{\nu_0} = \prod_{i=1}^{8} P(\Gamma_i) = P(\Gamma_a)P(\Gamma_b)P(\Gamma_c)P(\Gamma_d)$$

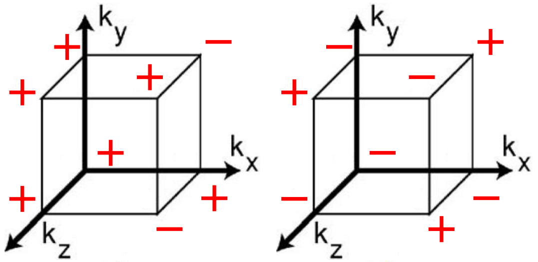


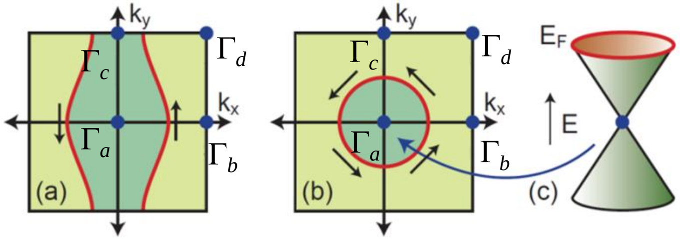


(001) plane projection

$$P(\Gamma_a) \equiv P(\Gamma_1)P(\Gamma_2)$$
$$P(\Gamma_b) \equiv P(\Gamma_3)P(\Gamma_4)$$
$$P(\Gamma_c) \equiv P(\Gamma_5)P(\Gamma_6)$$
$$P(\Gamma_d) \equiv P(\Gamma_7)P(\Gamma_8)$$

0 ;(0,1,1) 1 ;(0,0,0)





The product of TRP($P(\Gamma)$)

⇔ **The topology of surface states intersecting E_F**

$P(\Gamma_a)P(\Gamma_b) = -1$

⇔ **odd** number of surface bands between Γ_a and Γ_b

$P(\Gamma_a)P(\Gamma_b) = +1$

⇔ **even** number of surface bands between Γ_a and Γ_b

Strong topological insulator $\nu_0 = 1$

A single *P* differs in sign from the other three.

$P(\Gamma_a) = +1$ ➡ $P(\Gamma_b) = P(\Gamma_c) = P(\Gamma_d) = -1$

Surface state: 3D system with inversion symmetry

Fermi surface of the surface states on (001) surface

$$(-1)^{\nu_0} = \prod_{i=1}^{8} P(\Gamma_i) = P(\Gamma_a)P(\Gamma_b)P(\Gamma_c)P(\Gamma_d)$$

Strong topological insulator $\nu_0 = 1$

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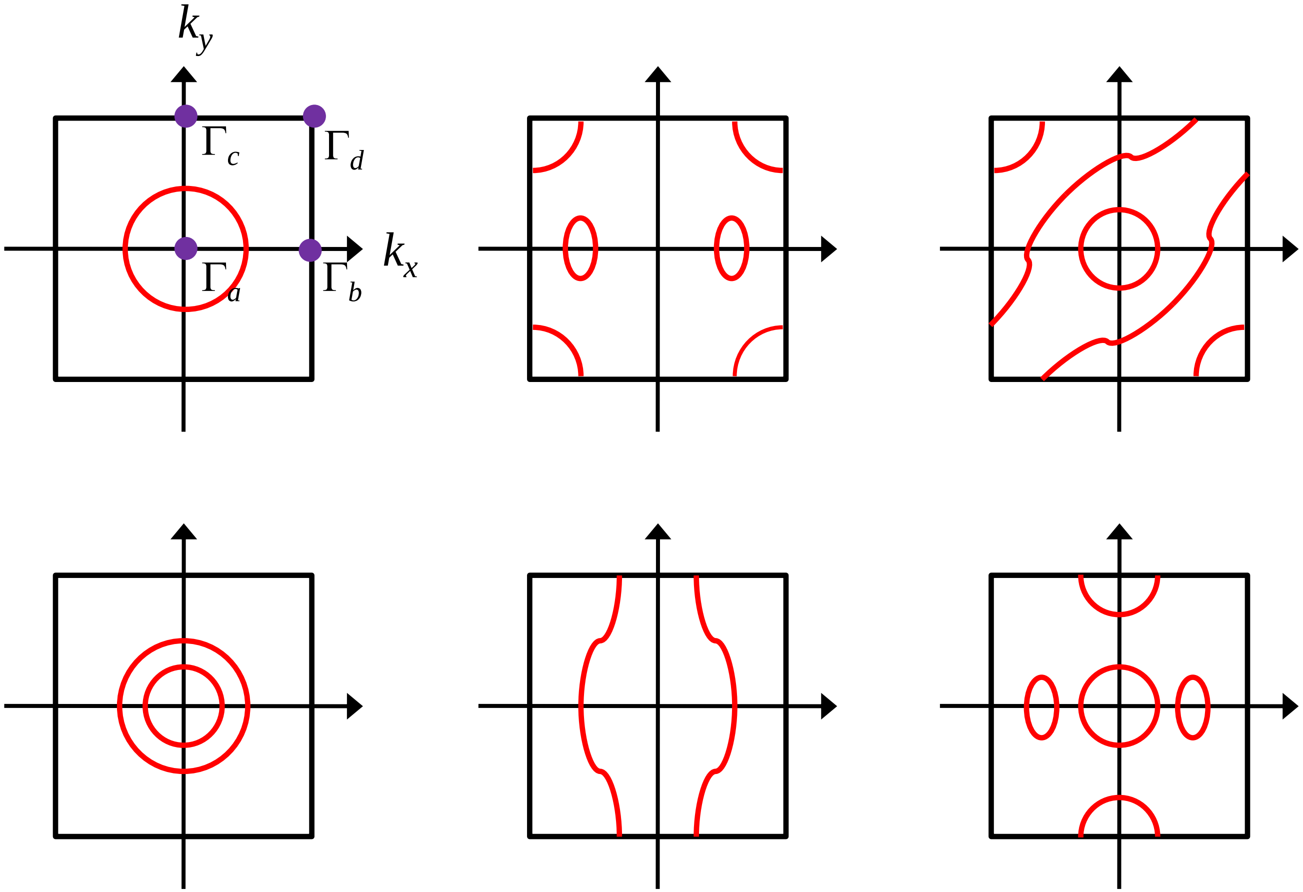


Surface state: 3D system with inversion symmetry

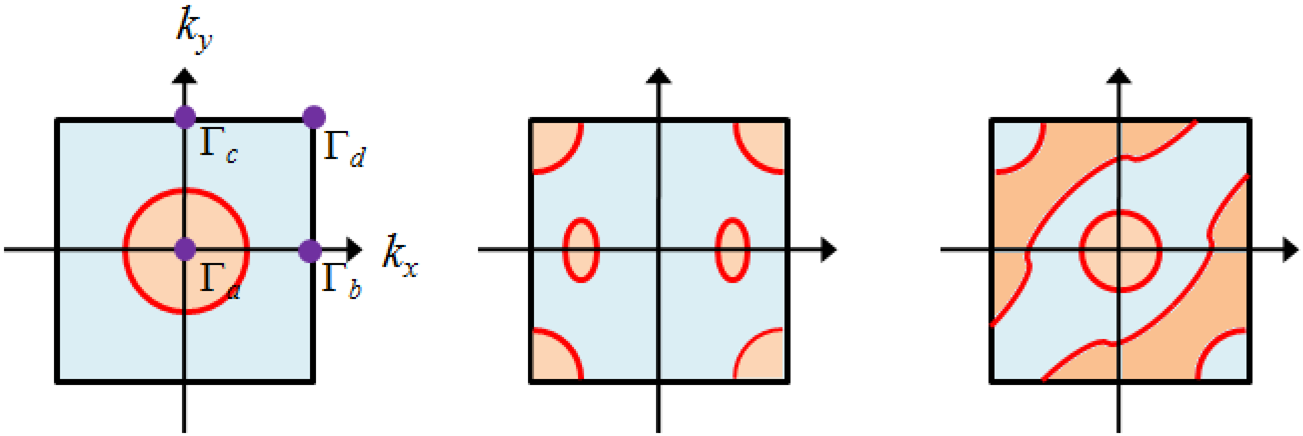
Fermi surface of the surface states on (001) surface

$$(-1)^{\nu_0} = \prod_{i=1}^{8} P(\Gamma_i) = P(\Gamma_a)P(\Gamma_b)P(\Gamma_c)P(\Gamma_d)$$

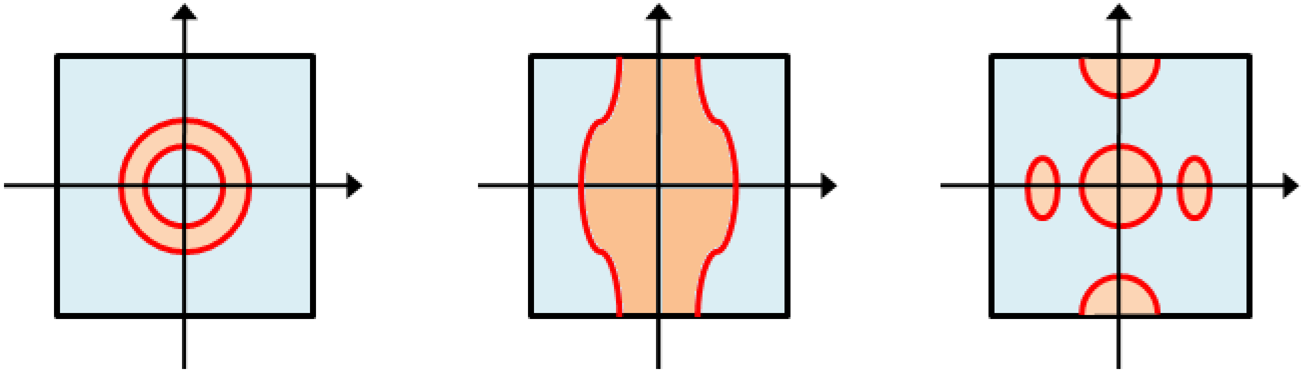
Strong topological insulator $\nu_0 = 1$

A single P differs in sign from the other three.

- $\nu_0 = 1$



- $\nu_0 = 0$



The surface Fermi arc encloses TRIM (Γ).

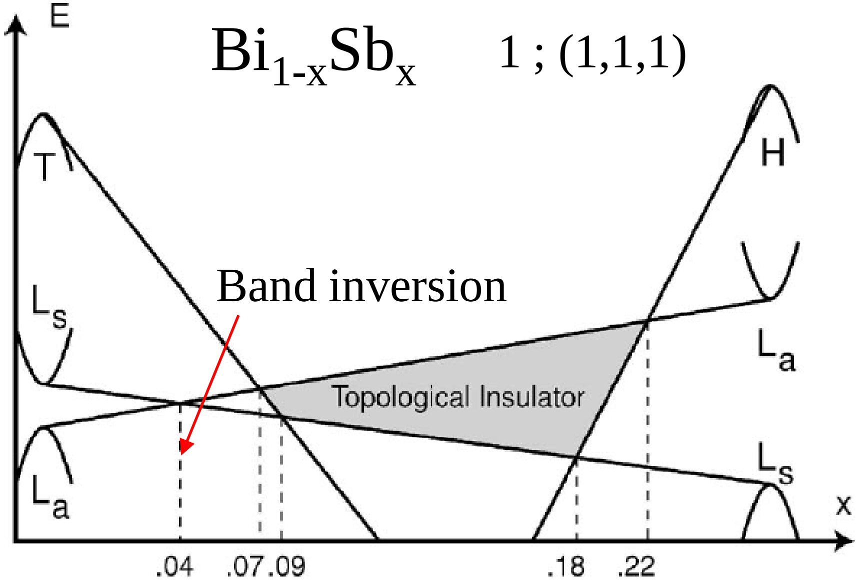
$\nu_0 = 1$: **odd** number (Berry phase π)

$\nu_0 = 0$: **even** number (Berry phase 0)

First Topological Insulator $Bi_{1-x}Sb_x$

3D topological insulator $Bi_{1-x}Sb_x$

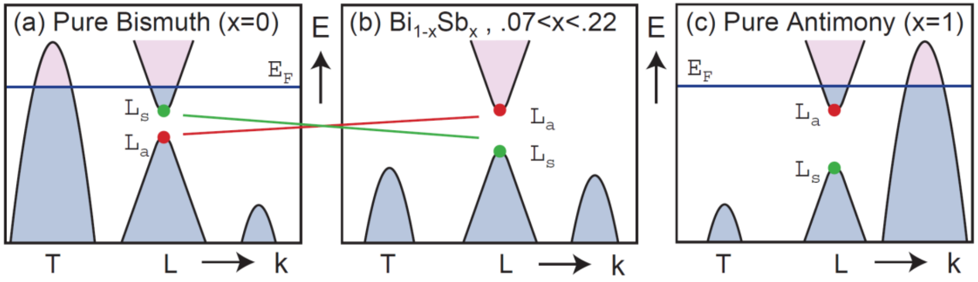
Fu & Kane, PRB (2007)


$Bi_{1-x}Sb_x$ 1 ; (1,1,1)

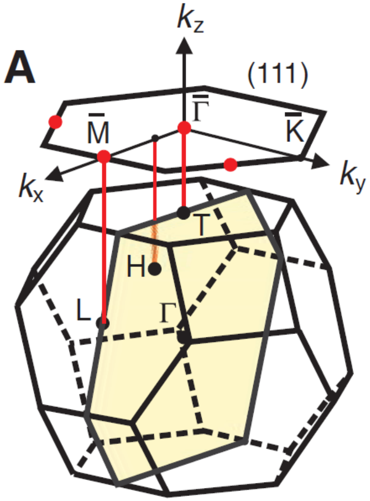
Band inversion

0 ; (0,0,0)

1 ; (1,1,1)



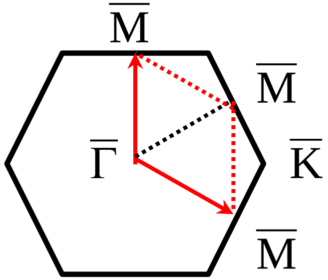
Bi ; rhombohedral crystal structure



TRIM

$\Gamma(0,0,0)$ $L(\pi,0,0)$ $H(\pi,\pi,0)$ $T(\pi,\pi,\pi)$

(111) plane projection



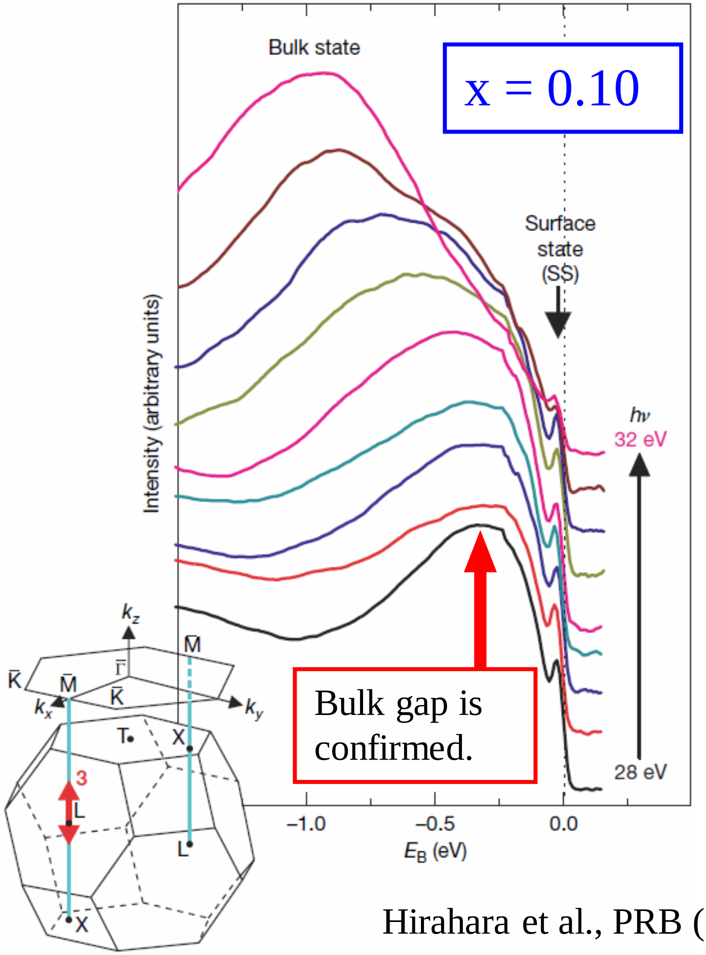
TRIM

one: $\bar{\Gamma}$ three: $\bar{M}$

Count the number of the surface Fermi arc enclosing TRIM (Γ).

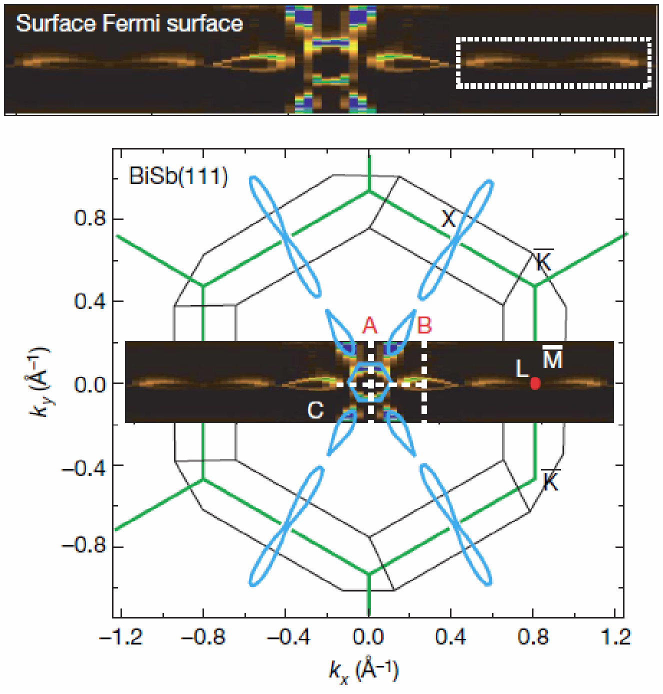
Hsieh et al., Nature (2008)

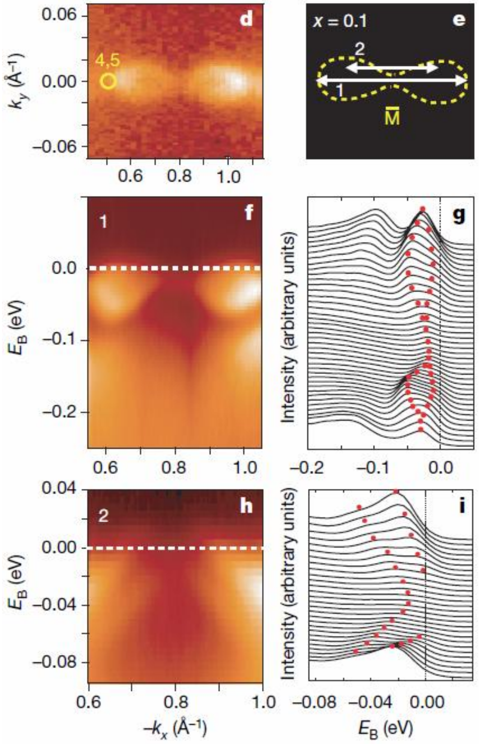
Surface State of $Bi_{0.9}Sb_{0.1}$

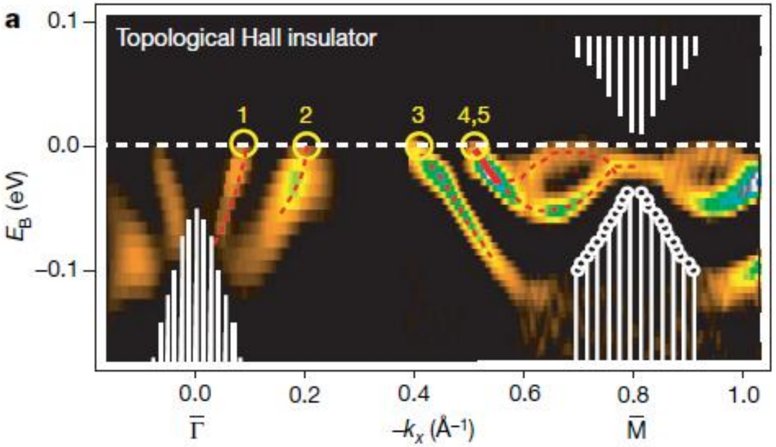


x = 0.10

Bulk gap is confirmed.



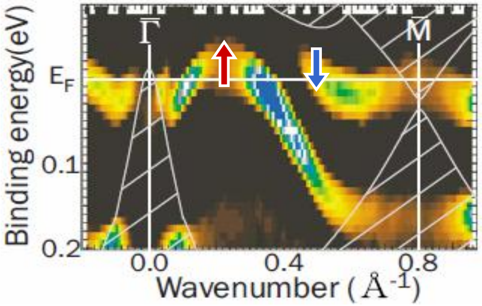




Hirahara et al., PRB (2007)

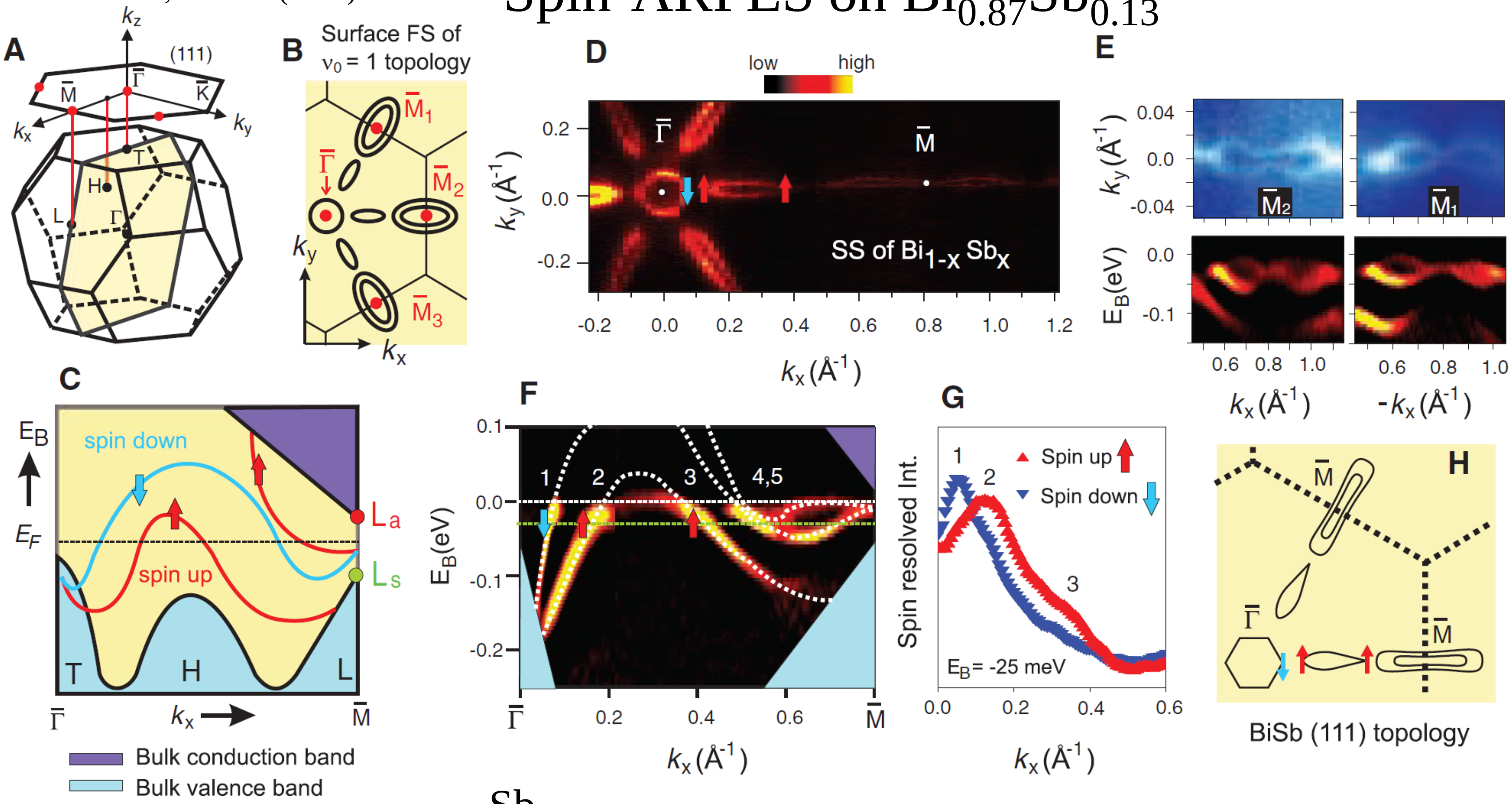
Pure Bi

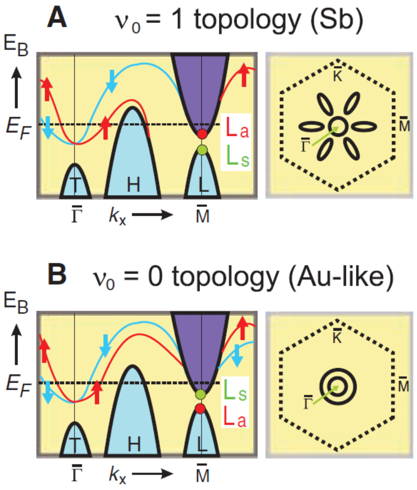
Spin-splitting of the surface states due to Rashba S-O int.



Spin-ARPES on $Bi_{0.87}Sb_{0.13}$

Hsieh *et al.*, Science (2009)





Sb

Topologically nontrivial

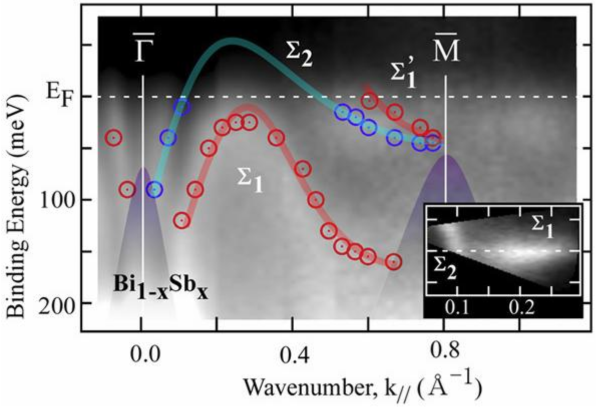
Au

Topologically trivial

$Bi_{0.87}Sb_{0.13}$

Γ is enclosed an odd number of times

$\nu_0 = 1$: topological insulator



Nishide, Taskin et al., PRB (2010)

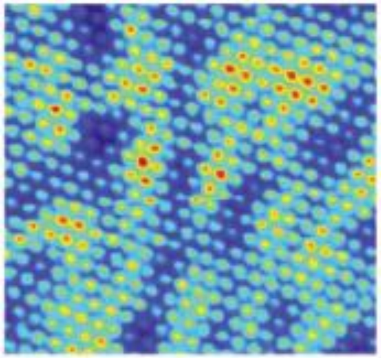
STS on Bi$_{1-x}$Sb$_x$ (backscattering suppresion)

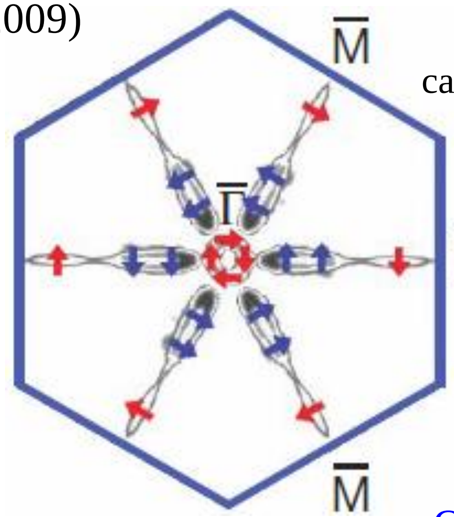
Joint Density of States

Spin-dependent Scattering Probability

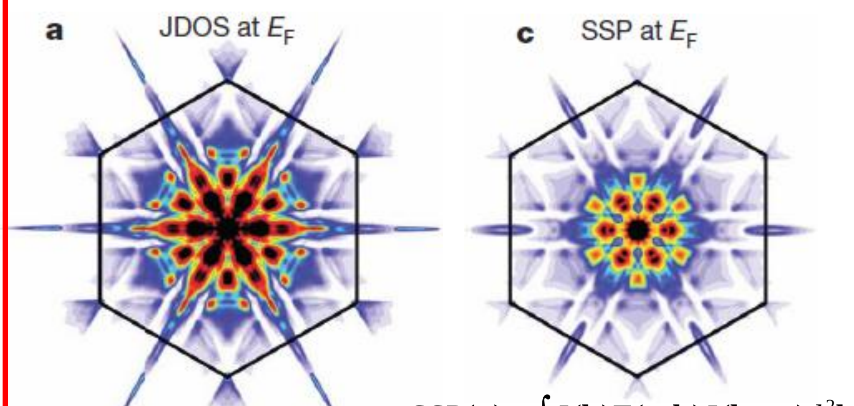
Roushan et al., Nature (2009)

Bi$_{0.92}$Sb$_{0.08}$ (STM)





calculation

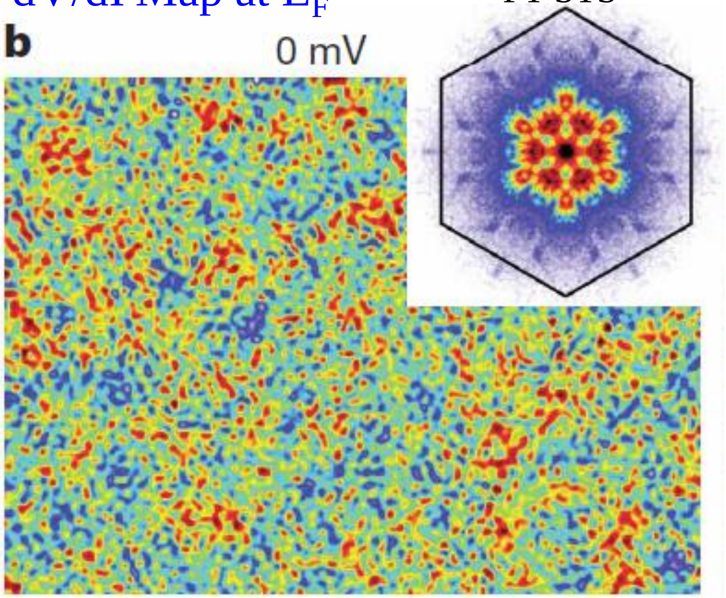


$$\mathrm{JDOS}(\mathbf{q}) = \int I(\mathbf{k}) I(\mathbf{k}+\mathbf{q}) d^2\mathbf{k}$$

$$\mathrm{SSP}(\mathbf{q}) = \int I(\mathbf{k}) T(\mathbf{q},\mathbf{k}) I(\mathbf{k}+\mathbf{q}) d^2\mathbf{k}$$

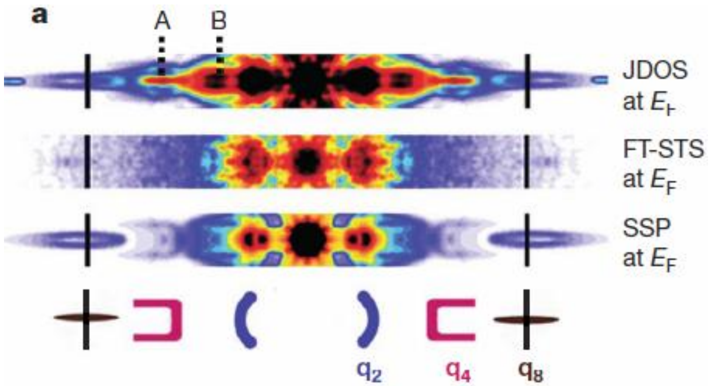
dV/dI Map at E$_F$

FT-STS

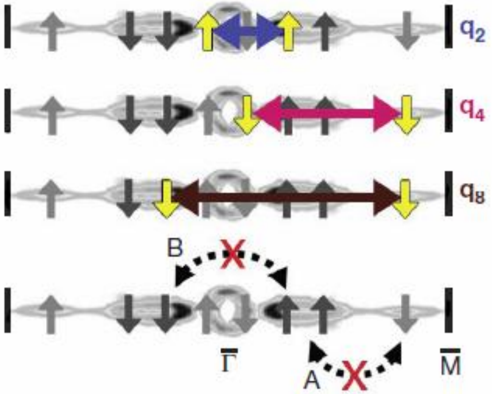


QPI Patterns along Γ-M

Scattering Vectors:

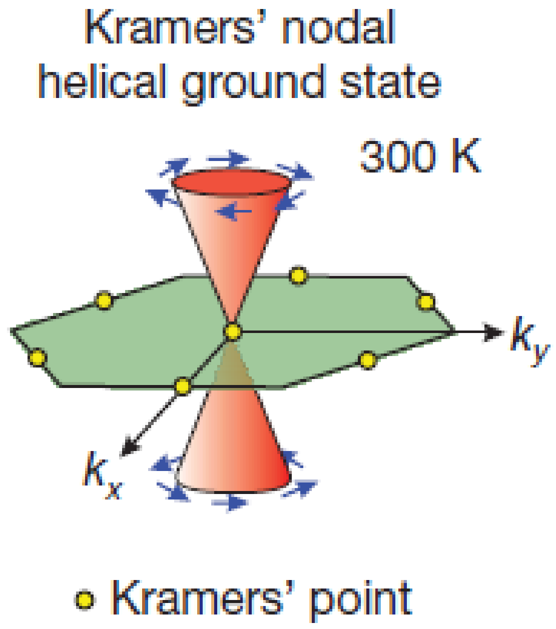


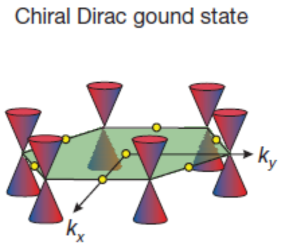
Allowed Scattering Processes



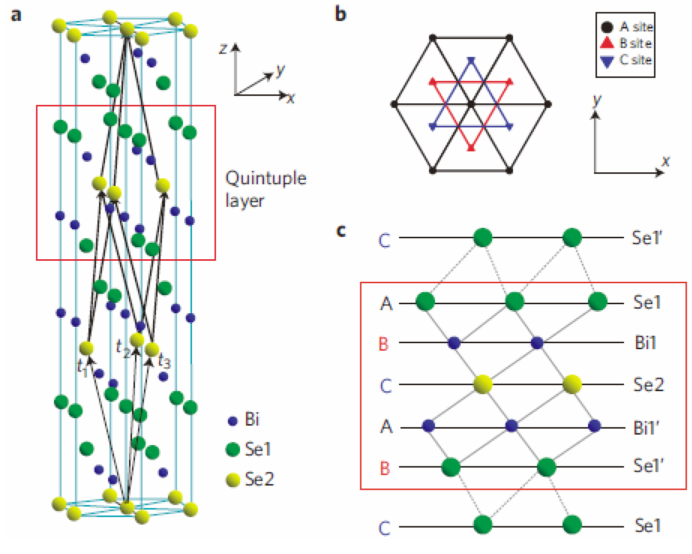
2nd-Generation Topological Insulators

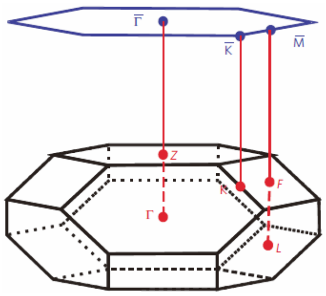
- Nearly idealized single Dirac cone
- Stoichiometric → high purity
- Large band gap $\sim$0.3eV





2nd-Generation TIs: Prediction

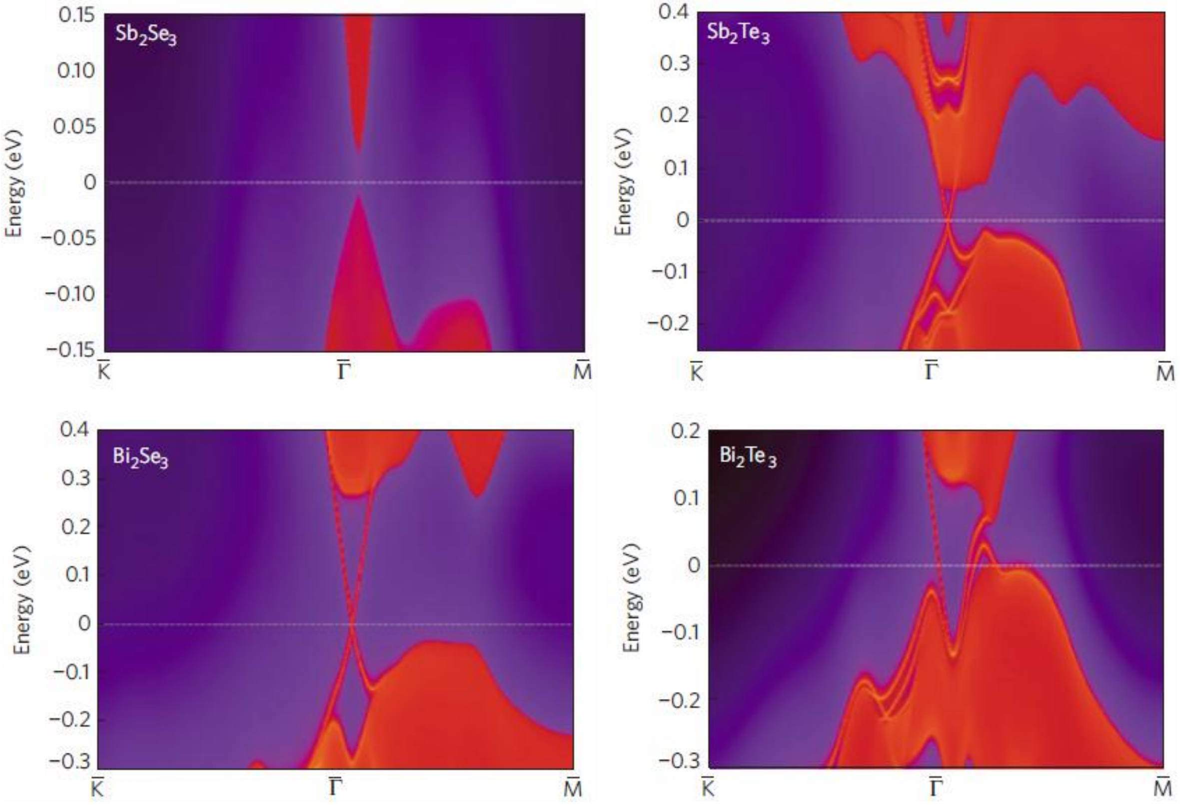


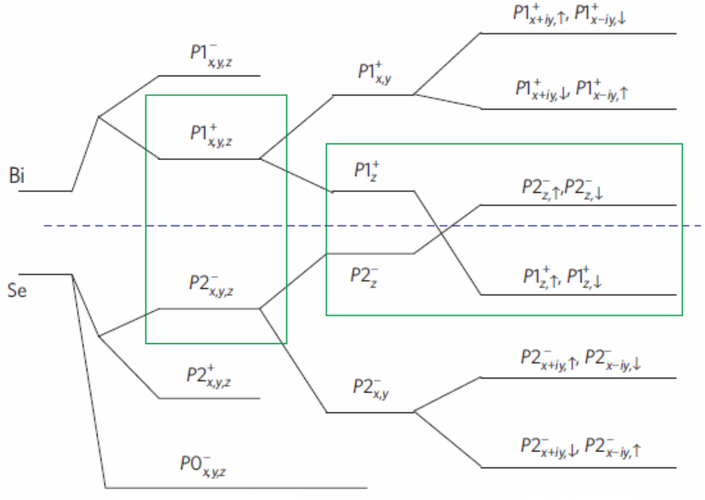


Bi_2Se_3 , Bi_2Te_3 , and Sb_2Te_3 should be topological insulators

1 ; (0,0,0)

Zhang et al., Nat. Phys. (2009)



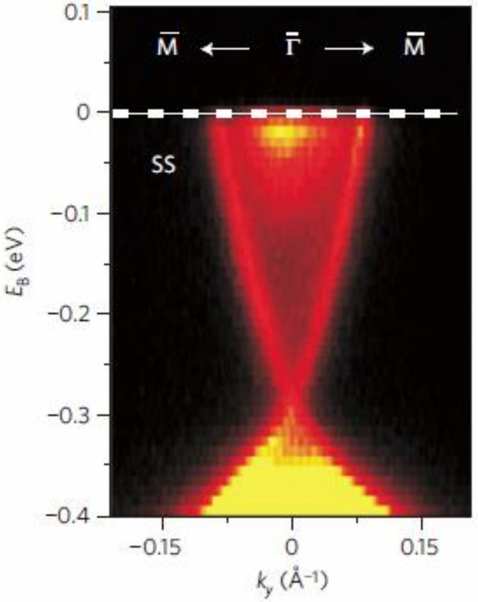


Chemical Bonding

Crystal Field

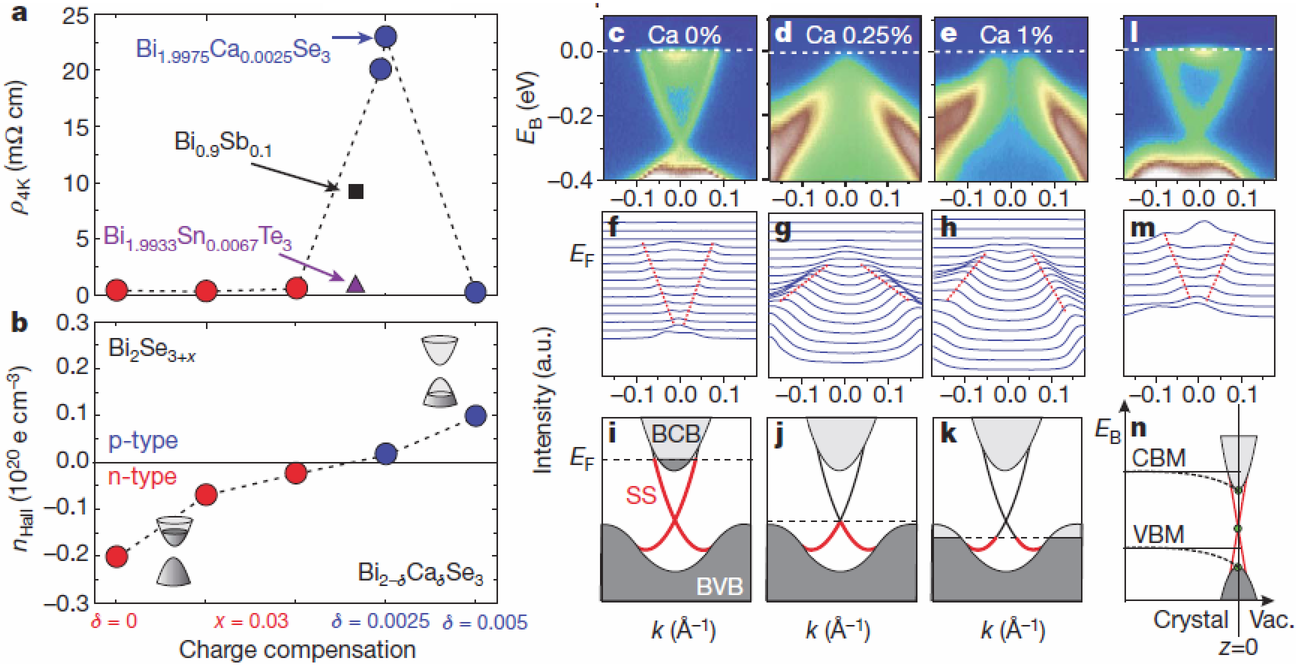
SOC

ARPES on Bi_2Se_3



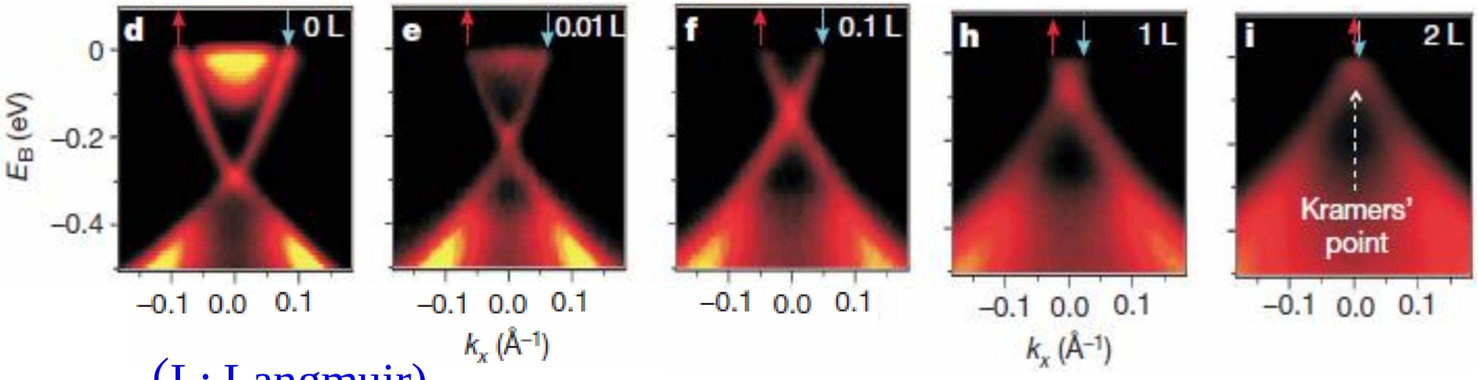
Xia et al., Nat. Phys. (2009)

Ca-doping lowers E_F

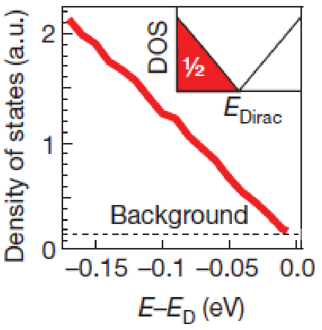


Hsieh et al., Nature (2009)

NiO_2 adsorption on $Bi_{2-\delta}Ca_\delta Se_3$ to tune E_F



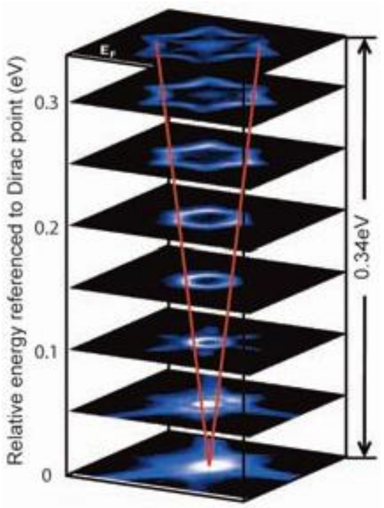
(L: Langmuir)



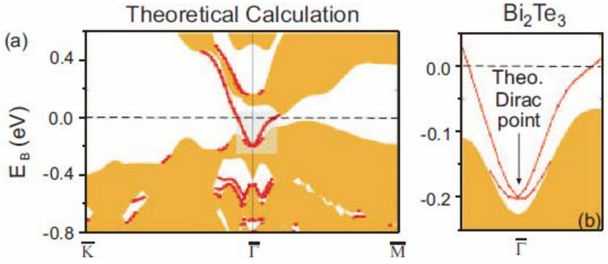
linear

2D massless Dirac Fermion

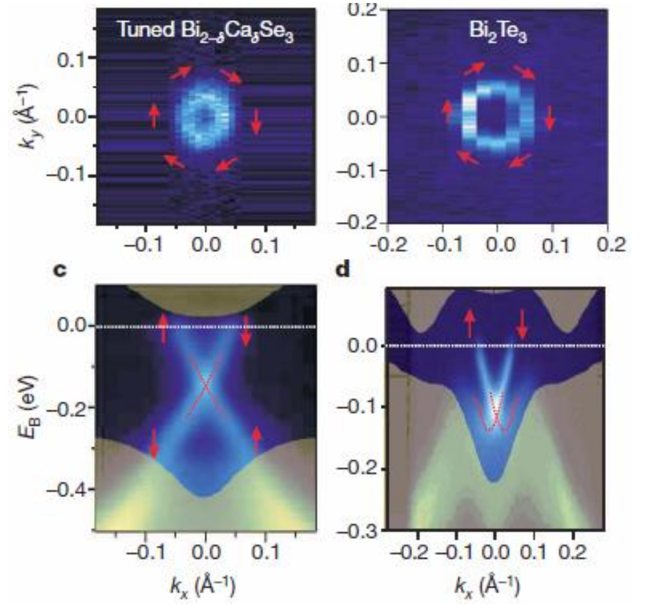
ARPES on Bi_2Te_3



Chen et al., Science (2009)

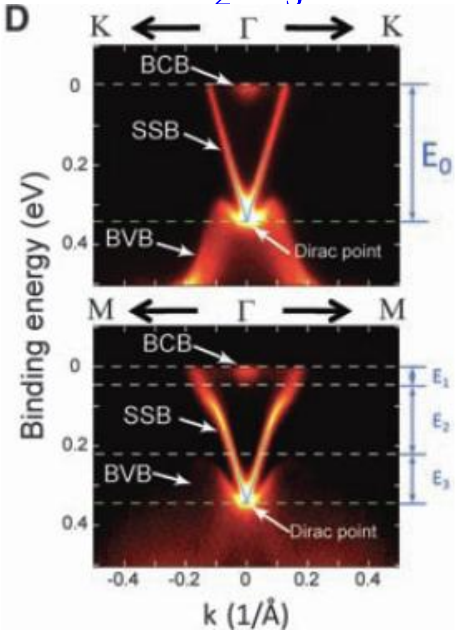


Xia et al., arXiv (2009)

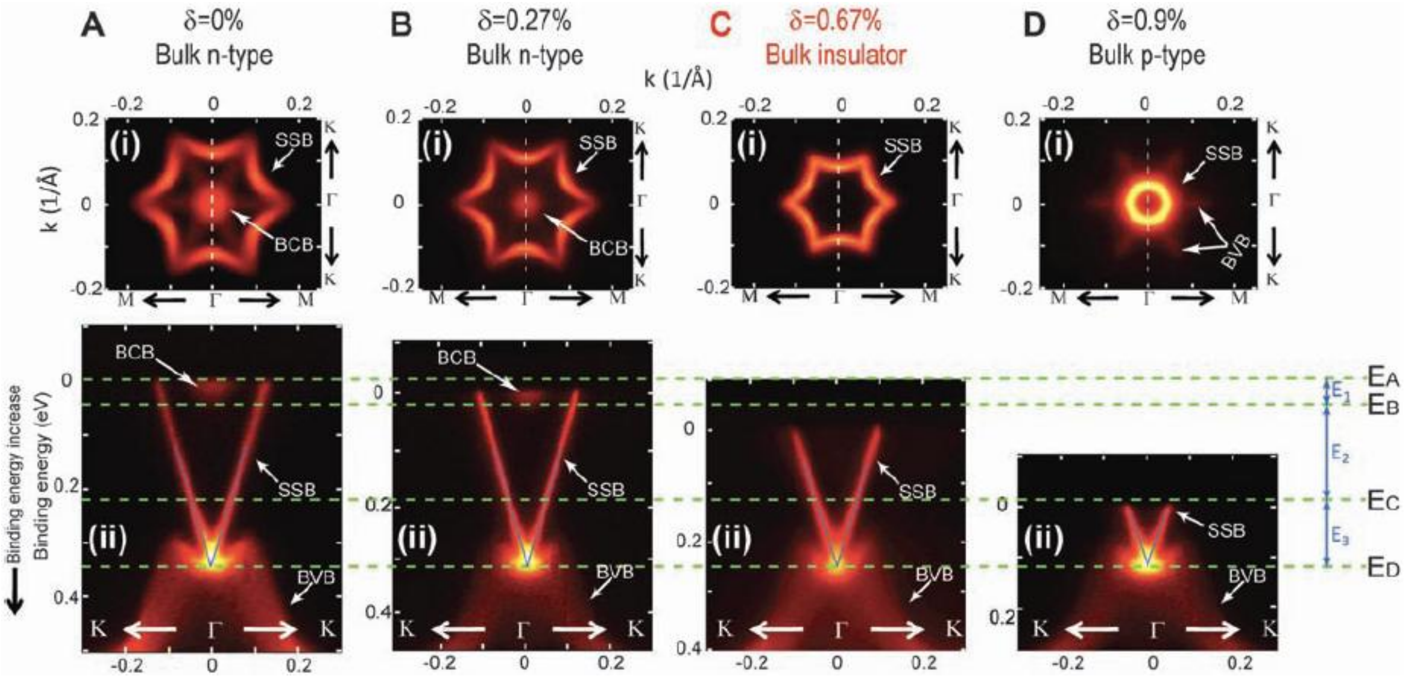


Hsieh *et al*., Nature (2009)

Bi_2Te_3

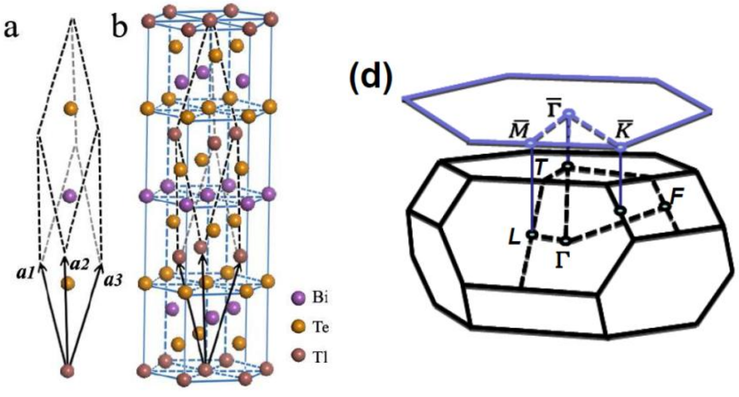


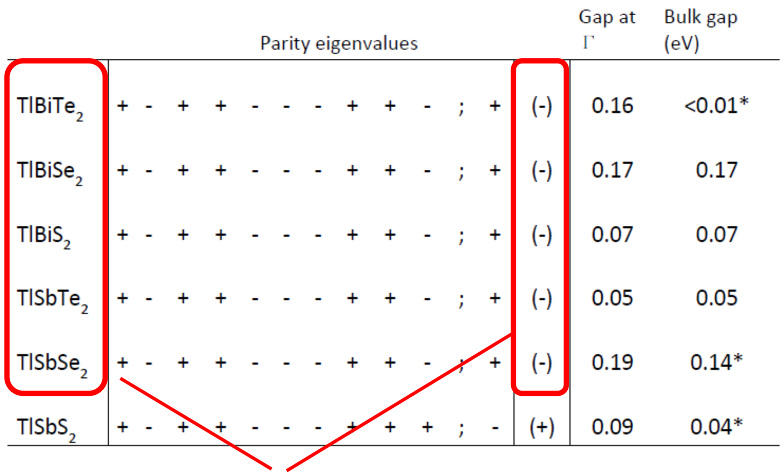
$Bi_{2-\delta}Sn_\delta Te_3$



Thallium-based Ⅲ-Ⅴ-Ⅳ$_2$ ternary chalcogenides

B. Yan *et al.*,arXiv:1003.0074

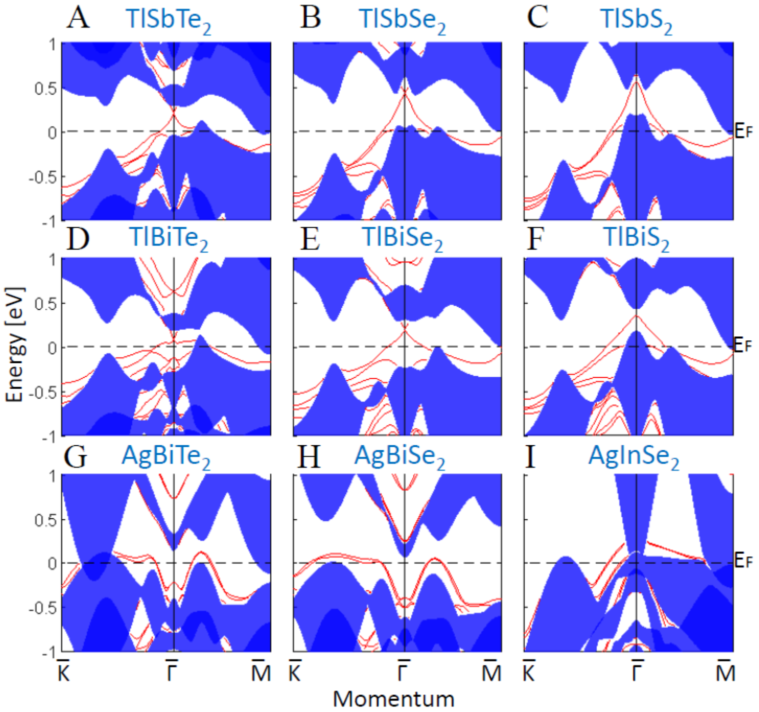




	Parity eigenvalues		Gap at Γ	Bulk gap (eV)
TlBiTe$_2$	+ - + + - - - + + - ; +	(-)	0.16	<0.01*
TlBiSe$_2$	+ - + + - - - + + - ; +	(-)	0.17	0.17
TlBiS$_2$	+ - + + - - - + + - ; +	(-)	0.07	0.07
TlSbTe$_2$	+ - + + - - - + + - ; +	(-)	0.05	0.05
TlSbSe$_2$	+ - + + - - - + + - ; +	(-)	0.19	0.14*
TlSbS$_2$	+ - + + - - - + + + ; -	(+)	0.09	0.04*

Topological insulator

H. Lin *et al.*,arXiv:1003.2615



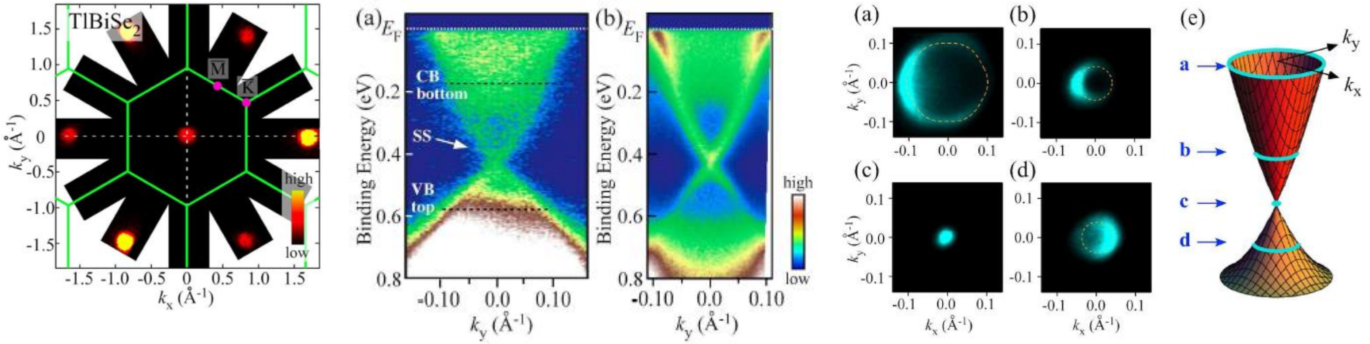
TlBiX$_2$ and TlSbX$_2$ (X=Te,Se,S)

All six compounds are topologically trivial by DFT-GGA calculation.

But

Their surface states may have Dirac-cone dispersions due to the band inversion.

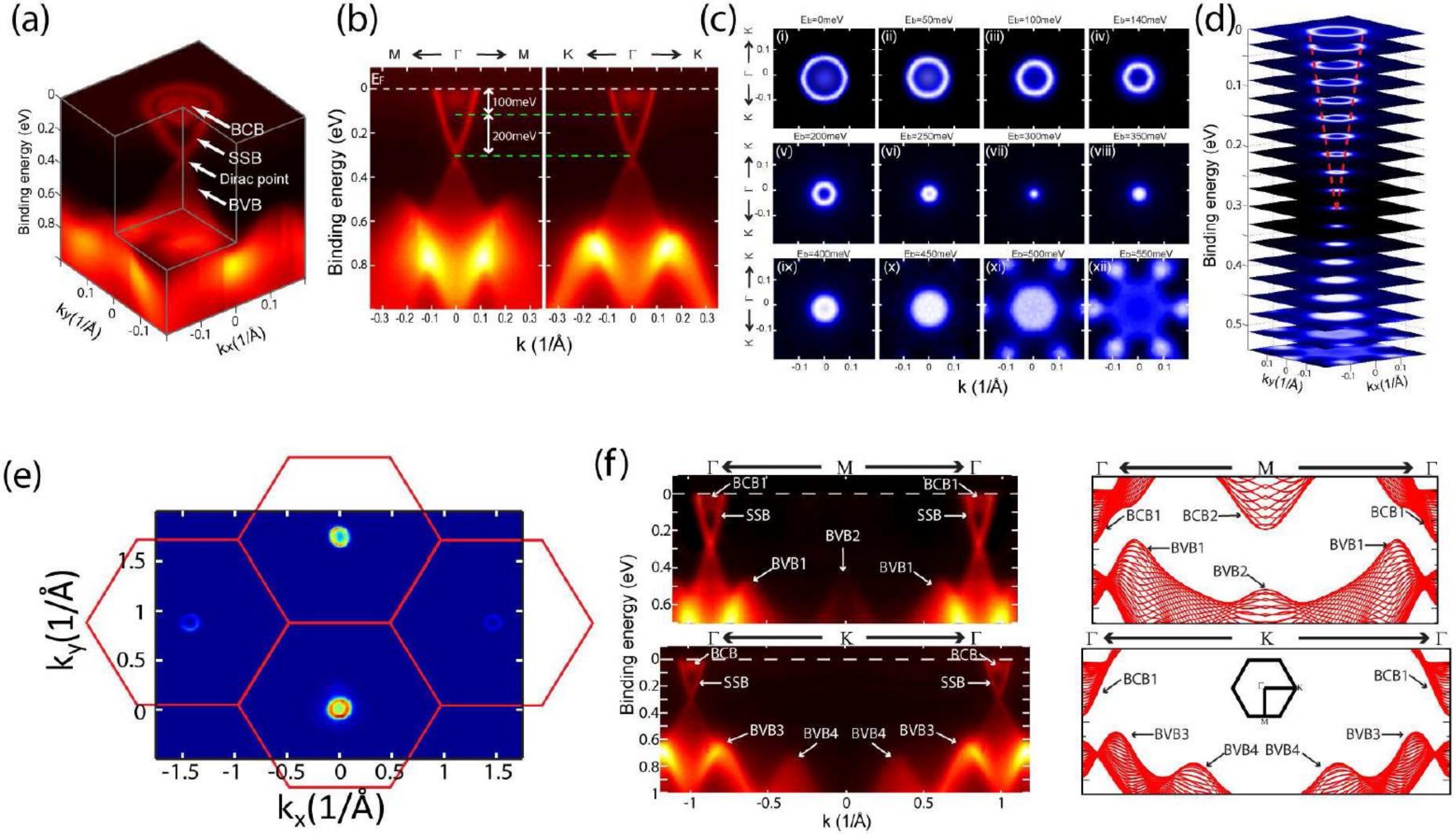
ARPES on $TlBiSe_2$



T. Sato *et al.*,
arXiv:1006.2437

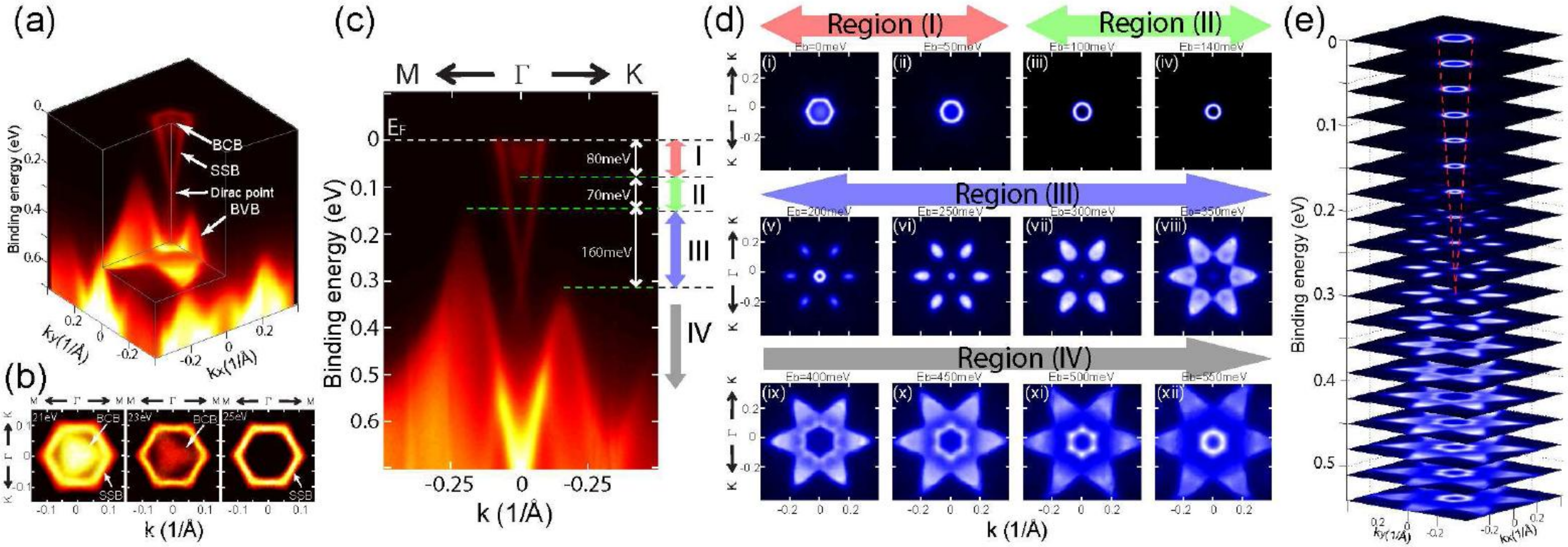
Bulk band gap 0.4eV largest

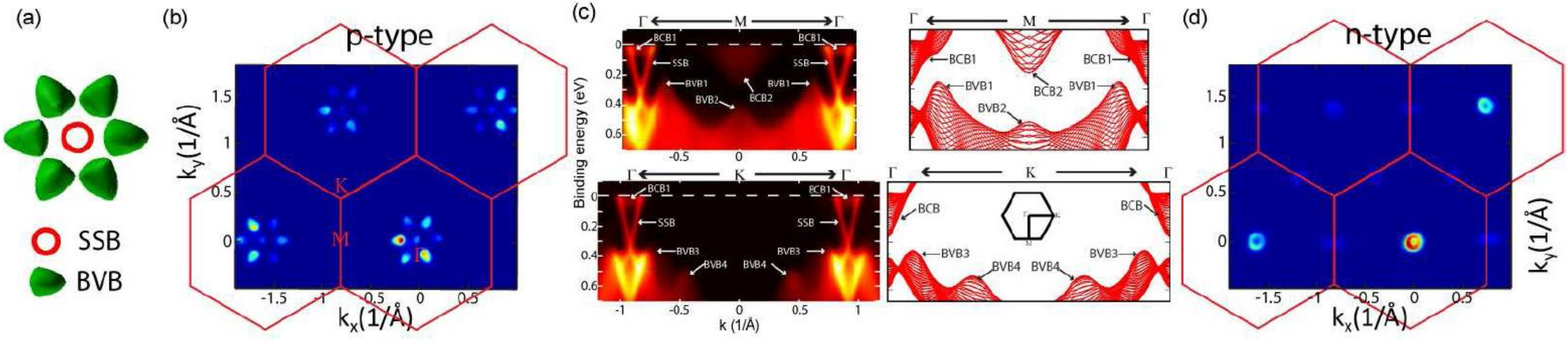
Y. Chen *et al.*,arXiv:1006.3843



ARPES on $TlBiTe_2$

Y. Chen *et al*.,arXiv:1006.3843





Conclusion

Topological insulator

2D system : Z_2 invariant

$\nu = 0$: trivial insulator
$\nu = 1$: QSH

Odd number of surface states intersect between TRIMs.

3D system : four Z_2 invariant

$\nu_0 ;(\nu_x, \nu_y, \nu_z)$

$\nu_0 = 1$: strong topological insulator (STI)
$\nu_0 = 0$: weak topological insulator (WTI)

Odd number of the surface Fermi arc enclosing TRIM

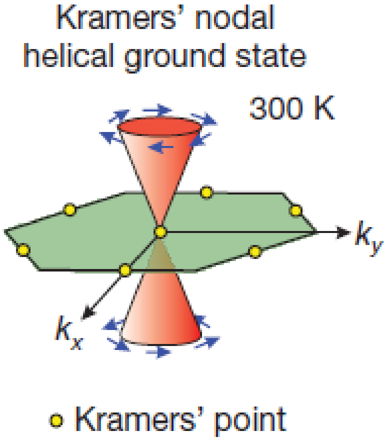
1-st

$Bi_{1-x}Sb_x$

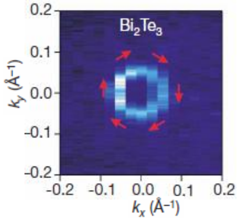
2-nd

Bi_2Se_3, Bi_2Te_3 , $TlBiSe_2$, $TlBiTe_2$

- Nearly idealized single Dirac cone
- Stoichiometric → high purity
- Large band gap ∼0.3-0.4eV

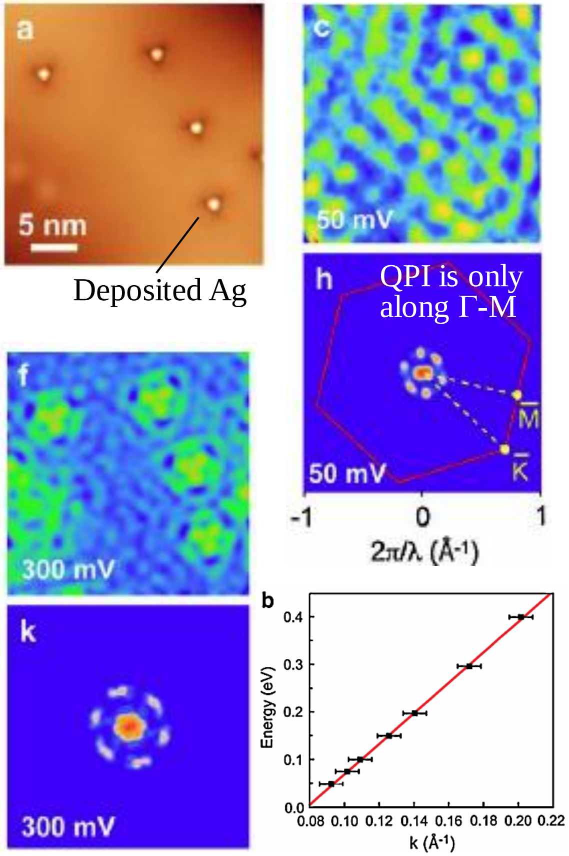


STS on Bi_2Te_3



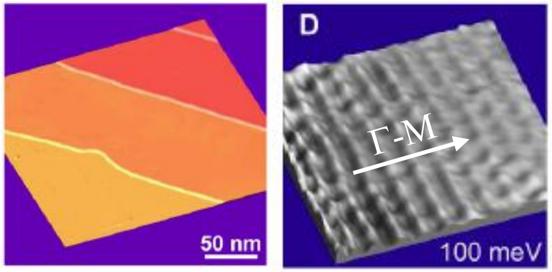
Hsieh et al.,
Nature (2009)

Zhang et al., PRL (2009)



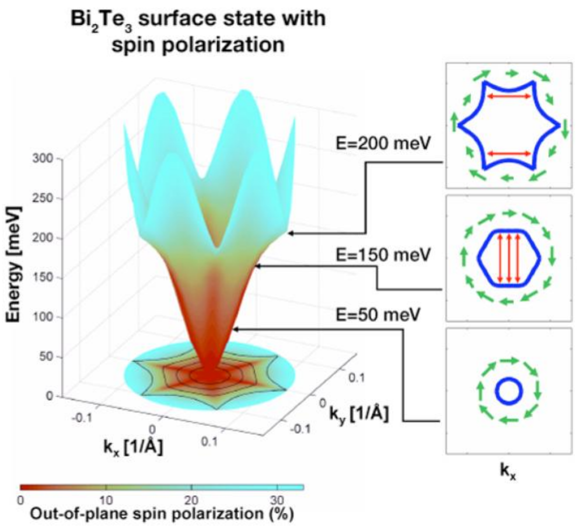
Deposited Ag

QPI is only along Γ-M

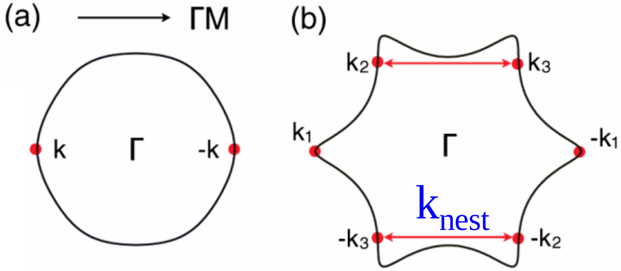


Γ-M

Hexagonal warping effect



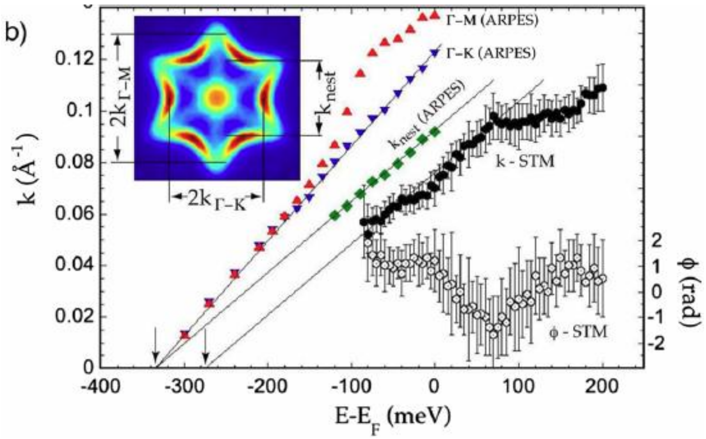
Fu, PRL (2009)

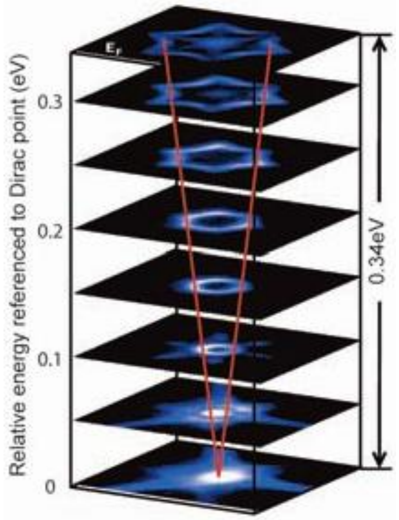


k_{nest}

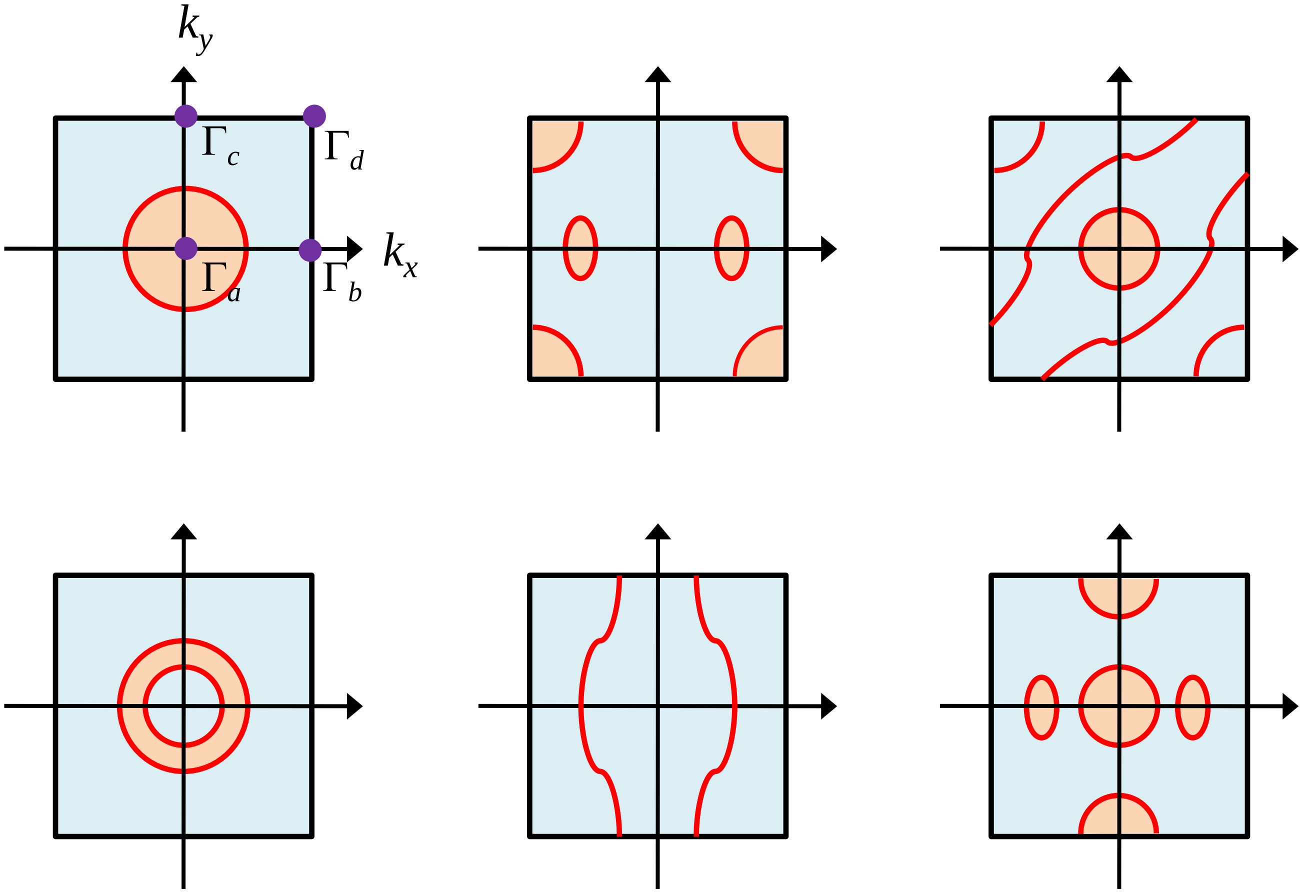
Backscattering between k's connected by the nesting vector k_{nest} (which is // Γ-M) is allowed.

Alpichshev et al., PRL (2010)





Chen et al., Science (2009)


k_y
Γ_c
Γ_d
k_x
Γ_a
Γ_b

Hofstadter's butterfly