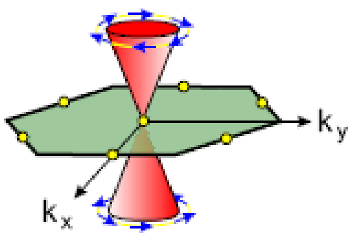
First observation of spin-textured helical Dirac cone in Topological Insulators

M Zahid Hasan
Department of Physics, Princeton University

Discovery of Strong Topological Insulator : Nature(2008), Science(2009)
(work done in 2007)

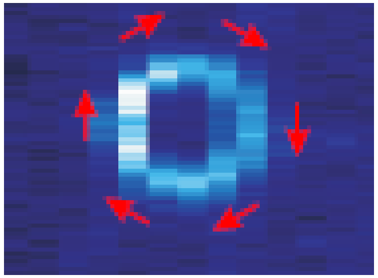
"Hydrogen Atom" of Topological Insulator Bi_2Se_3 (2008)
Observed (also Theoretically predicted) by Xia,Lin,MZH et.al.,
Nature Physics '09, N&V: Nat.Phys.'09

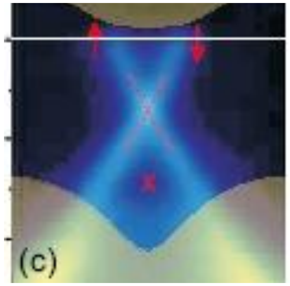


spin-Helical Dirac fermions in Topological Insulators
Hsieh, Xia, MZH et.al., **arXiv:0904.1260v1**

Direct signature of Topological Order

Bi_2Te_3

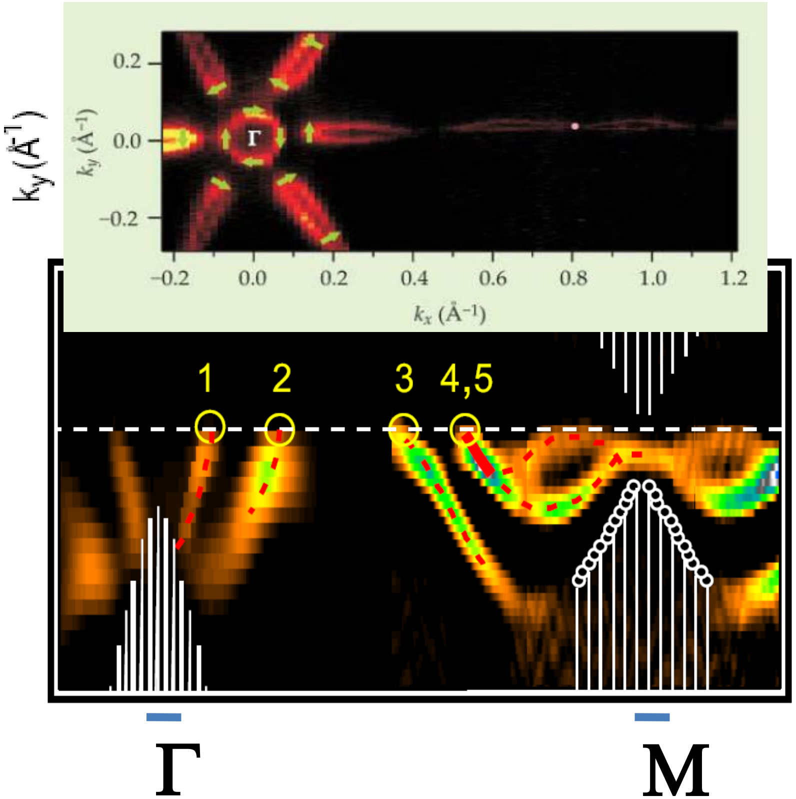




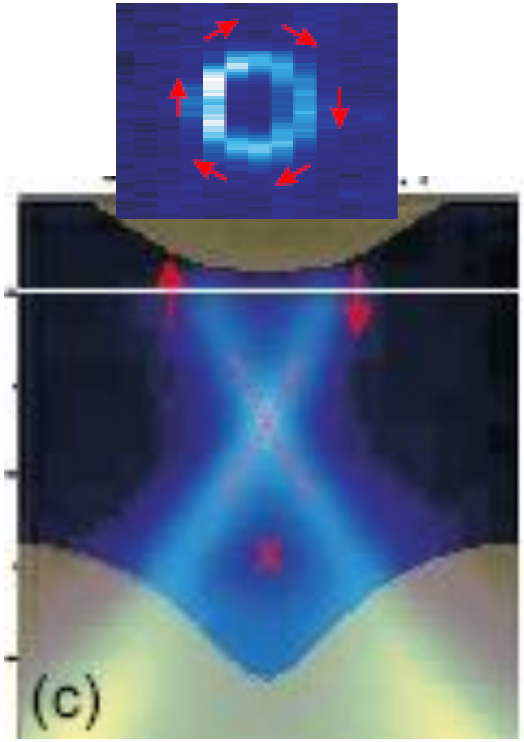
Bi_2Se_3

Experimental realizations of Strong Topo Insulators (Theta-Vacuum states) in nature :

Nature 08, Science 09



NatPhys 09, Nature 09



These two are actually 2 distinct types of strong topo insulators !

Physics Team

David Hsieh, Dong Qian, Andrew Wray, Matt Xia, MZH

Undergrads/JPs:

Cathy Kunkel
Matt Severson
Ram Shankar

High-purity Materials/Crystal Growth/Characterization

Y.S. Hor, R.J. Cava (Chem), J. Chechelsky, N.P. Ong (Physics),
D. Hsieh, Y. Xia, MZH (Physics), N.L. Wang (Beijing), H. Eisaki (Tokyo)

Acknowledgements :

Physics Experimental team : D. Hsieh, Y. Xia, D. Qian, L. Wray, A. Pal

Beamline/Detector/Instrumentation :

A. Fedorov, J. Osterwalder, L. Patthey, H. Dil, Y. Chuang

Quantum Hall effect/Topological Field Theory :

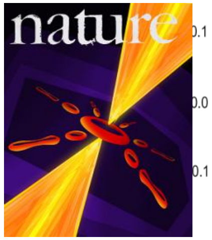
C.L. Kane, D. Haldane, J.E. Moore, F. Wilczek, A. Bernevig, X.-G. Wen, D. Tsui
Liang Fu, L. Balents, S.C. Zhang, D. Huse, N.P. Ong, B. Halperin, C. Callan

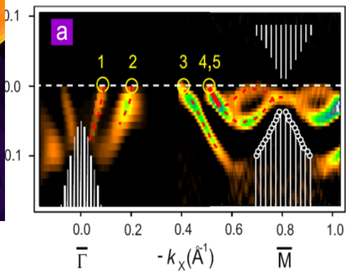
U.S. DOE, NSF, A.P.Sloan Foundation, R.H.Dicke Fdn (Princeton), MRSEC

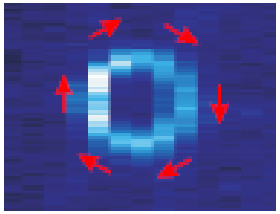
[Topological Insulators](#) *Quantum Spin Hall effect, Topological-Order, Spintronics*

*Angle-, Spin-*Resolved Spectroscopy

Nature (2008), N&V: Nature Phys (2008)
Science (2009), Nature Phys (2009)
Nature (acpt, 2009), Nature (in rev, 2009)



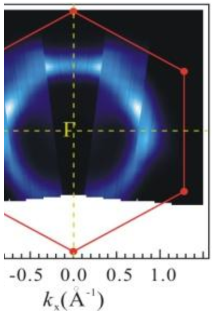


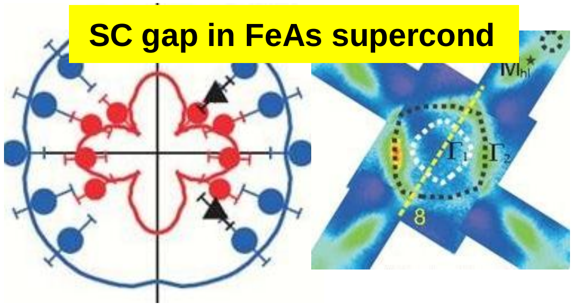


[Exotic Superconductors](#) *Fermi surface, Spontaneous SB, SC gap, Self-energy*

Photoemission, Resonant X-ray Scattering

Nature (in rev) (2009), Phys.Rev.Lett.(2009)
Phys.Rev.Lett.s (2007a,b,c), PRL/B (2008)
Phys.Rev.Lett.s (2006 a,b,c)
Science (2000), Phys.Rev.Lett.(2004)

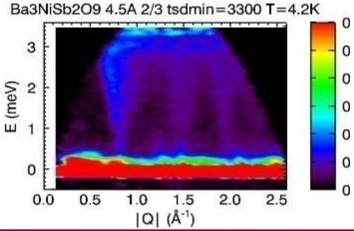


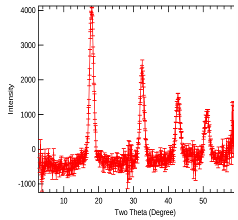


[Frustrated Magnetism](#) *Spinon dynamics, Quantum Criticality*

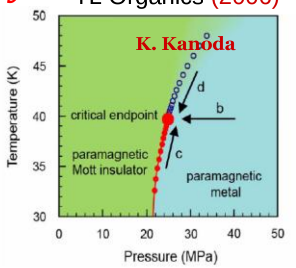
Polarized Neutron Scattering

Phys. Rev.Lett. (subm.) (2009)
Z. Tan Senior-Thesis, P.U. (2005)



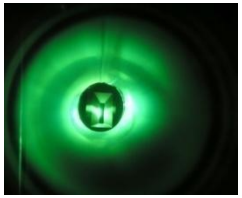


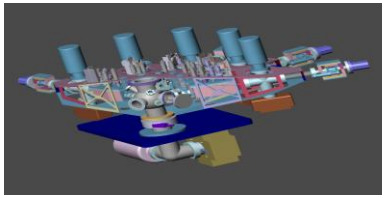
Quantum Spin-liquid
TL Organics (2006)

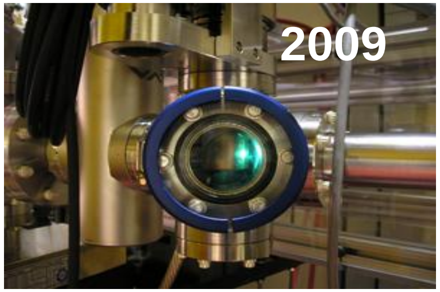


Spectrometer development

MERLIN Project
Spin detector Project
Projects at LBNL & SLAC

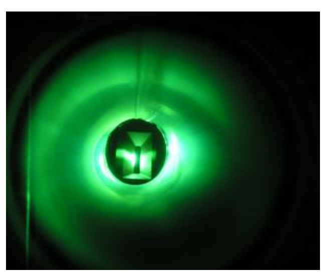


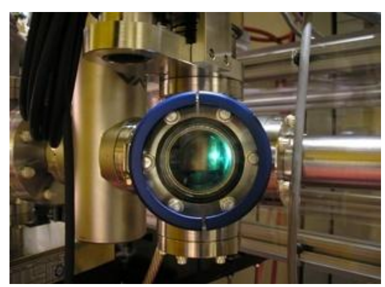


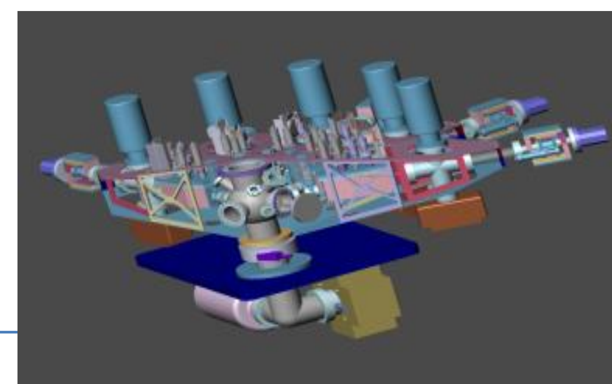


Accelerator Facilities

Beamline/Spectrometer/Detector development :







Collaboration with LBNL(ALS)

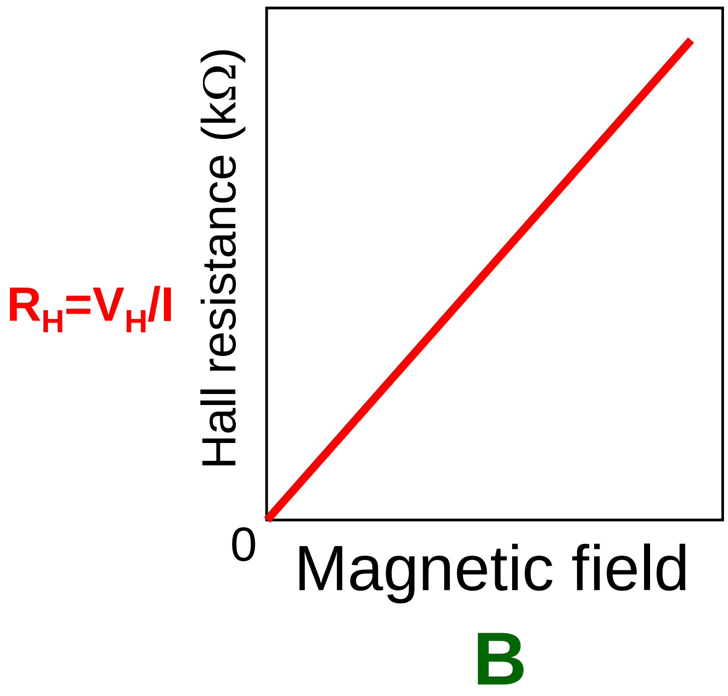
~~ Outline ~~

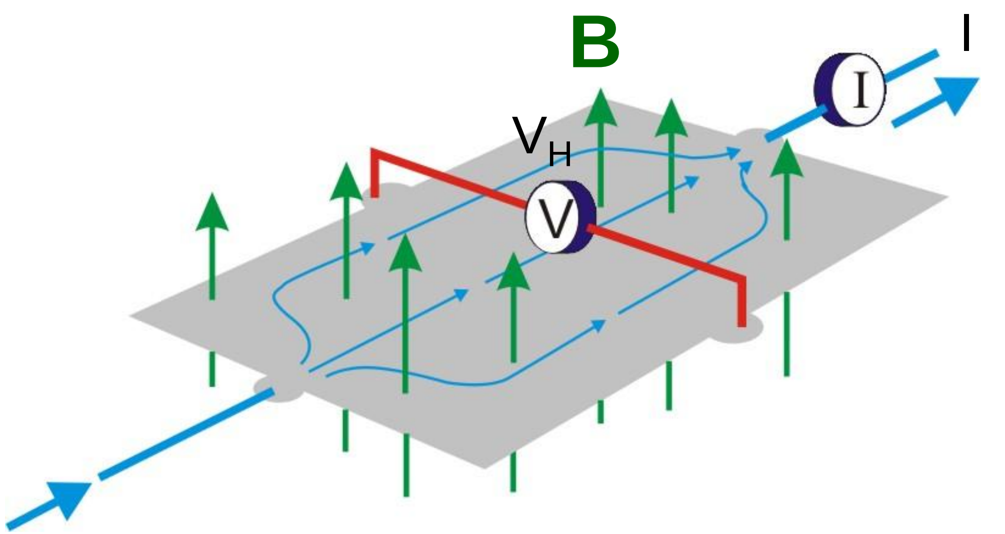
- QHE & Topological Invariants
- How to measure Topo Quantum numbers?
- Spin-resolved-photoemission (spin-ARPES)
- Observation of Topo Insulators
- Determination of non-trivial Berry's phase
- Future Directions (Topo. QC, TEC etc.)

Metals feature no gap: current can flow (no energy gap):
How many carriers ? what sign ?

Hall Effect

Edwin H. Hall (1879)

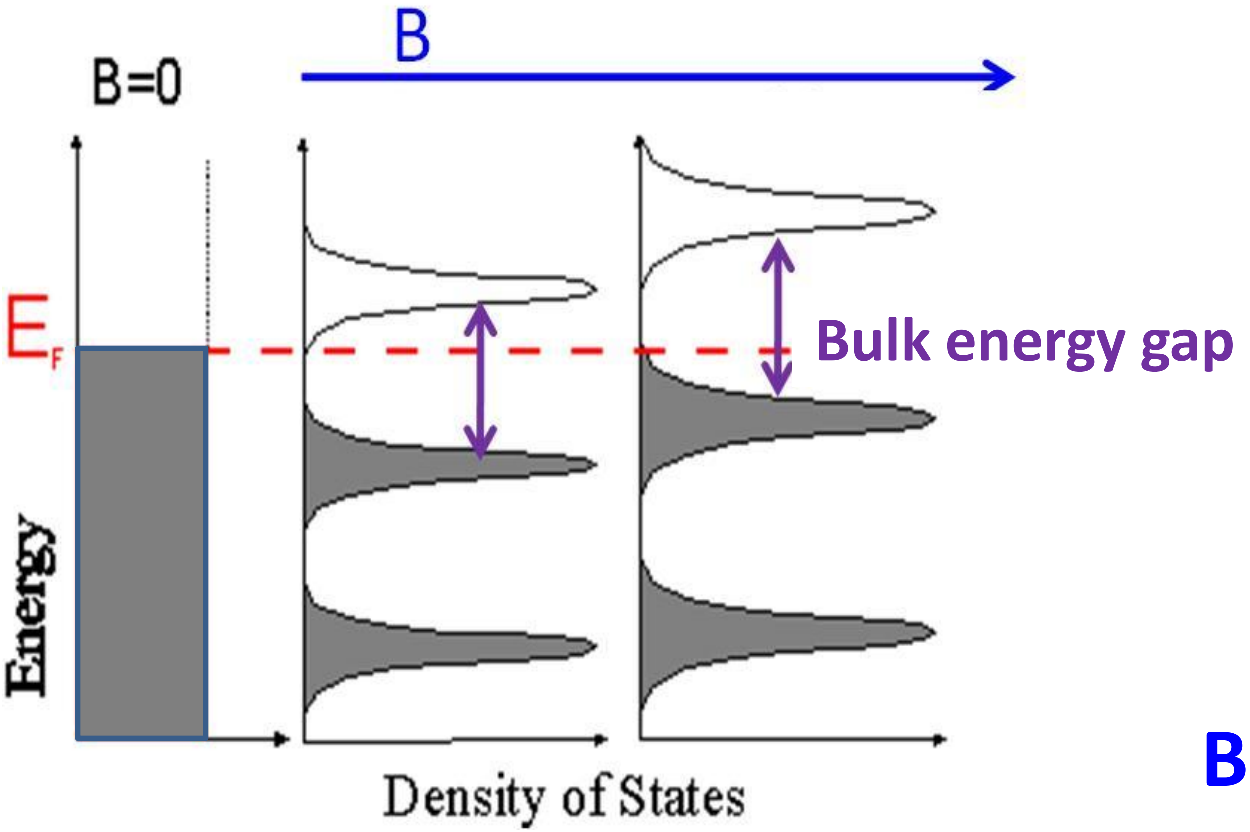




Hall resistance $R_H=V_H/I$

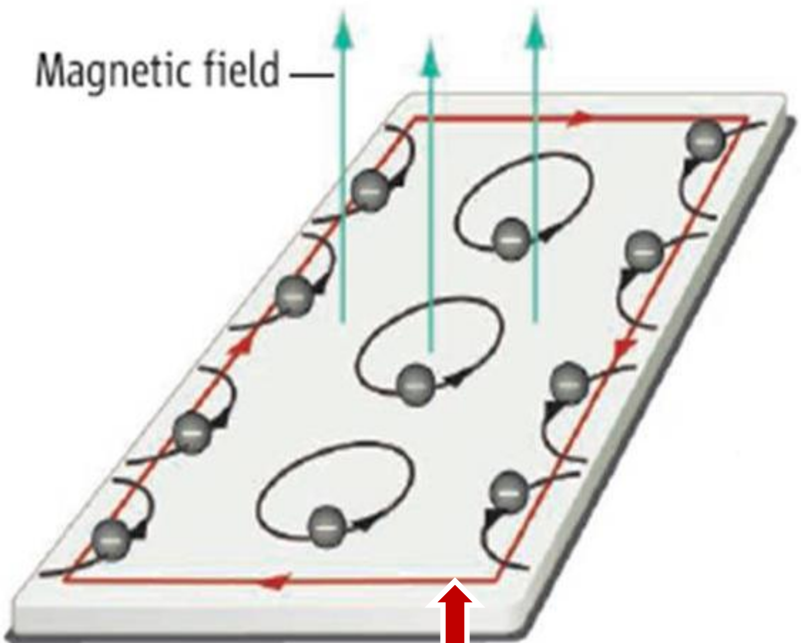
Hall Effect at **high** magnetic fields

Electrons + strong magnetic field → Discrete Energy Levels



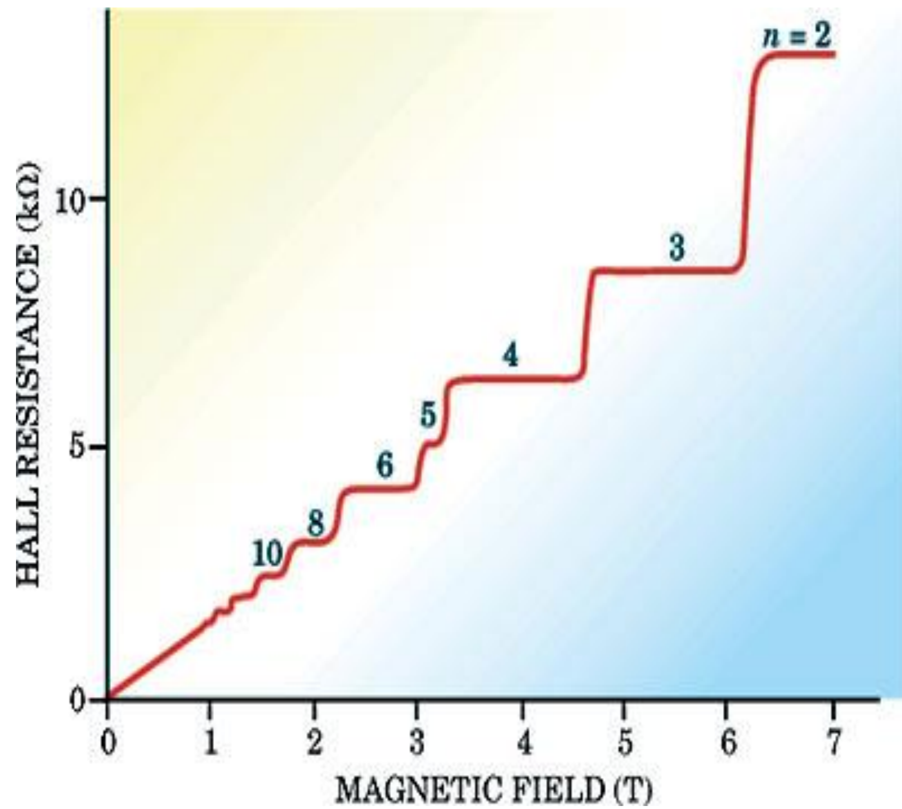
Band Insulator?

Bulk Insulator but **Conduction through the Edge**



Conduction through the boundary

Finite Hall Conductivity

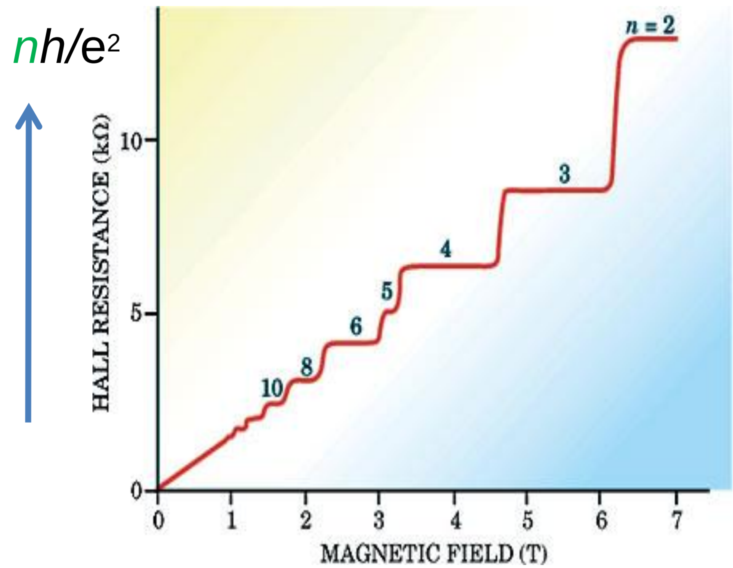


Quantum Hall Effect

K. von Klitzing et.al., (Nobel Prize, '85)

D.C. Tsui et.al.,(Nobel Prize, '98)

Quantum Hall State : Topological, TR-breaking



Hall conductance:

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

n = Chern no. (**Edge** states)

S. Chern : Quantum version (Hilbert space) of Gauss-Bonnet formula

Topological Property

$$n = \frac{1}{2\pi}\int_{BZ}[\nabla_{\mathbf{k}} \times \mathbf{A}(k_x, k_y)]_z d^2\mathbf{k}$$

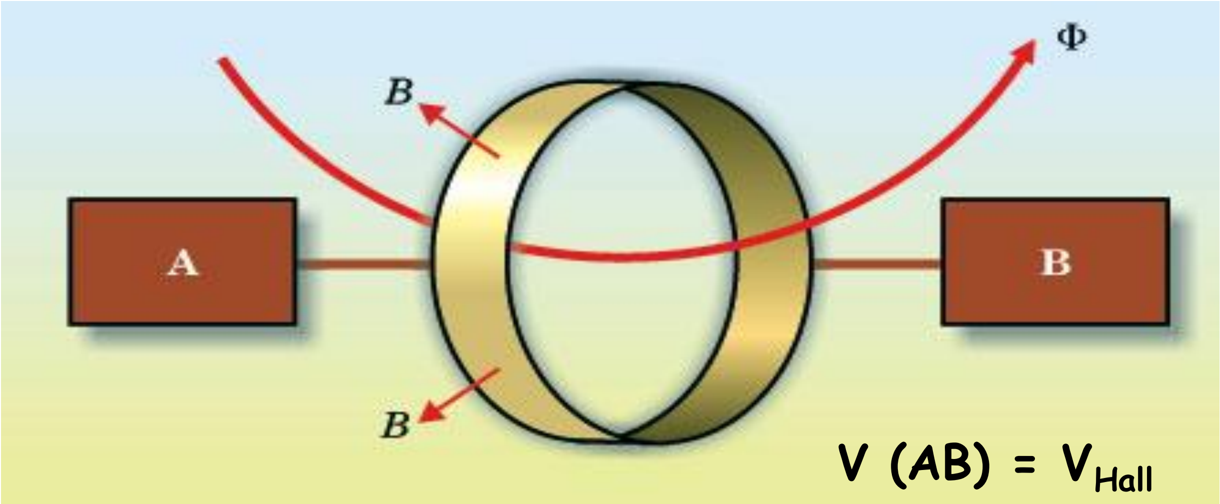
TKNN invariant

$$\mathbf{A} = -i\langle u_{\mathbf{k}}|\nabla_k|u_{\mathbf{k}}\rangle$$

Electron-occupied **Bulk** bands

Finite ***n*** → **topologically "protected" edge-states**

Laughlin cylinder : Quantum Hall State (IQH)



ϕ=h/e inserted through the cylinder (at filling N) results in a transfer of N electrons from one end of the cylinder to the other (quantum charge pump). Change in charge polarization.

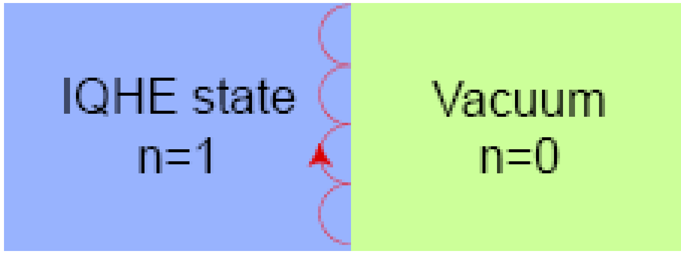
A generalization of Gauss-Bonnet formula to the geometry of the eigenstates parameterized on a surface (geometry <-> topology/#handles). A topological invariant the Chern integer characterizes the IQHE state precisely. It characterizes this quantized change in charge polarization. Weak sensitivity to disorder.

No SBS, no local OP.

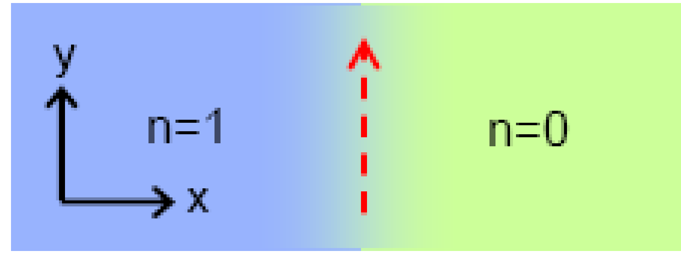
Avron Phys. Today. (2003)

Edge States

Gapless states must exist at the interface between topologically distinct phases



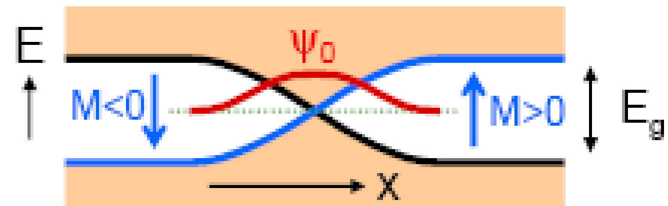
Edge states ~ skipping orbits



Smooth Interpolation

2 Band Model : Dirac Eq.

$$H = -iv(\sigma_x \partial_x + \sigma_y \partial_y) + M(x)\sigma_z$$



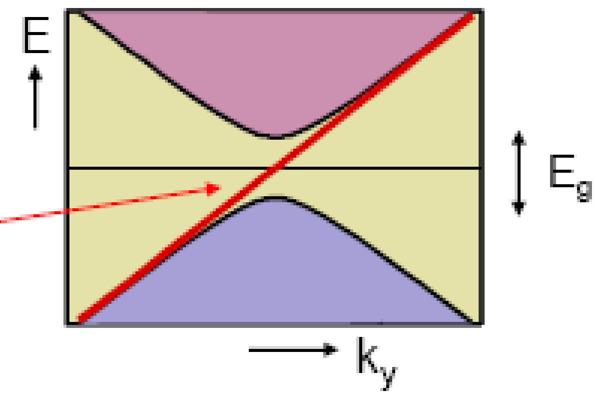
$M(x) = M_0$: Gap $E_g = 2M_0$

$$E(k_x, k_y) = \pm\sqrt{v^2 |k|^2 + M_0^2}$$

Gapless Chiral Fermions

$M(x) \sim M_0$ sgn(x) : "Domain Wall bound state"

$$\psi_0(k_y, x) \sim e^{ik_y y} e^{-M_0 |x|/v} \begin{pmatrix} 1 \\ i \end{pmatrix} \qquad E_0(k_y) = vk_y$$



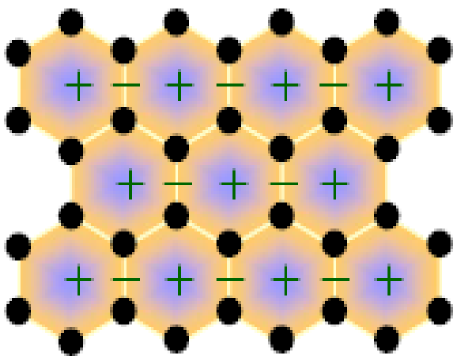
Slide from C. Kane

"Quantum Hall Effect" without Magnetic Field?

Haldane Model (1988)

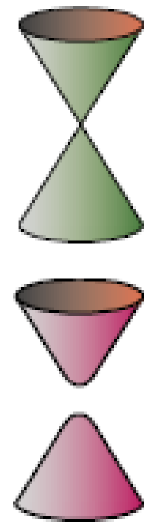
Alternating field but net magnetic field is zero

Bulk band-structure



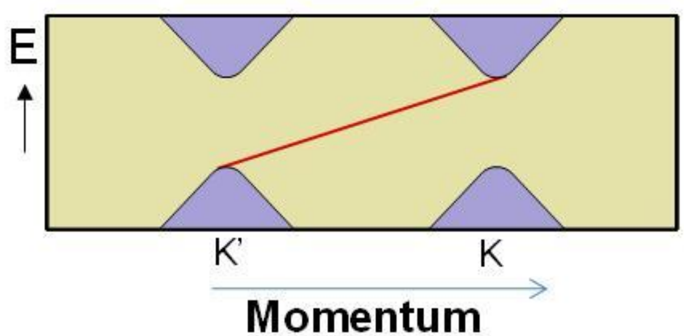
$B(r) = 0$
Zero gap,
Dirac point

$B(r) \neq 0$
Energy gap
$\sigma_{xy} = e^2/h$



Dirac point

Massive Dirac particles



Edge structure

Chiral fermions

Hall Transport is determined by band-structure
Edge <-> Bulk

Do QHE-like topological phases exist in nature that are time-reversal invariant?

Topological state in 2D (spin Hall state)

Kane & Mele (2005), Bernevig & Zhang (06), Murakami (06)
Sheng, Haldane et.al.(2006) also others

Distinct new Topo state in 3D (Theta-vac, Axionic state)

Moore & Balents (07), Fu, Kane & Mele (07), Roy (09)
Qi, Hughes, Zhang (08), Essin, Franz, Moore, Vanderbilt, X.G. Wen (08)
Ryu, Ludwig, Schnyder (08), Kitaev (08) and others
Earlier work by Wilczek, Callan, Witten and others (70-80s)

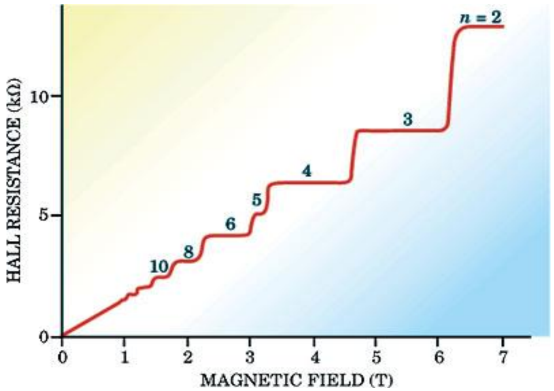
Experimental realization : Nature 08, Science 09, NatPhys 09

Topological Theta vacuum (3D) is distinct from spin Hall state (2D).
This is not the case for quantum Hall state. 2D and 3D QH states are the same!
Theta vacuum (3D) or the 3D Topological Insulator is the most exotic state!

QHE phases

$\sigma_{xy} = ne^2/h$

Topological quantum number



Transport

Topo Insulators

How to experimentally "measure" the topological quantum numbers (ν_i) associated with the quantum spin Hall (QSH) or Strong Topological Insulator (STI) phases?

No quantized transport!

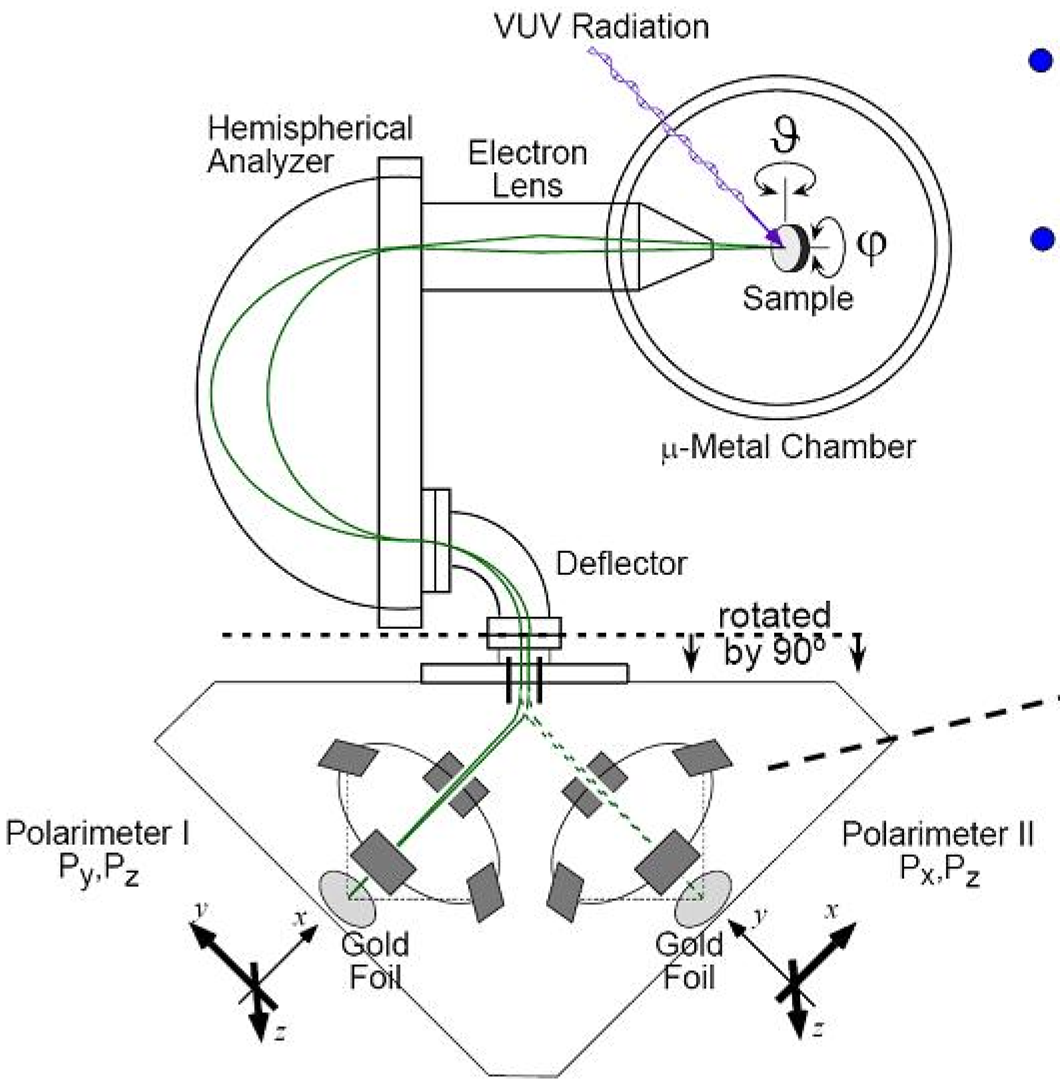
$\{\nu_i\}$

Topological quantum number

?

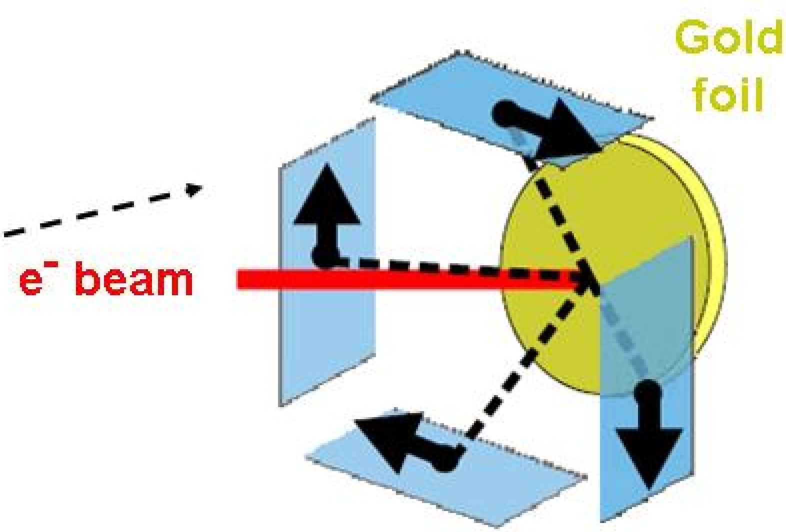
Spin-sensitive Momentum-resolved Measurements!

Double Mott detector configuration



M. Hoesch

- Each Mott detector measures 2 orthogonal spin components
- Double Mott detector captures 4 (3 indep.) spin components



SLS set-up (2008)

First generation materials:

Gap too small *Graphene*

No SS in *Pb(Sn)Te*

2D
(spin Hall state)

Hg(Cd)Te

<u>Charge Transport</u>
measurements of
edge-states
Konig et.al., (Molenkamp).
SCIENCE (2007)

3D
(Theta-vac state)

$Bi_{1-x}Sb_x$

<u>spin-ARPES (spin-sensitive)</u>
measurements of edge-states
Hsieh et.al., (Hasan).
NATURE (2008)
SCIENCE (2009)

Second generation : "hydrogen atom" materials

Bi_2Se_3

"Hydrogen Atom" of Topological Insulator
Xia et.al., arXiv:0812.2078v1
NATURE PHYSICS (2009)

Sb

SCIENCE (2009)

Sb_2Te_3

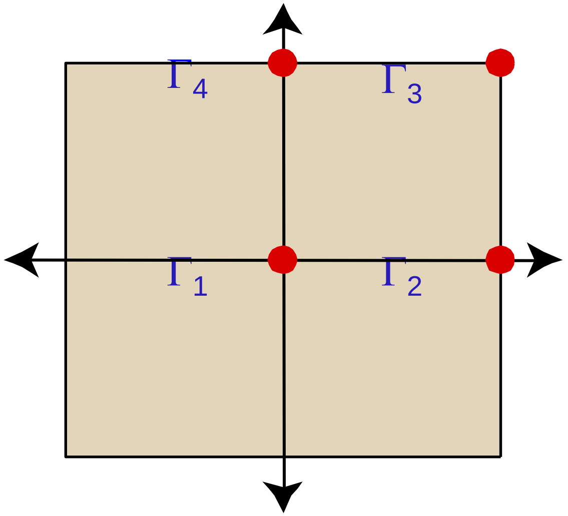
Bi_2Te_3

see my **KITP talk** (2008)

Hsieh et.al., **arXiv:0904.1260**

Topological (Z_2) invariants :

Inversion Symmetry : **Parity of occupied Bloch states** at $\Gamma_{1,2,3,4}$



Bulk Brillouin Zone

$$P|\psi_n(\Gamma_i)\rangle = \xi_n(\Gamma_i)|\psi_n(\Gamma_i)\rangle$$

$$\xi_n(\Gamma_i) = \pm 1$$

$$(-1)^{\upsilon} = \prod_{i=1}^{4} \prod_{n} \xi_{2n}(\Gamma_i)$$

ν = 0 or 1

In 3D (8 bulk KPs) there are **4 Z_2 invariants: ($\nu_0 ; \nu_1 \nu_2 \nu_3$)**
Characterizing the bulk. These determine how edge states Connect → 16 topological phases!!

Moore & Balents, Fu, Kane & Mele (2007), Roy (2009)

Direct/unique Detection of Topological Order

via

Direct Imaging of Edge-structure

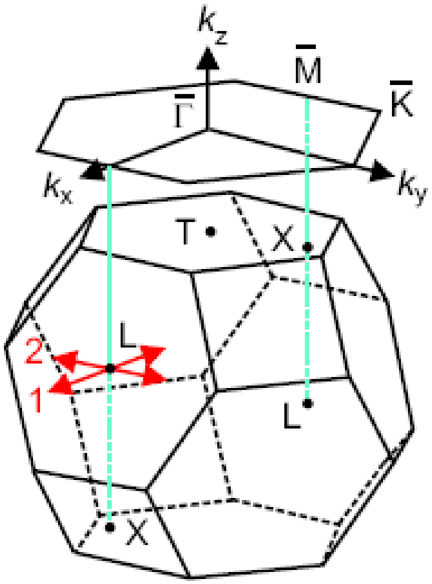
*Surface/Interface **Dirac Fermions***

***Spin Texture** of surface/edge electrons*

Bulk** band-structure, **parity set

Insulating bismuth-Antimony

Band inversions at 3 L points
T point is not inverted



Bulk Low-lying states(Bi)

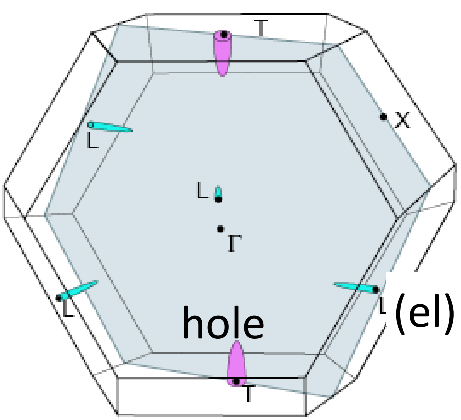
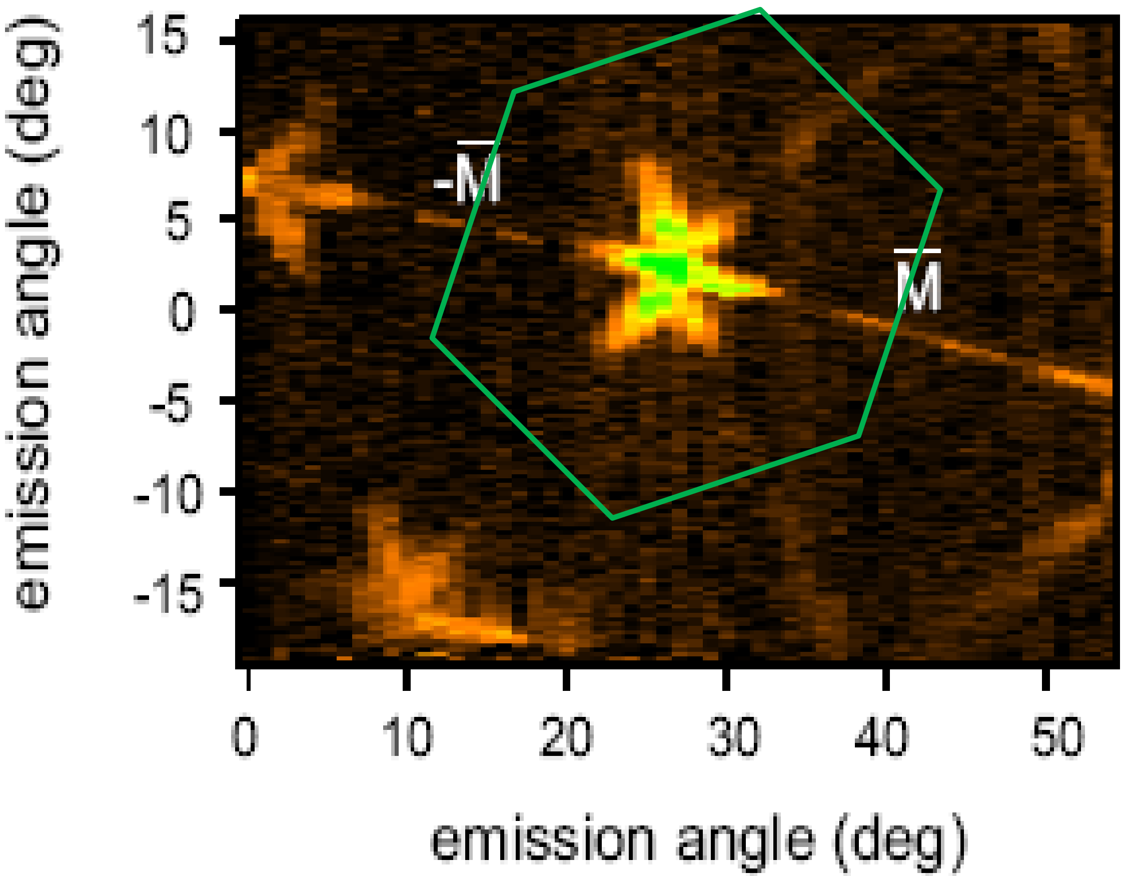
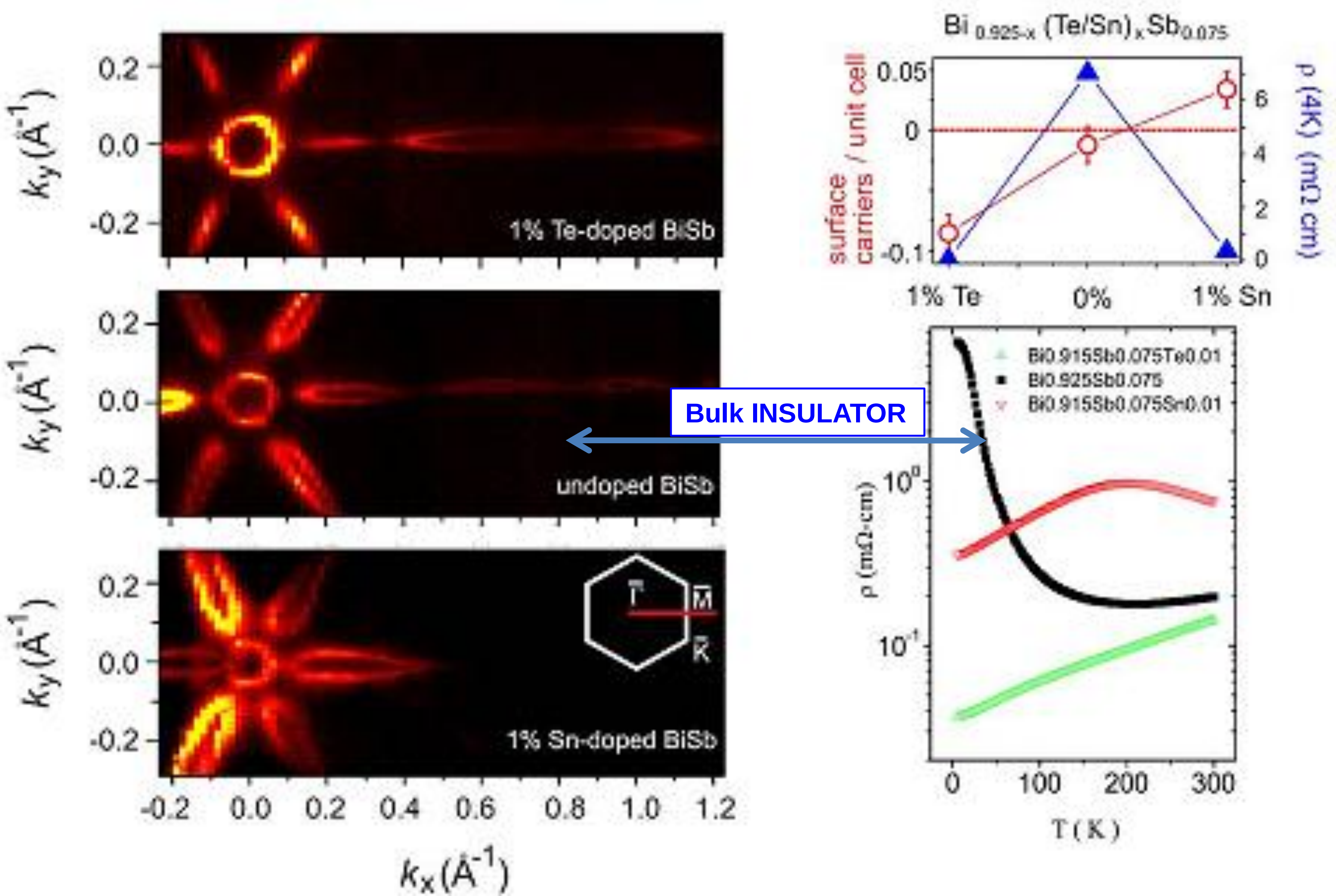


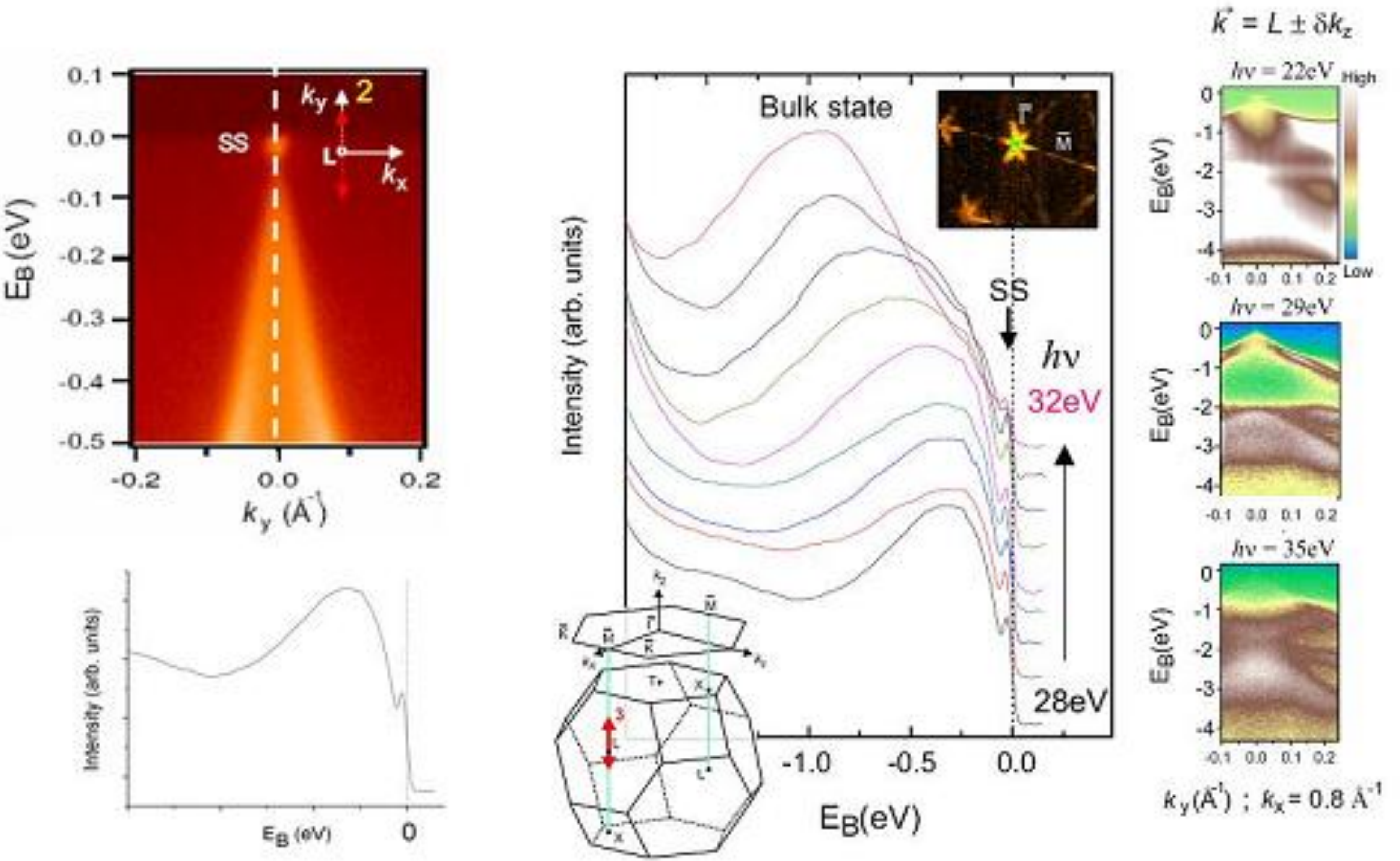
Photo-Emission intensity at Fermi level

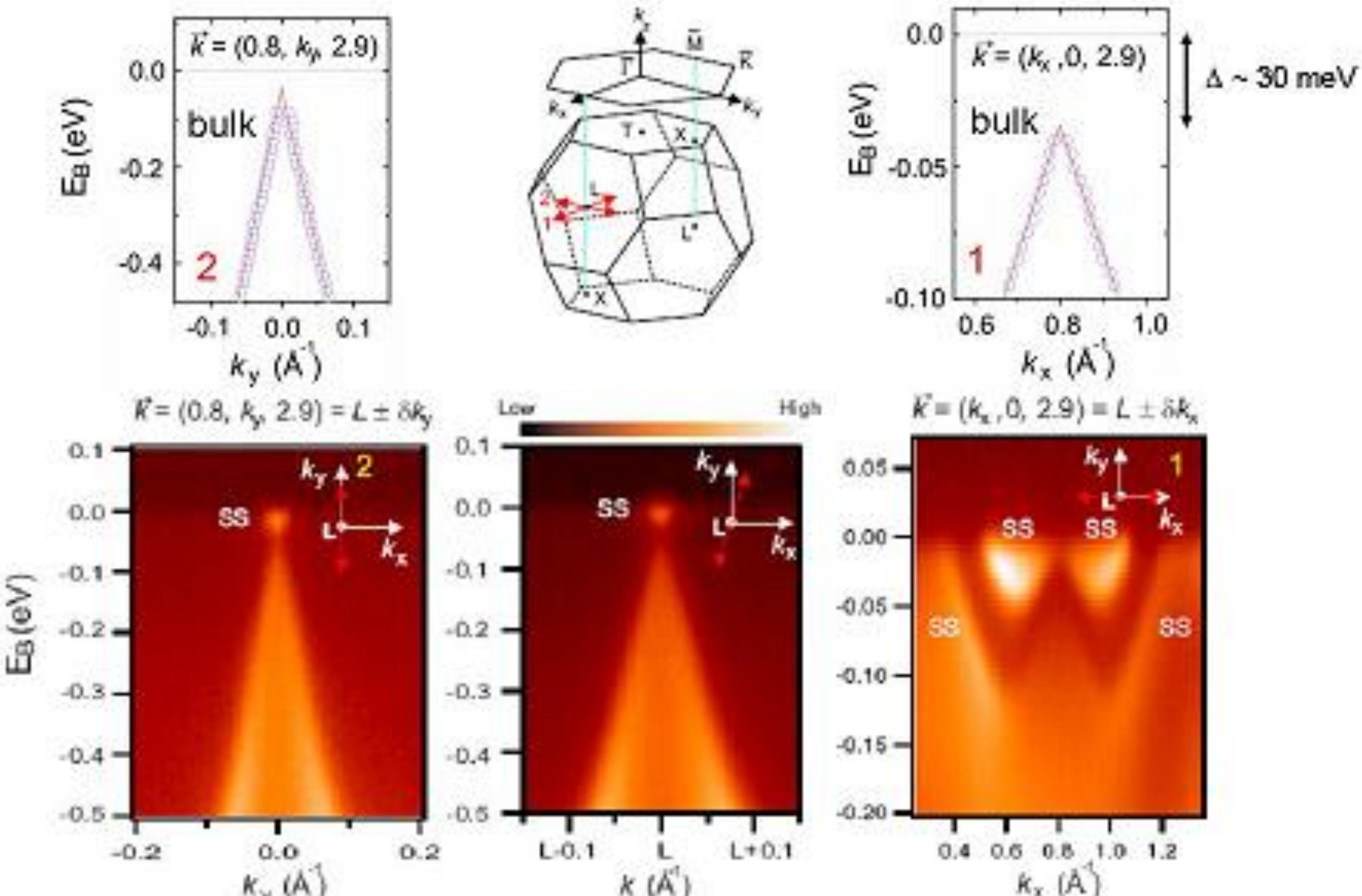


Tuning to the topological insulator regime in $Bi_{1-x}Sb_x$



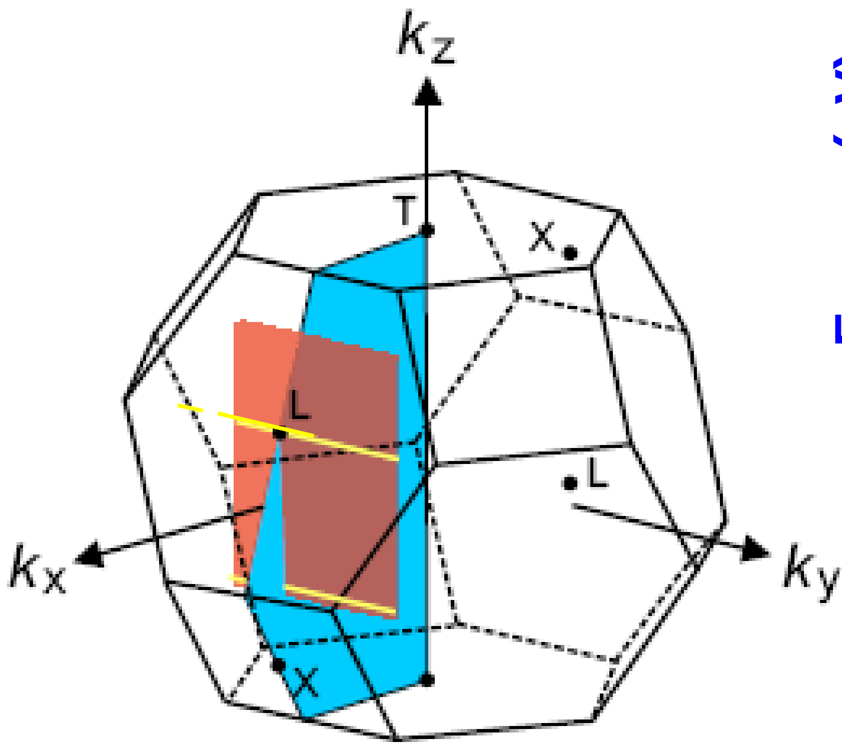
How to isolate Bulk vs. Surface states ?

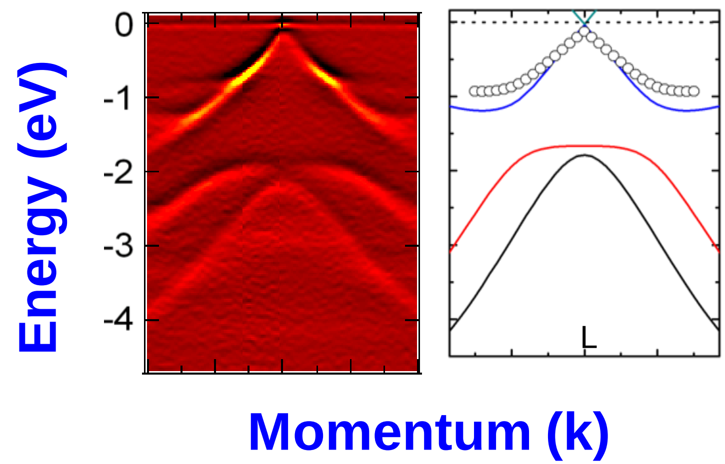


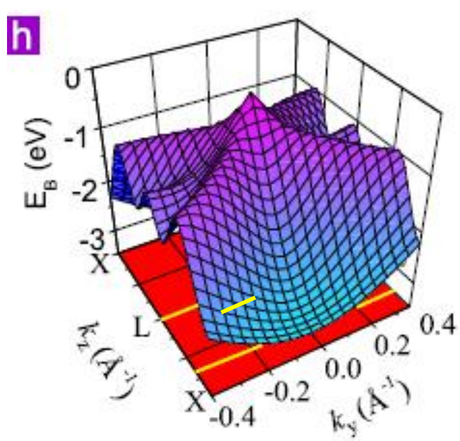


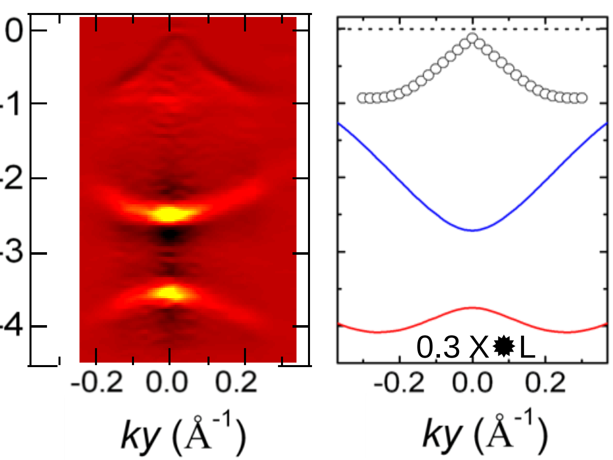
k⃗ = (0.8, ky, 2.9)
bulk
2
EB (eV)
ky (Å-1)
kz
M̄
Γ̄
R̄
kx
ky
T
X
L
L*
X
1
2
k⃗ = (kx ,0, 2.9)
bulk
1
Δ ~ 30 meV
kx (Å-1)
k⃗ = (0.8, ky, 2.9) = L ± δky
Low
High
k⃗ = (kx ,0, 2.9) = L ± δkx
SS
ky
kx
L
k (Å-1)
L-0.1
L+0.1

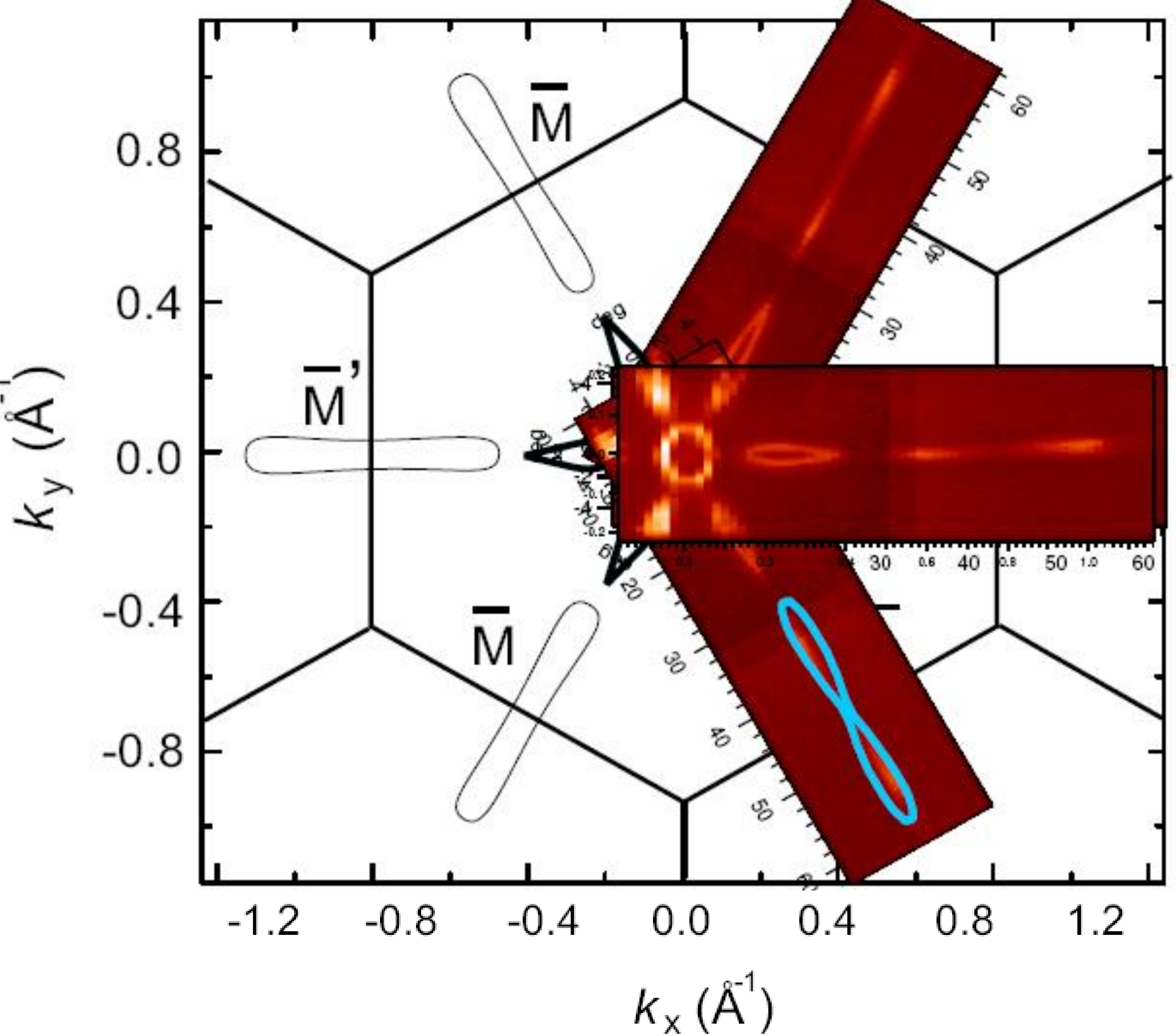
Expt. data vs. bulk band calculation







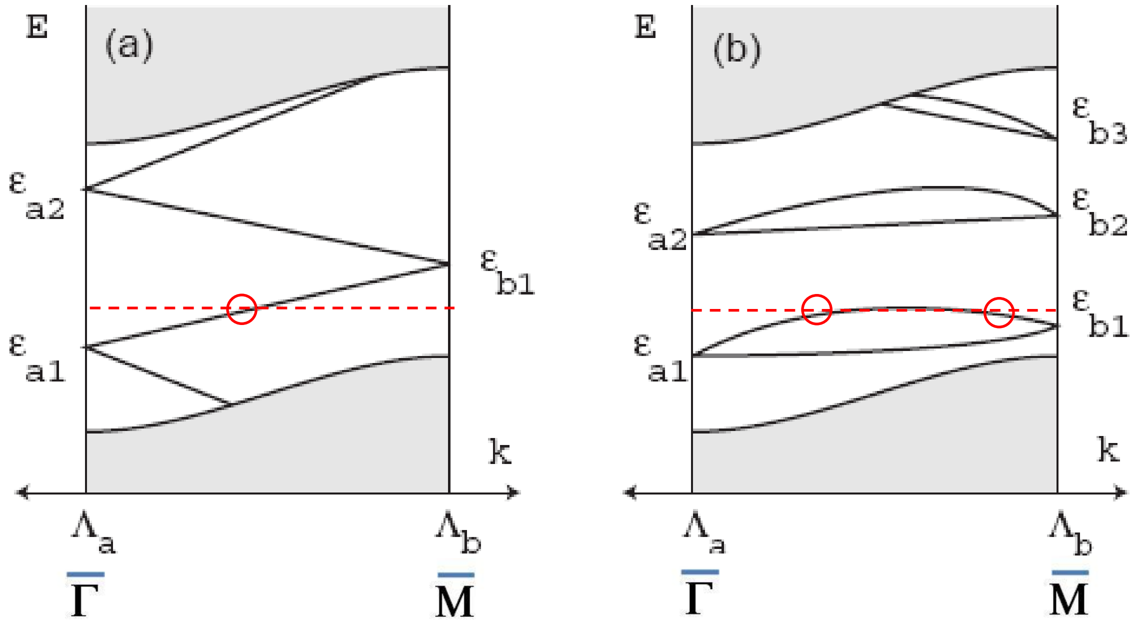




0.8
0.4
0.0
-0.4
-0.8
-1.2
-0.8
-0.4
0.0
0.4
0.8
1.2
k_y (Å^{-1})
k_x (Å^{-1})
M̄
M̄'
M̄
30
40
50
60

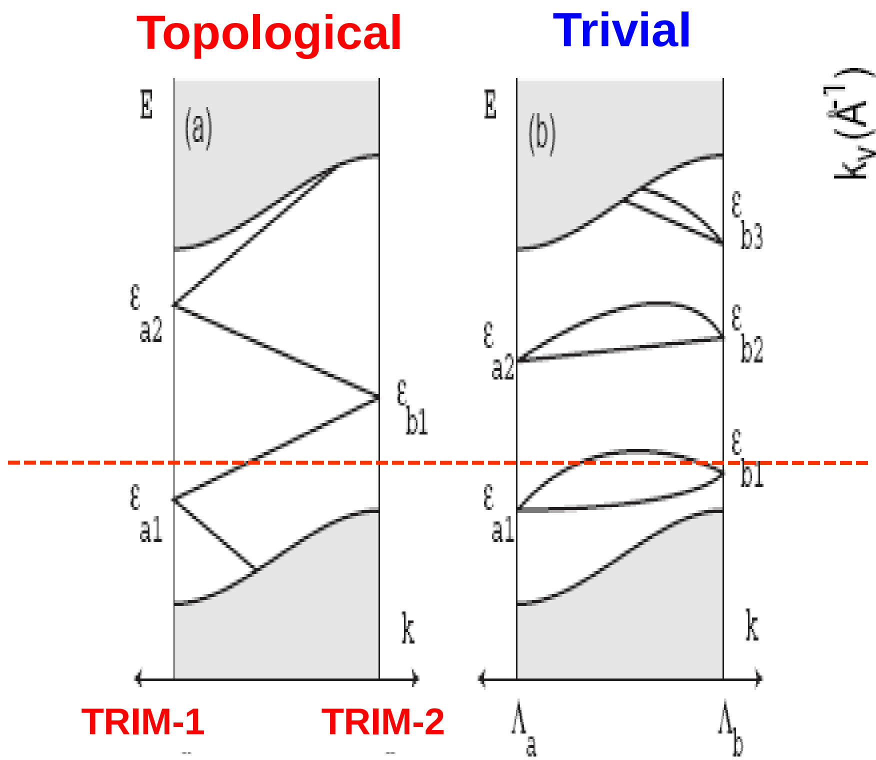
Signatures of the Topological edge states

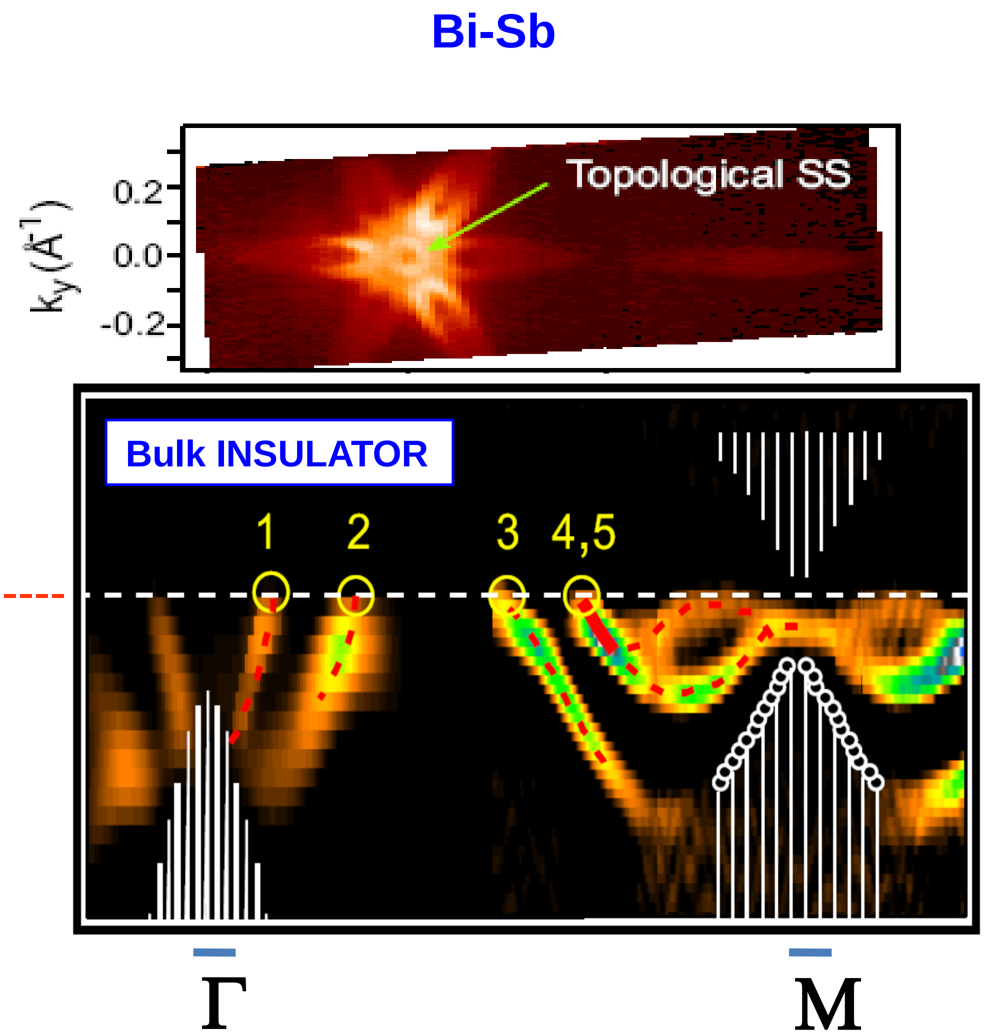
Z_2 invariant characterizes the presence or absence of Kramers degeneracy associated with a boundary

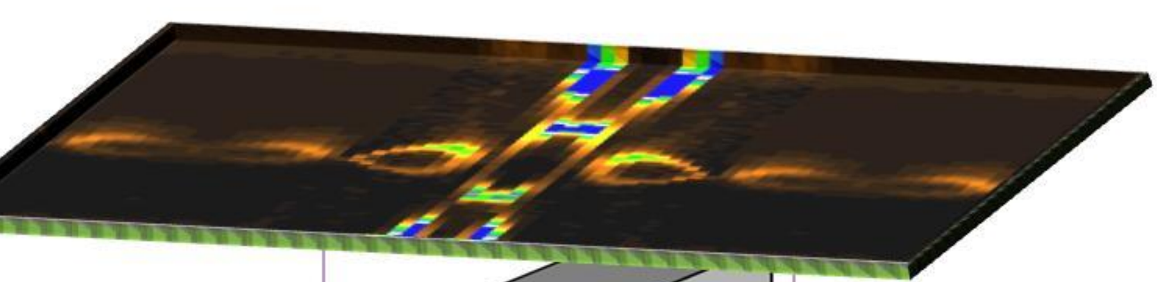


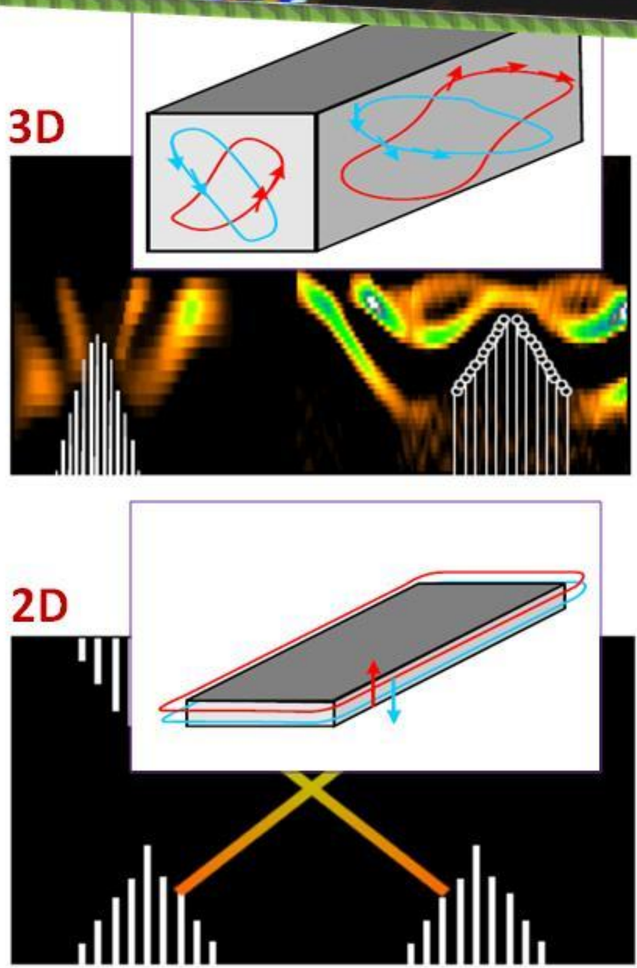
# crossing between TRIM	odd	even
Z_2 class	-1	+1
Protected bulk crossing	yes	no

Gapless odd number modes at the boundary

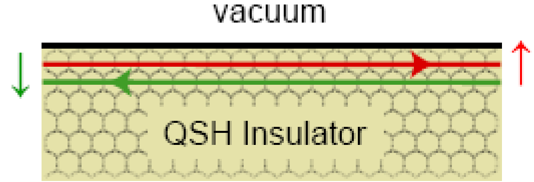




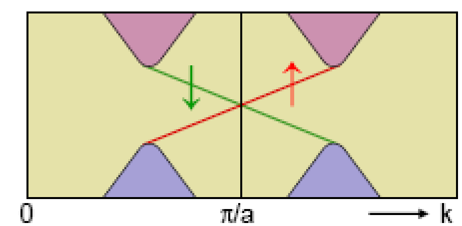




Spin Filtered edge states

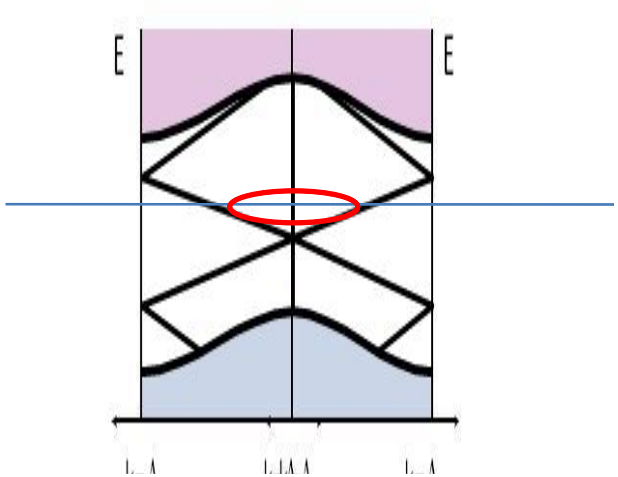


Edge band structure



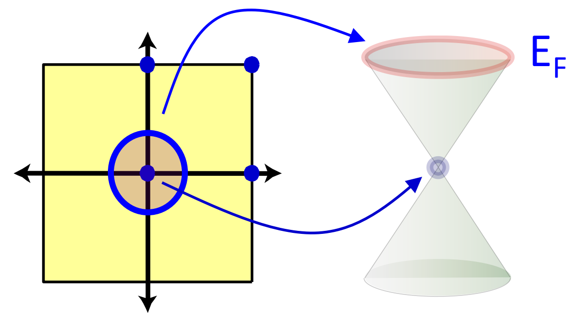
Edge states form a unique 1D electronic conductor

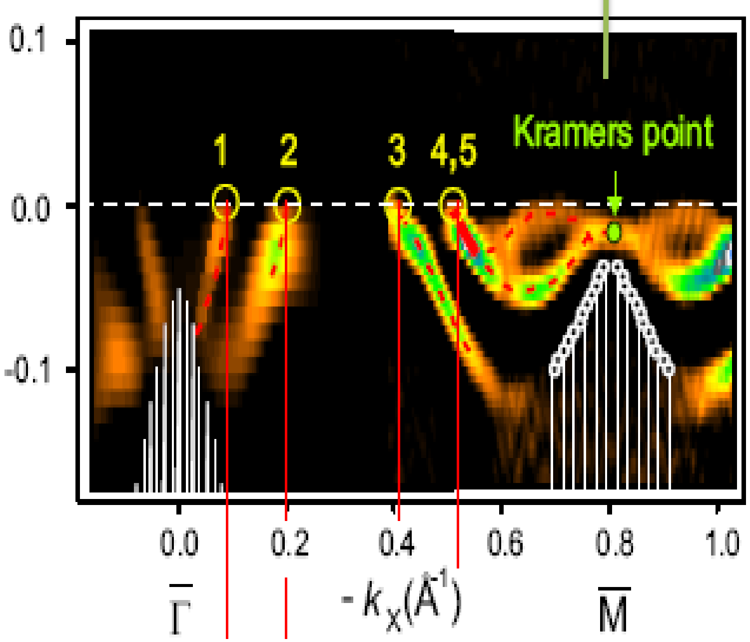
- HALF an ordinary 1D electron gas
- Protected by Time Reversal Symmetry (conservation of S_z is NOT essential)
- Elastic Backscattering is forbidden. No 1D Anderson localization

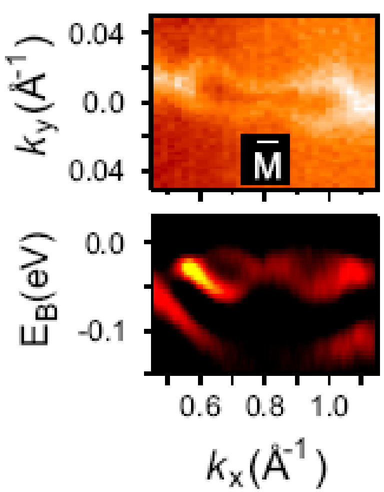


Topological Insulators

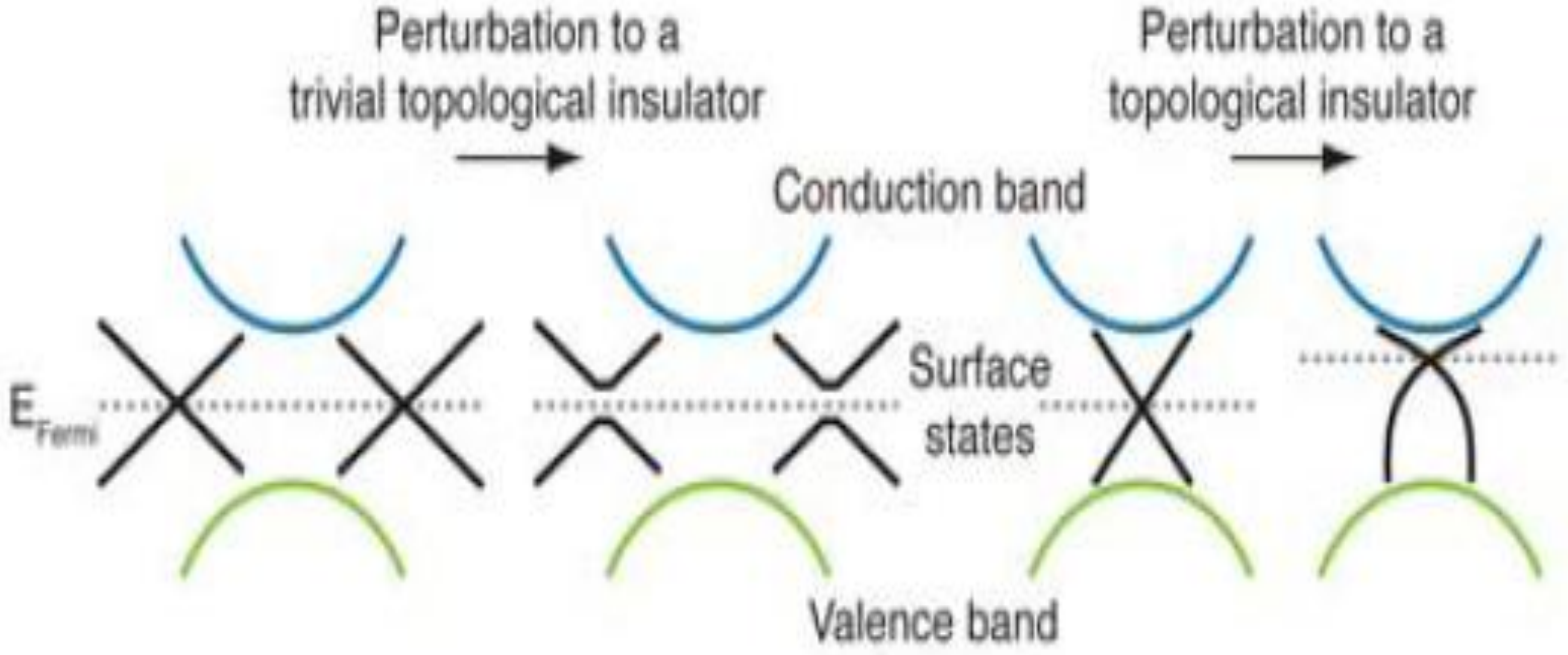
Surface Fermi pockets must enclose ODD number of Kramers points (Dirac points)





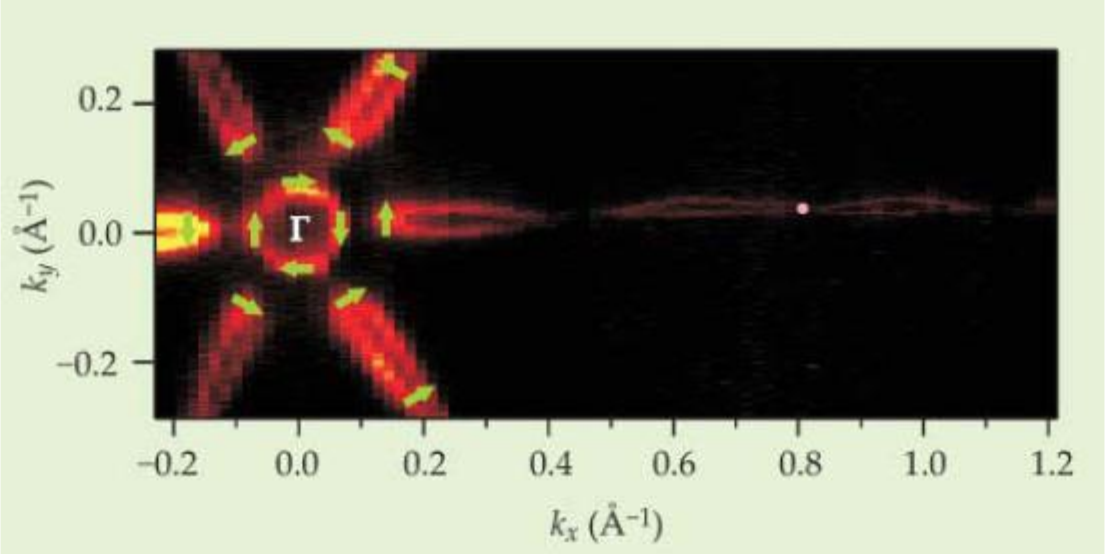


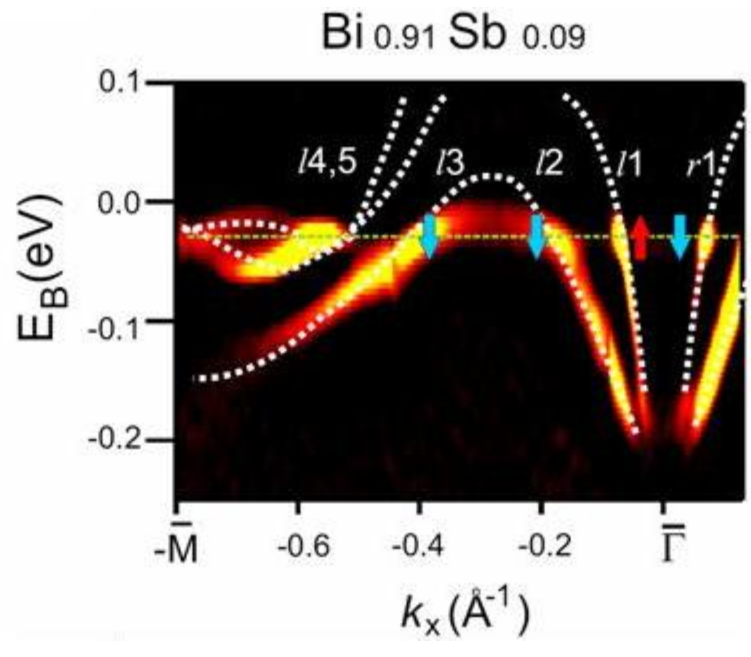
Why Dirac cone is distorted ?

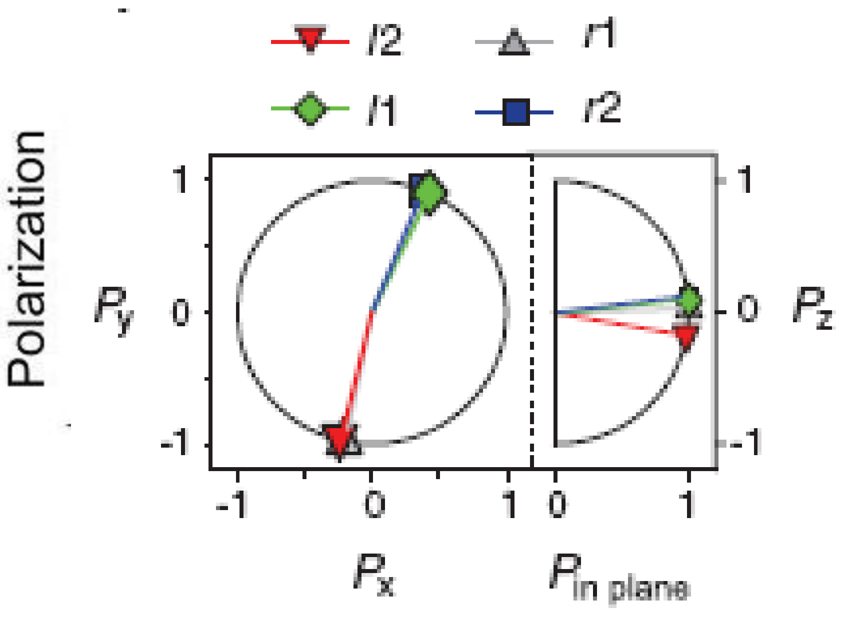


S.C Zhang (on BiSb) : Physics [APS news&views] (2008)

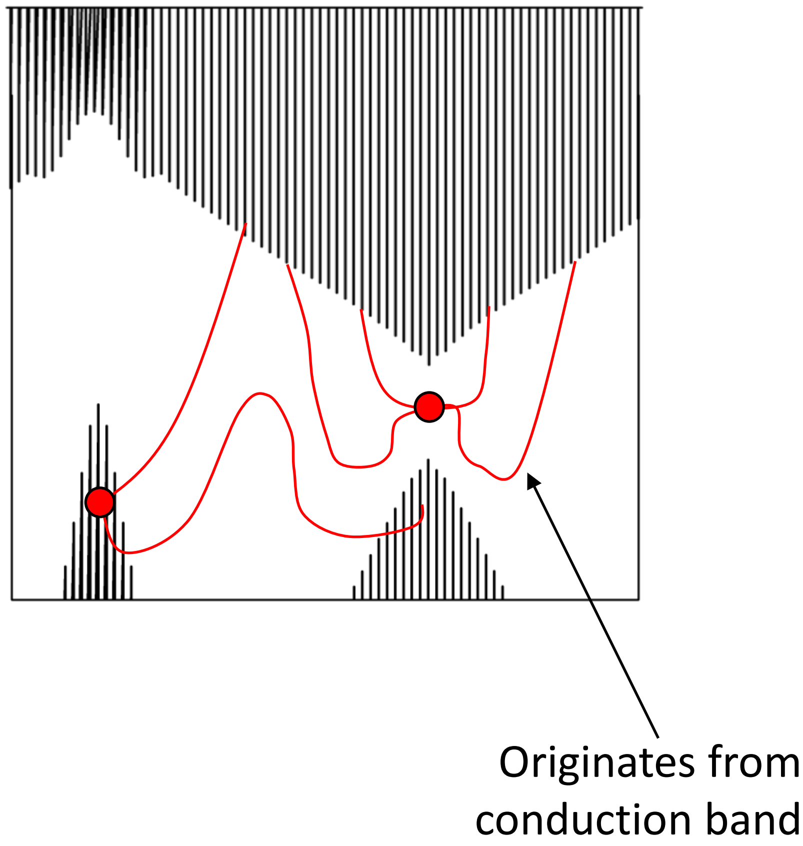
Surface state spin-textures







Which one is the "Knot" band?



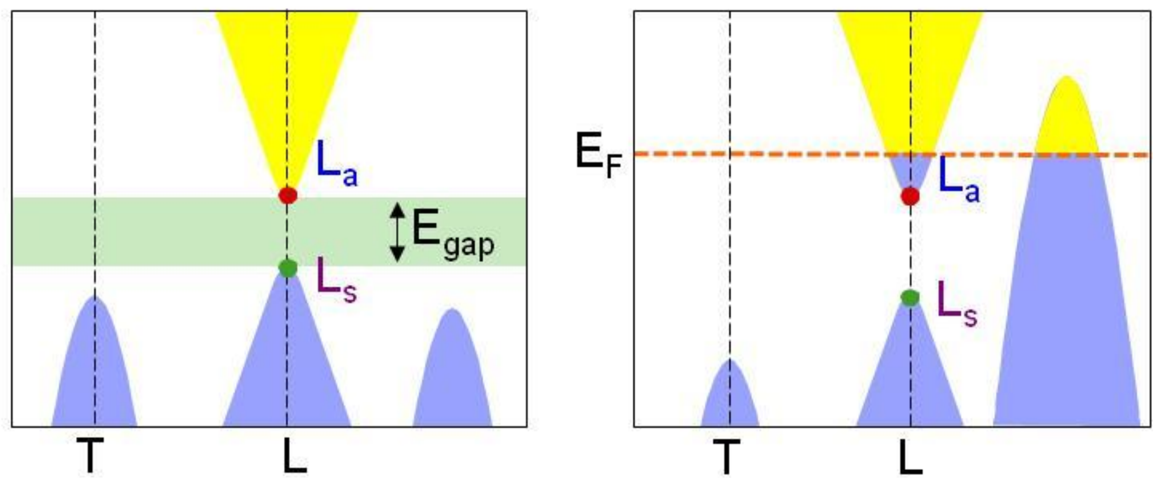
Parity Table for $Bi_{1-x}Sb_x$

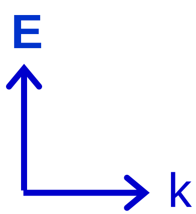
Alloy : .09<x<.18

Band gap ~ 30-50 meV

Pure Antimony

semimetal



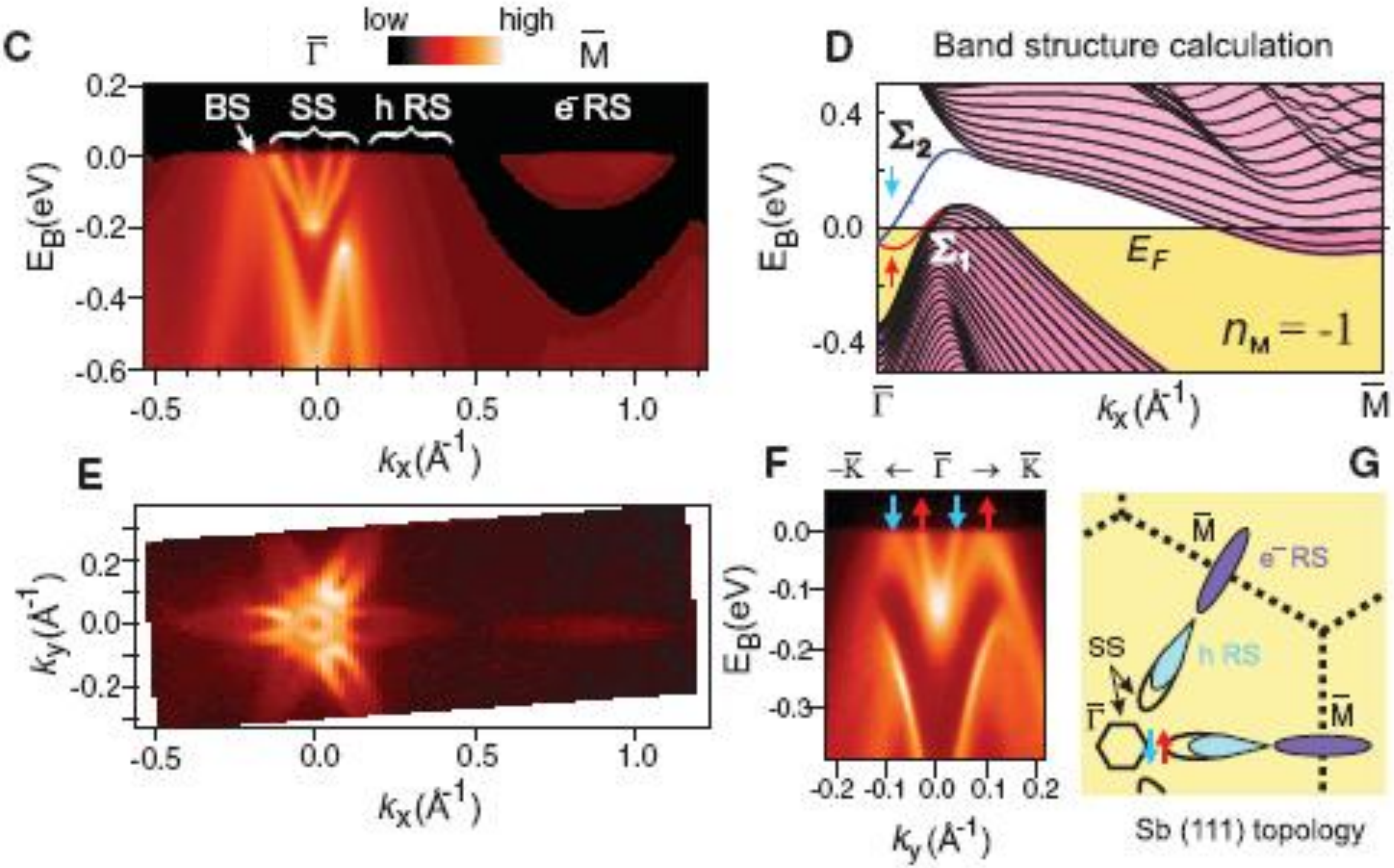


Inversion symmetry ⇒

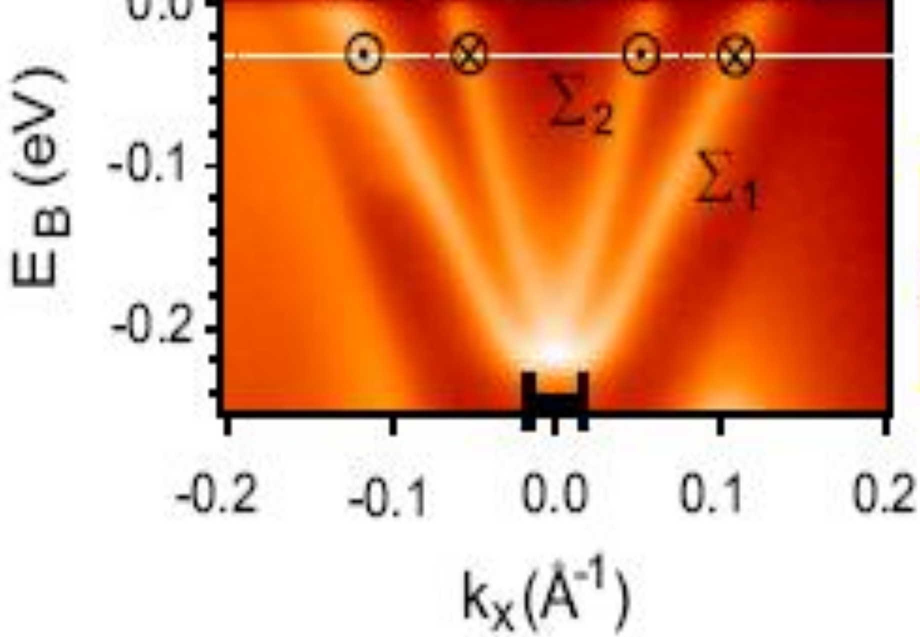
$$(-1)^{\nu_0} = \prod_{i=1}^{8} \prod_{n} \xi_{2n}(\Gamma_i)$$

Antimony

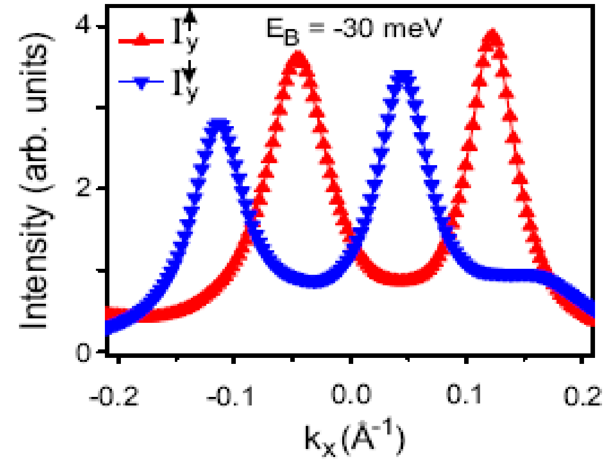
1Γ	$\Gamma_6^+ \quad \Gamma_6^- \quad \Gamma_6^+ \quad \Gamma_6^+ \quad \Gamma_{45}^+$	$-$
$3L$	$L_s \quad L_a \quad L_s \quad L_a \quad L_s$	$+$
$3X$	$X_a \quad X_s \quad X_s \quad X_a \quad X_a$	$-$
$1T$	$T_6^- \quad T_6^+ \quad T_6^- \quad T_6^+ \quad T_{45}^-$	$-$
	Z_2 class	$(1;111)$

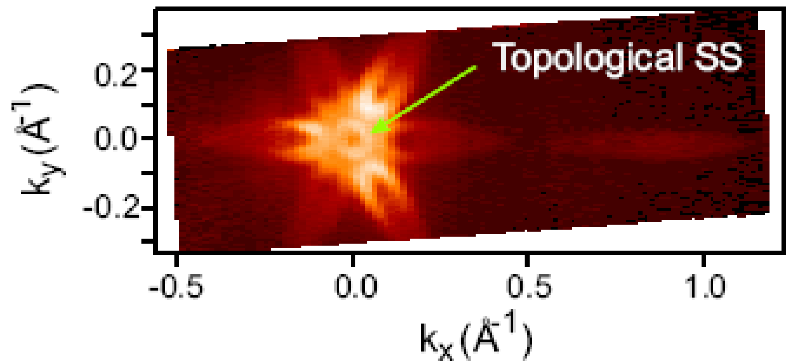


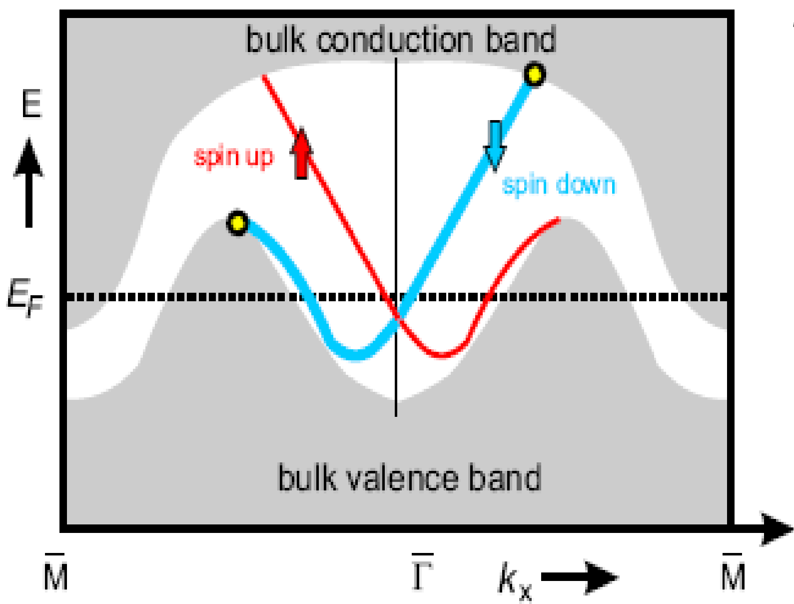
C
low
high
$\bar{\Gamma}$
$\bar{M}$
BS
SS
h RS
e⁻RS
E_B(eV)
k_x(Å^{-1})
D
Band structure calculation
Σ_2
Σ_1
E_F
n_M = -1
E
k_y(Å^{-1})
F
−K̄ ← Γ̄ → K̄
G
e⁻ RS
h RS
SS
Sb (111) topology

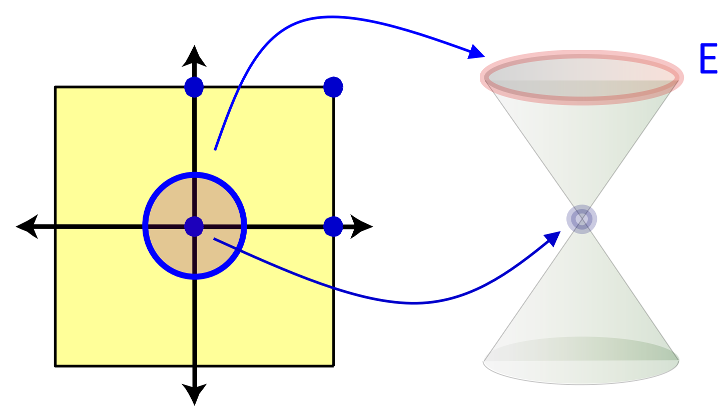

Σ2
Σ1
0.0
-0.1
-0.2
E_B (eV)
-0.2
-0.1
0.0
0.1
0.2
k_x (Å^-1)


l1
Γ̄
r1

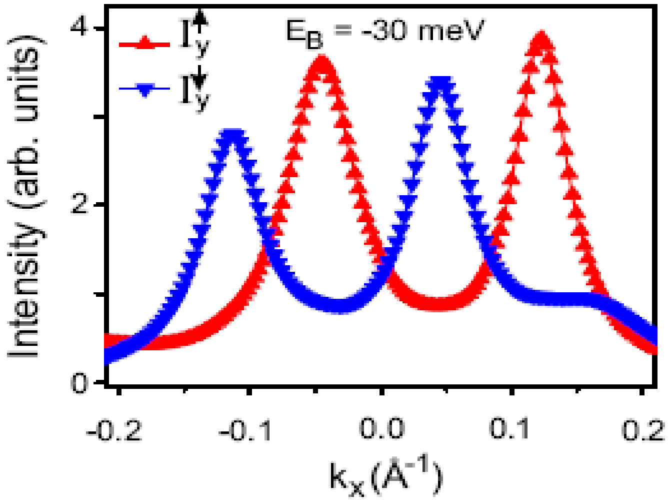

I_y^↑
I_y^↓
E_B = -30 meV
Intensity (arb. units)
4
2
0
-0.2
-0.1
0.0
0.1
0.2
k_x (Å^-1)

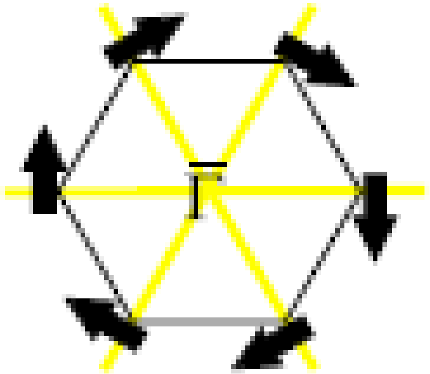

Topological SS
k_y (Å^-1)
0.2
0.0
-0.2
-0.5
0.0
0.5
1.0
k_x (Å^-1)


bulk conduction band
E
spin up
spin down
E_F
bulk valence band
M̄
Γ̄
k_x
M̄


E_F

Spin Chirality & Topological Berry's Phase



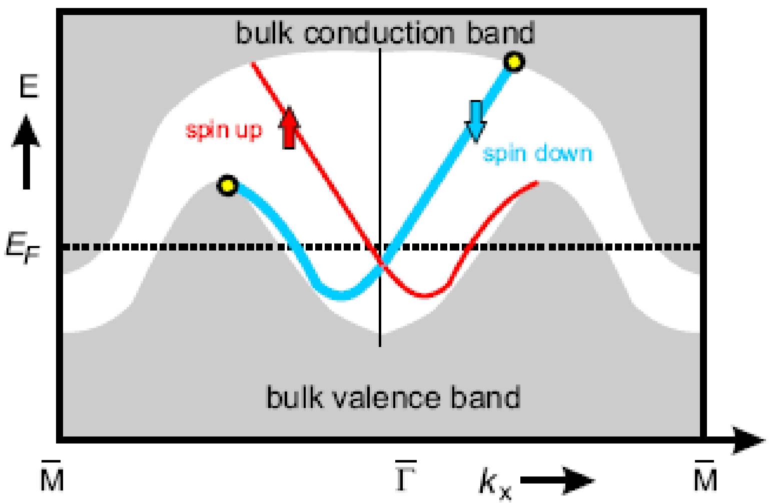


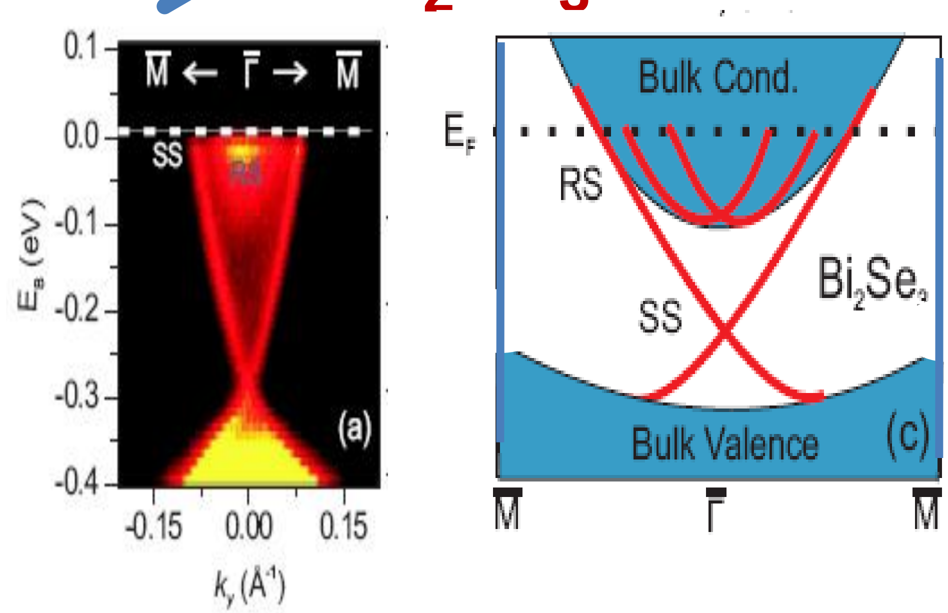
$$e^{i\phi(\Gamma)} = \exp i \oint_{\Gamma} \mathcal{A}_\mu dg^\mu$$ **= -1**

$$\oint_{\Gamma} \mathcal{A}_\mu(\boldsymbol{g}) = -i\langle\Psi(\boldsymbol{g})|\partial_\mu\Psi(\boldsymbol{g})\rangle \sim \pi$$

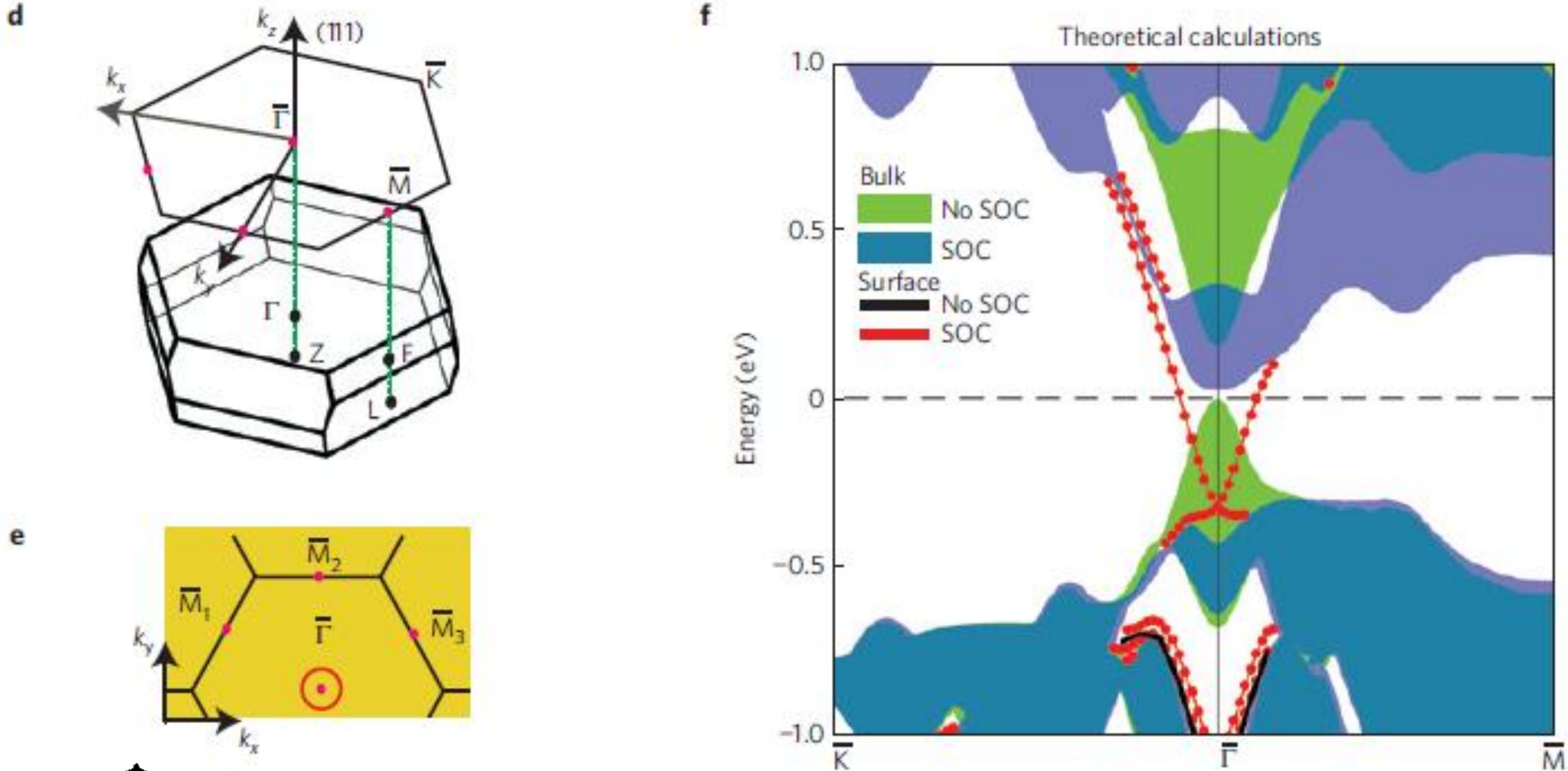
Can we make an insulating version of Sb?

Pure Sb → Bi_2Se_3



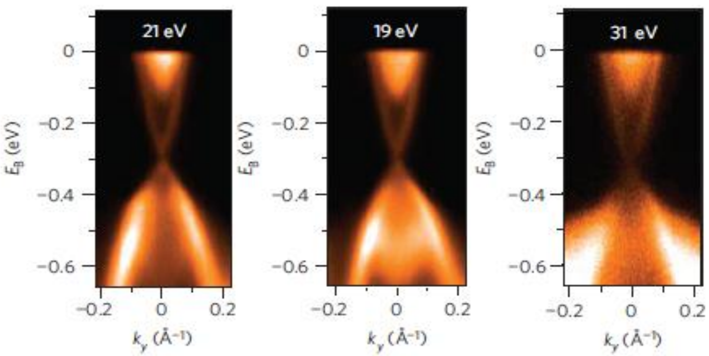


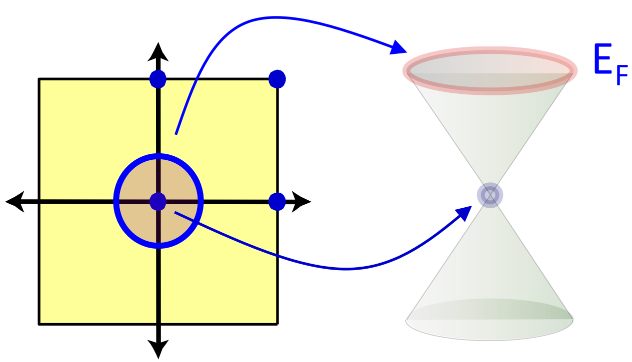
Our theoretical prediction of Topological Dirac fermions in Bi_2X_3 class

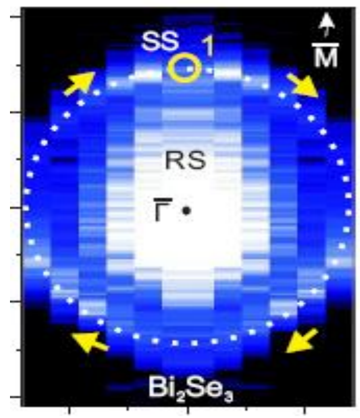


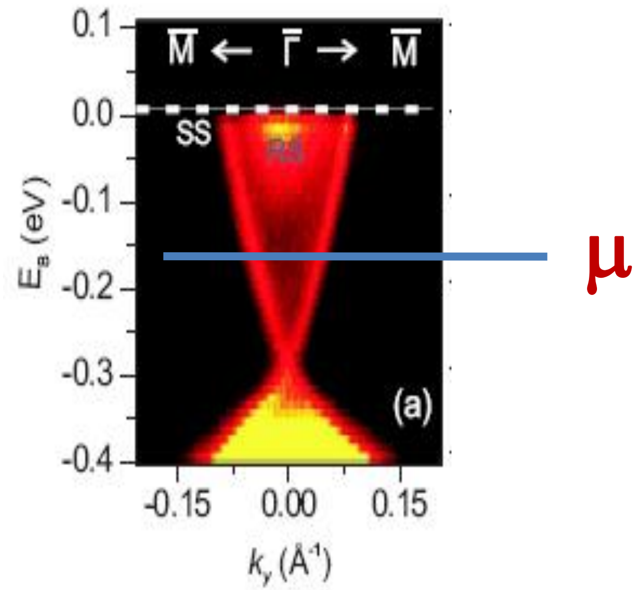
Xia et.al., **Nature Physics** 5, 398 - 402 (2009)
Published online: 10 May 2009 | doi:10.1038/nphys1274

Experimental Observation of "Hydrogen atom" of Strong Topological Insulator





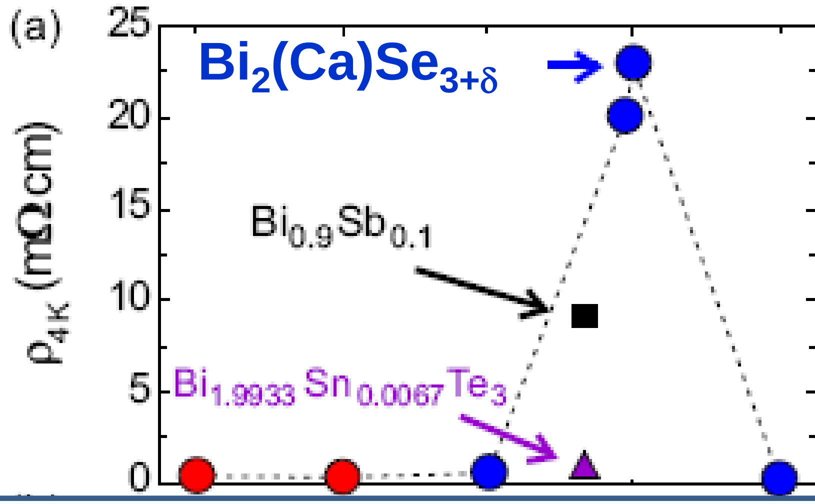




Xia et.al., **Nature Physics** 5, 398 - 402 (2009)
Published online: 10 May 2009 | doi:10.1038/nphys1274

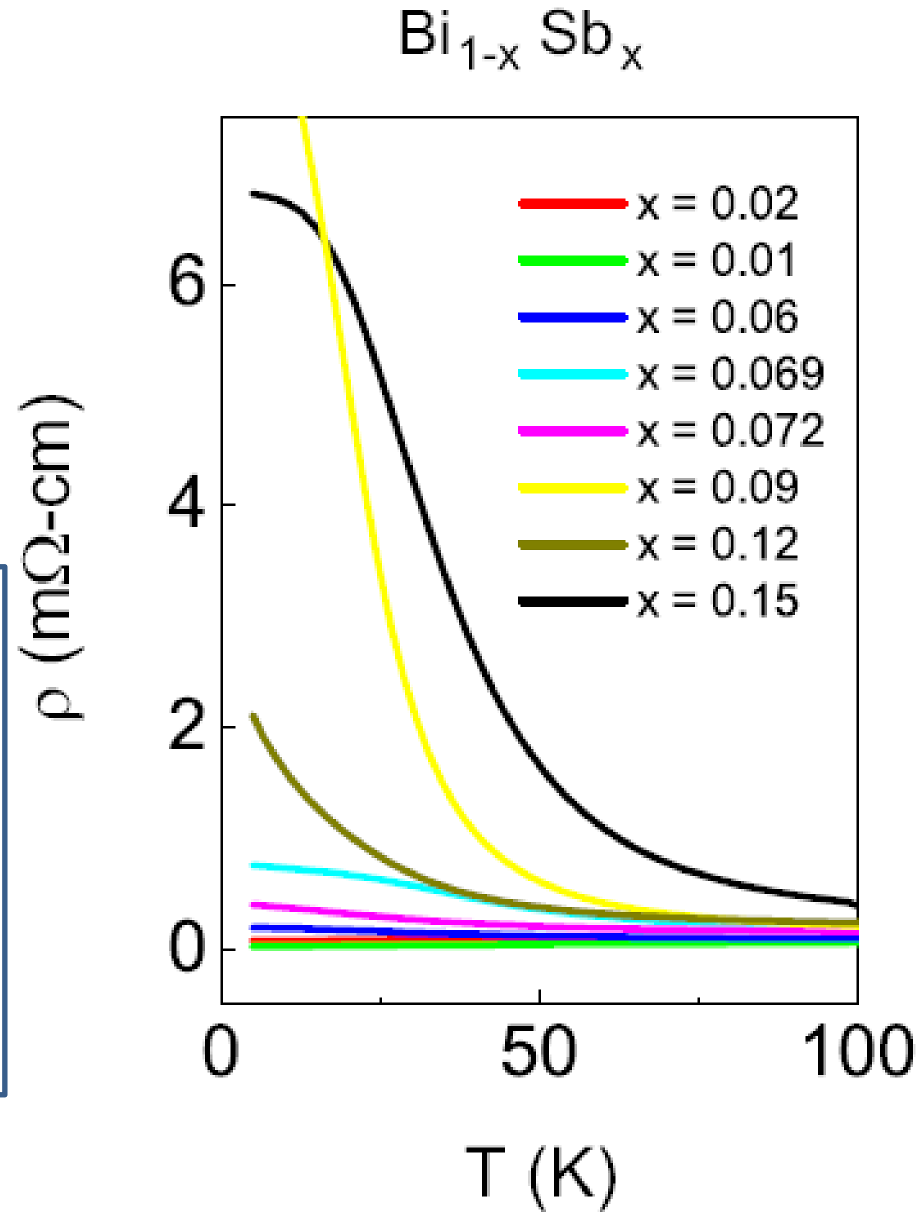
News & Views : http://www.nature.com/nphys/journal/v5/n6/full/nphys1294.html

Bulk Insulator

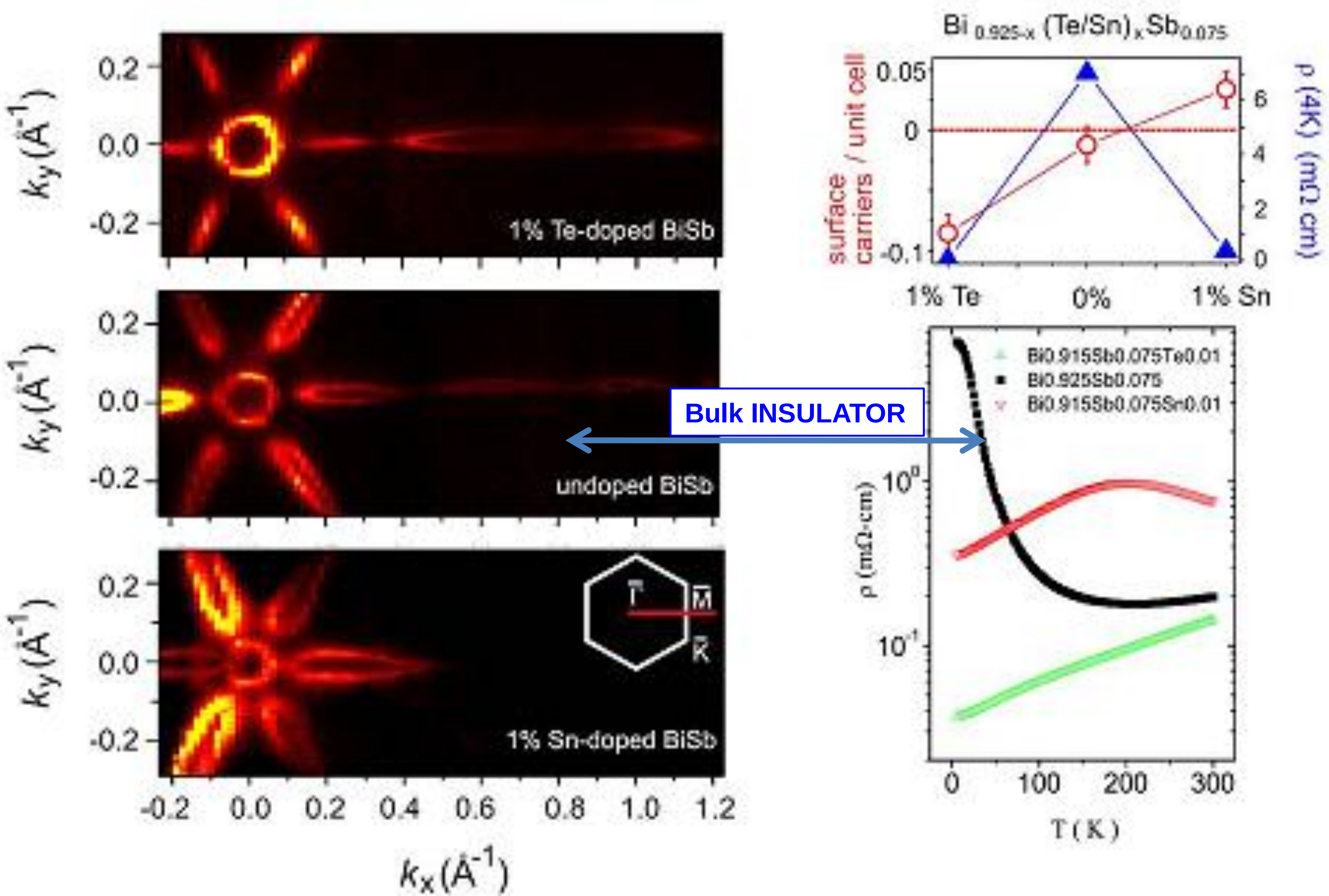


Data by Checkelsky & Ong (2009)

Charge compensation

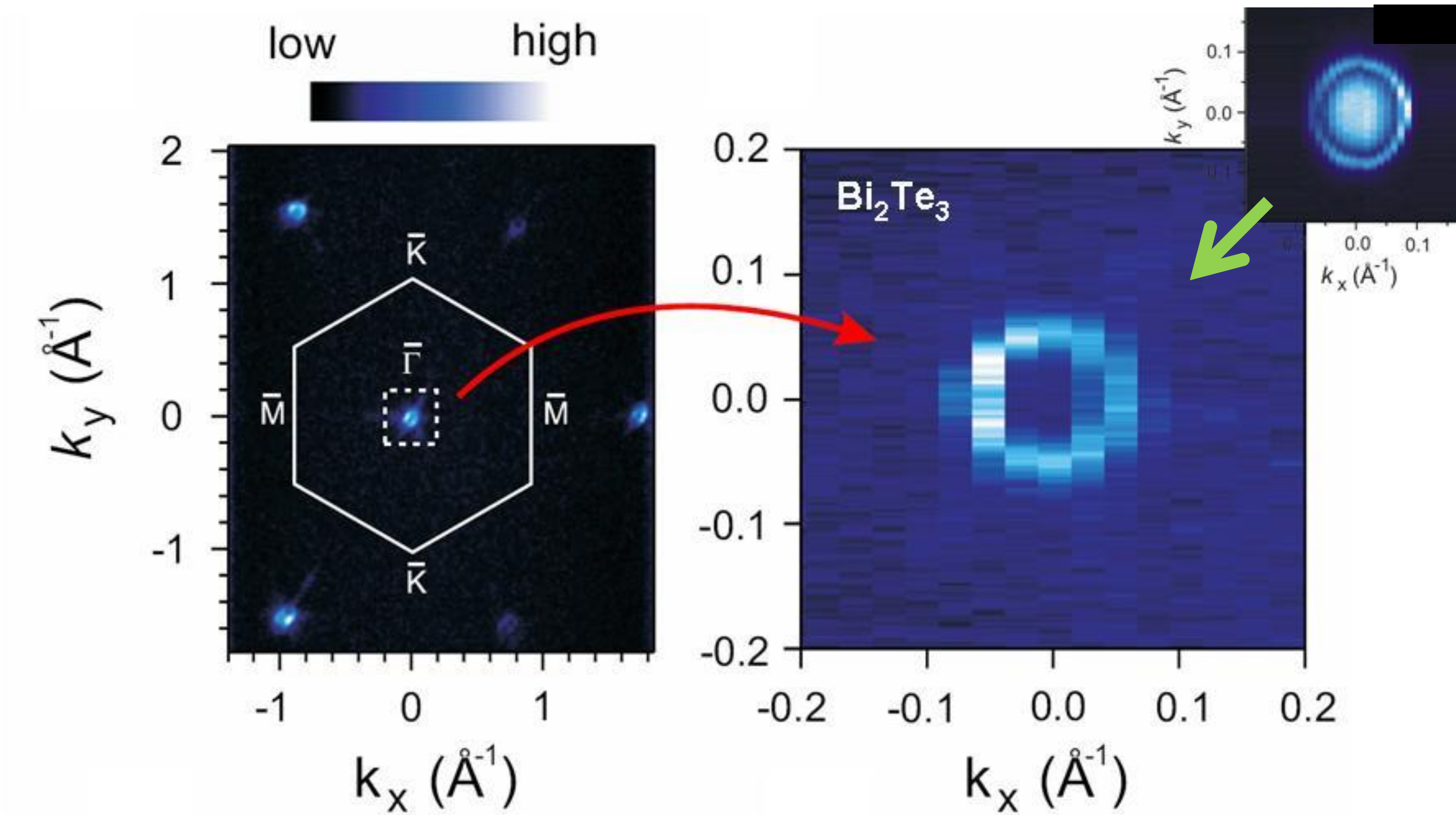


Tuning to the topological insulator regime in $Bi_{1-x}Sb_x$



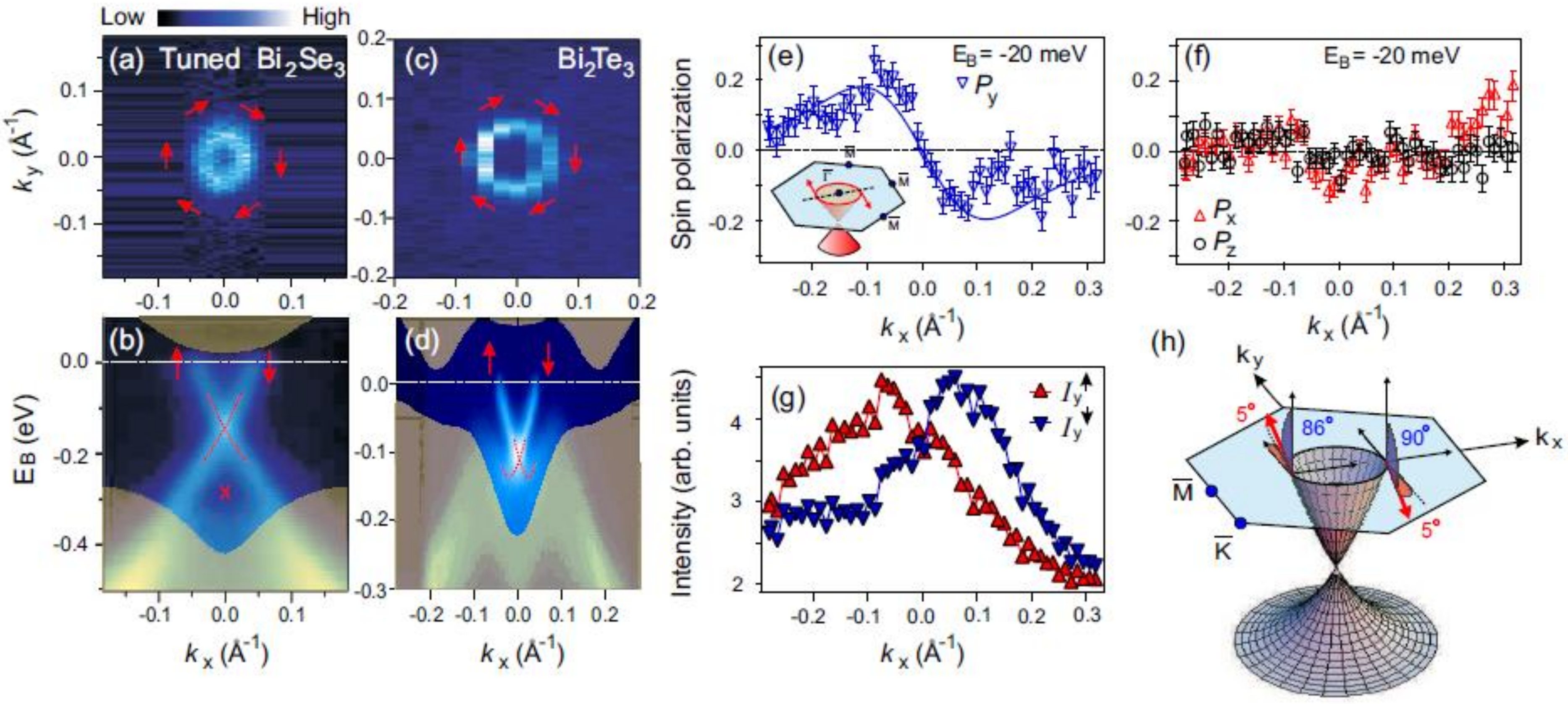
First observation of spin-Dirac fermions and topological insulator phase in Bi_2Te_3 probed by spin-ARPES **(previous work, Noh et.,al. was not spin polarized detection):**

Hsieh et.al., http://aps.arxiv.org/abs/0904.1260



Helical Dirac fermions

Spin-momentum locking



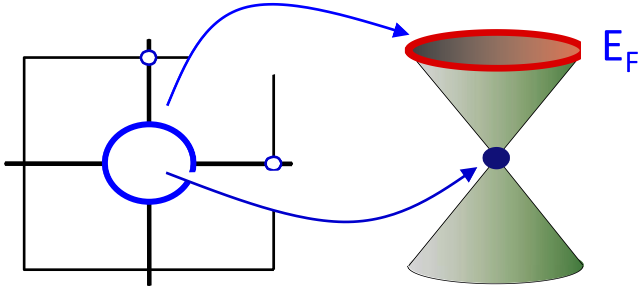
Hsieh et.al.,
http://aps.arxiv.org/abs/0904.1260

Strong Topological Insulator ($\nu_0 = 1$)

Boundary Fermi pocket encloses **odd** number of Dirac points

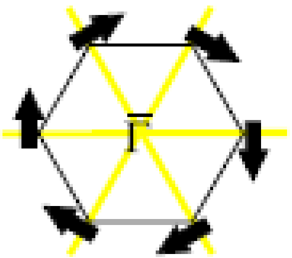
Surface states form a "Topological Metal" phase :
This topological state is fundamentally different from conventional 2D matter (2DEG) and the integer QHE state.

- Berry's phase π around the Fermi pocket
- Half-integer charge QHE
- Opposite to Anderson Localization (weak "anti-localization")



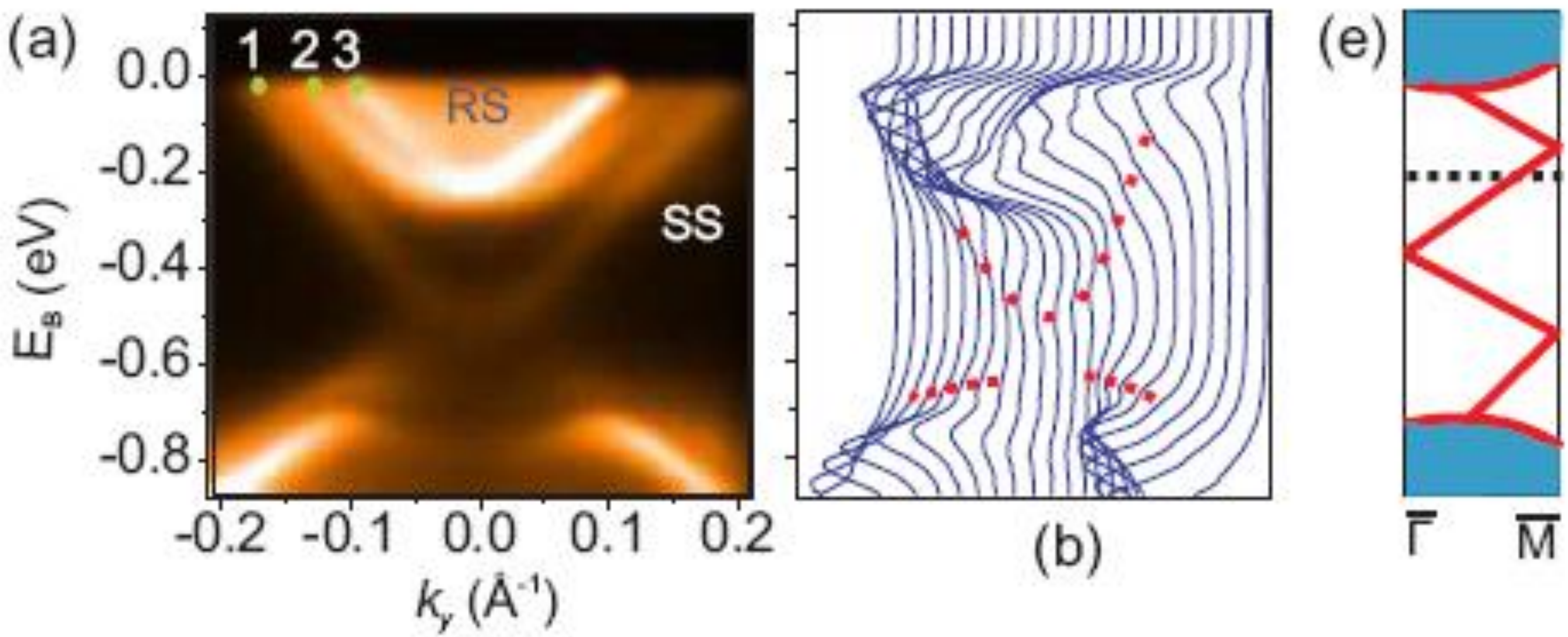
Spin-textured Dirac cone

$n_M = -1$



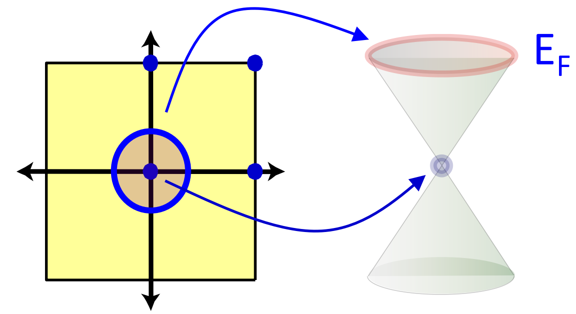
Mirror Chern number

Deposit a magnetic submonolayer on STI



See our preprint for details : Xia, Hasan et.al., arXiv:0812.2078v1 (2008)

<u>Strong</u> Topological Insulator (ν_0 = 1)



Fermi arc encloses <u>odd</u> number of Dirac points

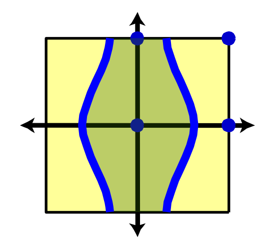
Dirac structure has unique <u>spin-texture</u>

Leading to π Berry's phase

<u>Weak</u> Topological Insulator (ν_0 = 0)

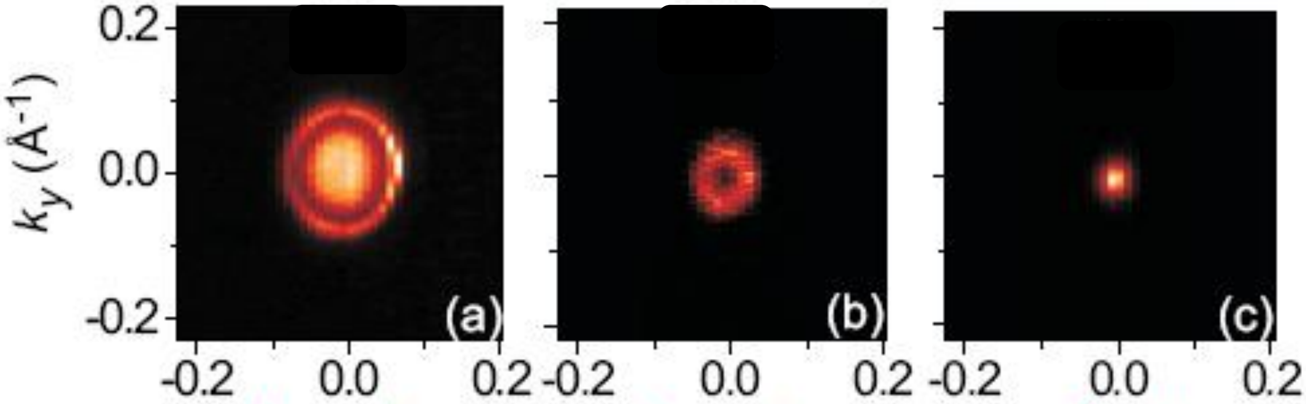
Fermi arc encloses <u>even</u> number of Dirac points

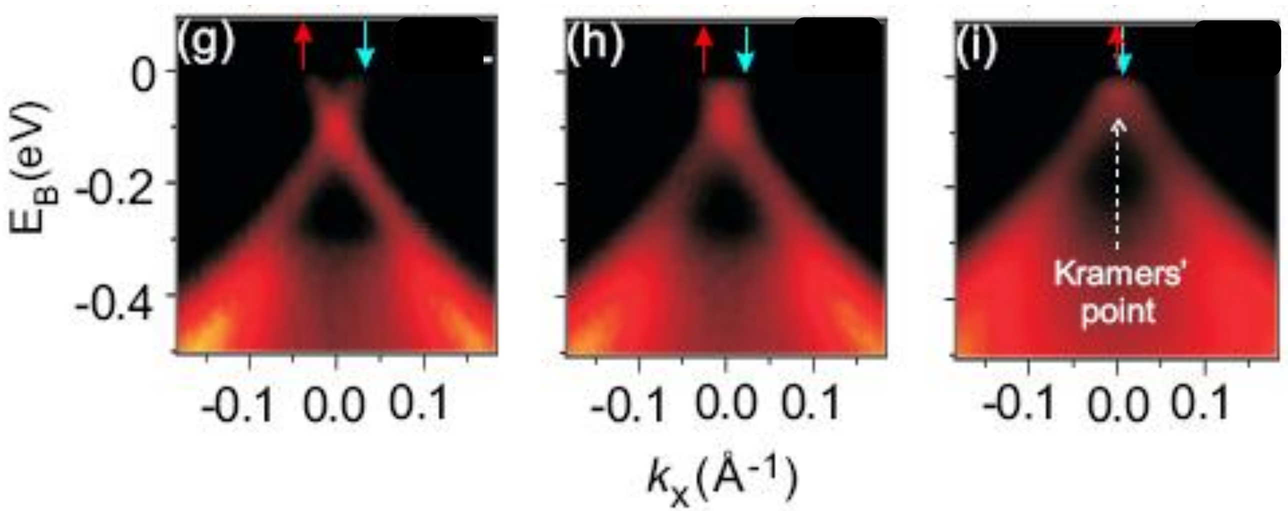
Dirac structure has spin-texture but trivial phase



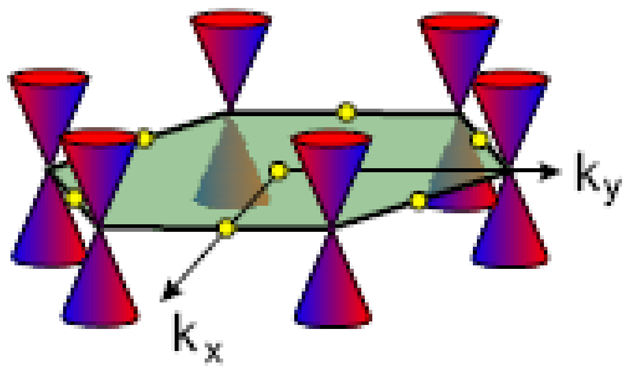
Trivial 3D Generalization of 2D QSH phase

TOPOLOGICAL "Graphene"

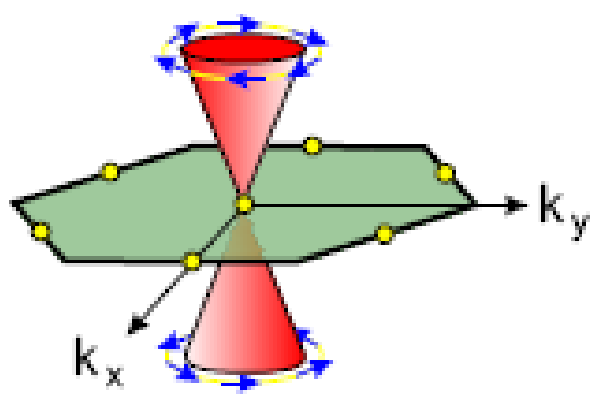


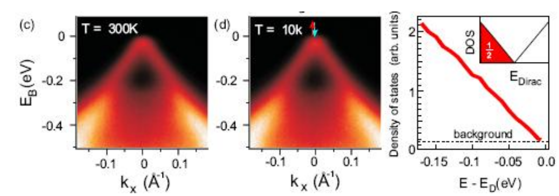


Chiral Dirac ground state

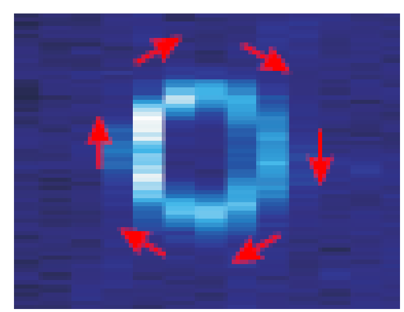


Graphene





Topo Insulator



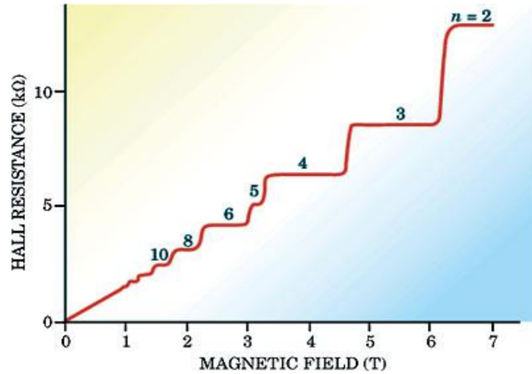
Quantum Hall effect

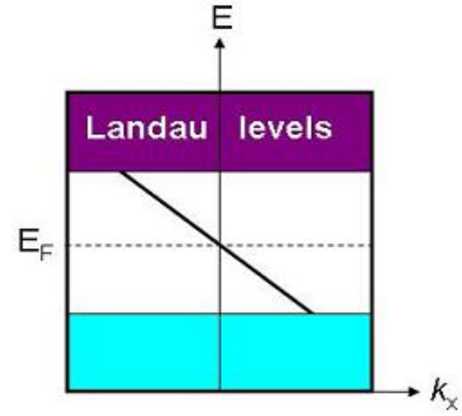
Chiral degenerate fermions

$\sigma_{xy} = ne^2/h$

↑

Topological quantum number





Topological Insulators

Helical spin-Dirac fermions

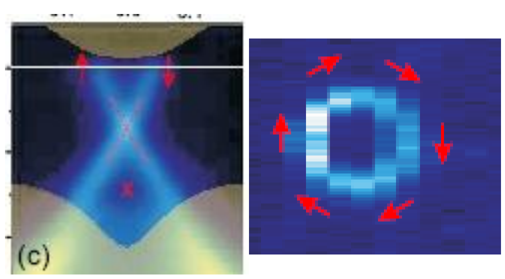
How to experimentally "measure" the topological quantum numbers (ν_i) associated with the quantum spin Hall or Strong Topological Insulator (STI) phases?

No quantized transport!

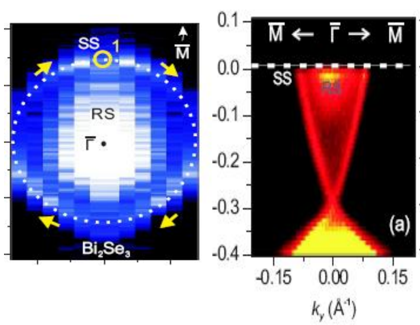
$\{\nu_i\}$

↑

Topological quantum number

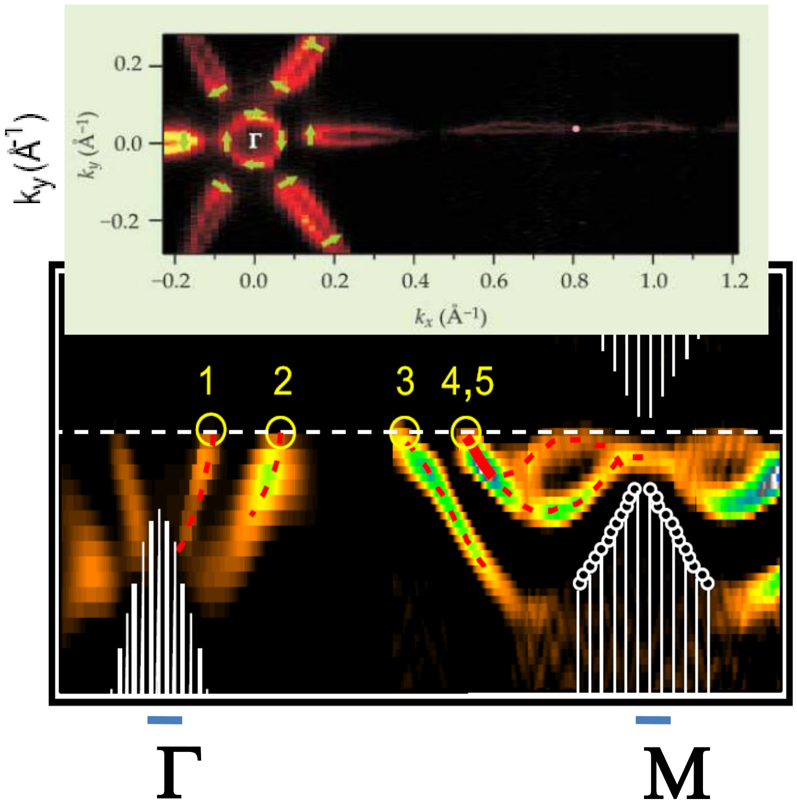


Spin-textured Dirac

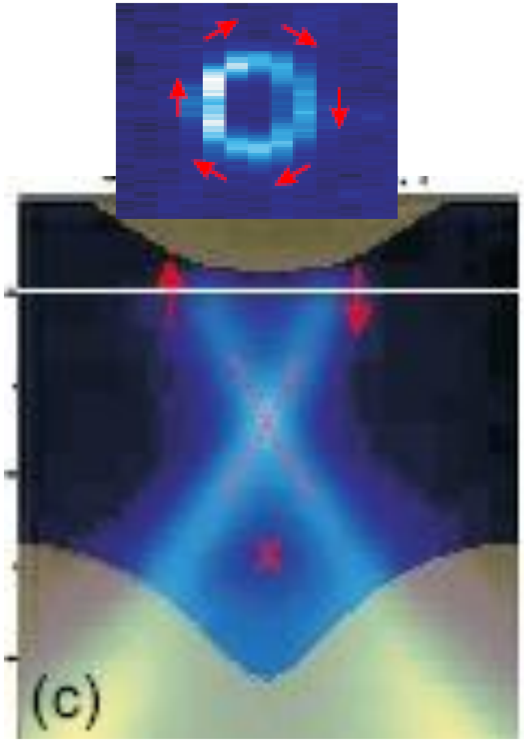


Experimental realizations of Strong Topo Insulators (Theta-Vacuum states) in nature :

Nature 08, Science 09



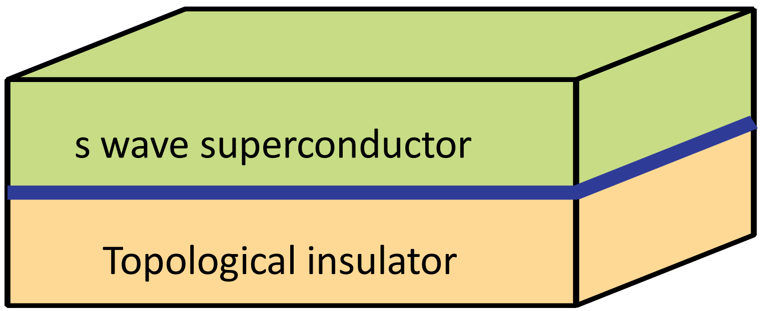
NatPhys 09, Nature 09



These two are actually 2 distinct types of strong topo insulators !

STI/Superconduct interface

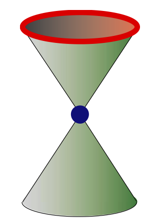
Kane-Fu proposal



2D interface state with energy gap and exotic topological order

Resembles 2D spinless p_x+ip_y superconductor but does not violate time reversal symmetry

$$H = \psi^\dagger(-iv\vec{\sigma}\cdot\vec{\nabla} - \mu)\psi + \Delta\psi_\uparrow^\dagger\psi_\downarrow^\dagger + \Delta^*\psi_\downarrow\psi_\uparrow$$



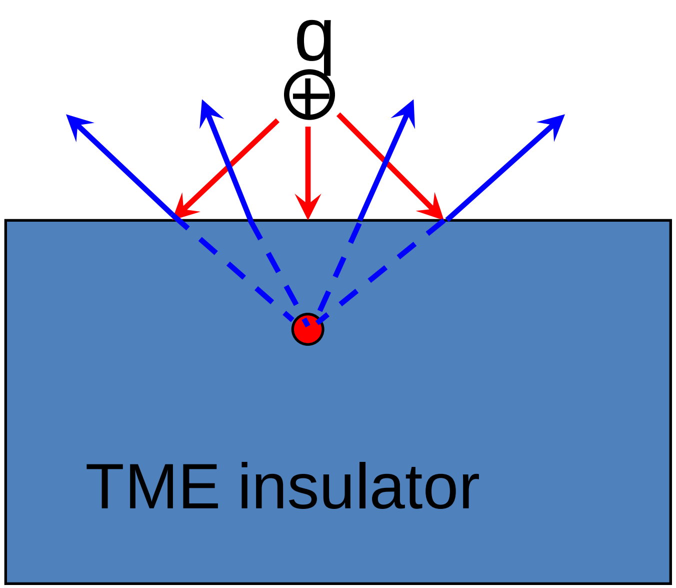
Dirac surface states
(no spin degeneracy)

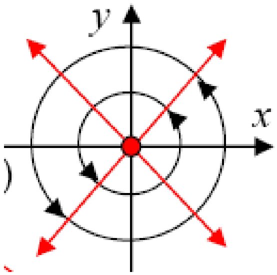
proximity induced
superconductivity

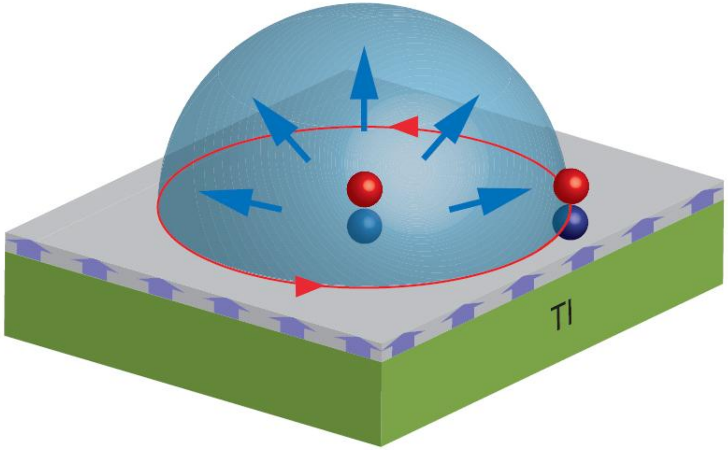
Majorana bound state at a vortex : $\Delta = \Delta(r)e^{i\theta}$

- bound state solution to BdG equation at exactly zero energy
- $c_0 = c_0^\dagger$ (electron=hole) Majorana fermion = "1/2 a state"
- Also predicted in ν=5/2 FQHE, Sr_2RuO_4, cold atoms, etc

Seeing the magnetic monopole thru the mirror of a TME insulator, (Qi, Zhang et al, Science 323, 1184, 2009)



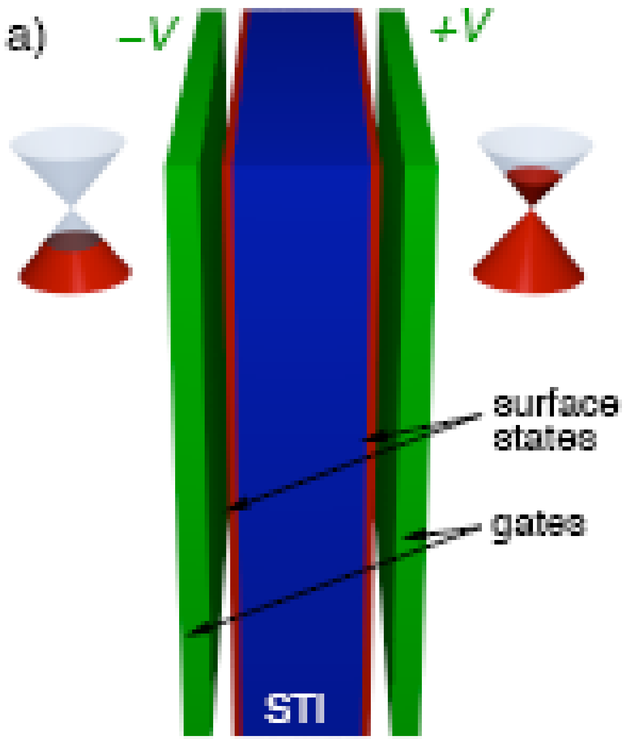




Magnitude of B:

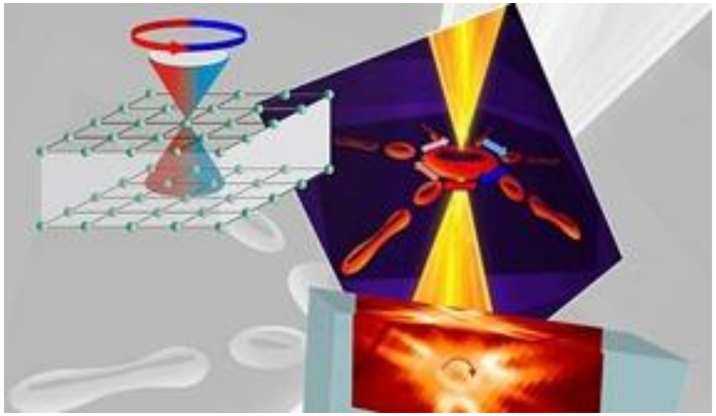
$10^6 V/m \rightarrow 0.25G$

Topological Exciton Condensation:



B. Seradjeh,[1] J.E. Moore,[2,3] and M. Franz[4]

An odd number of gapless Dirac fermions is guaranteed to exist at a surface of a strong topological insulator. We show that in a thin-film geometry and under external bias, electron-hole pairs that reside in these surface states can condense to form a coherent exciton condensate, similar in general terms to the exciton condensate recently argued to exist in a biased graphene bilayer, but with different topological properties. Such a 'topological' exciton condensate (TEC) exhibits a host of unusual properties; the most interesting among them is the fractional charge $\pm e/2$ carried by a singly quantized vortex in the TEC order parameter.



Future Directions :

Strong Topological Insulators are expected to exhibit :

- Half-integer charge quantum Hall effect
- Opposite to Anderson localization (weak anti-localization)
- Superconducting proximity: Majorana Fermions :
  Fu, Kane et.al., Beenakker et.al., Kitaev
- Magnetoelectric/ Axion effects: Moore, Franz et.al,
- Topo exciton (BEC) condensates: Moore, Franz et.al,
- Magnetic proximity effect, Monopole: Qi, Zhang et.al,
- Helical-metal in Dislocations: Ran, Vishwanath et.al.,
- Topological (fault-tolerant) quant.computing Kitaev, Kane, Beenakker

Our Expts on Topological Insulator

(Theta-vacuum or Axionic state)

Spin-sensitive direct edge-state imaging methods

"A topological Dirac insulator in a Quantum Spin Hall Phase"
NATURE (2008)

"Spin-textures & Berry's phase in a Topo Insulator" [Bi-Sb series]
SCIENCE (2009)

"Charge compensation in a Topo Insulator" [$Bi_2(Ca)Se_3$]
Phys. Review B (2009)

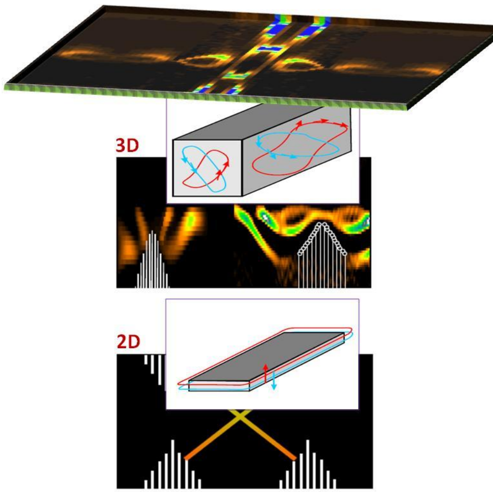
"A large-gap Topological with single Dirac cone" [Bi_2Se_3]
NATURE PHYS (2009)

"A new Topological Insulator"
NATURE (in review) (2009)

Conclusion :

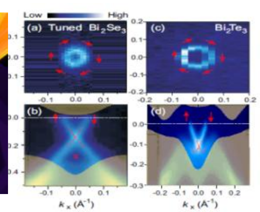
A fundamentally new quantum phase of matter ($z_2 = -1$, $v_o = 1$ θ-vacuum state) has been observed (Topological Insulator) which is distinct from the quantum Hall effect phase yet topological in nature.

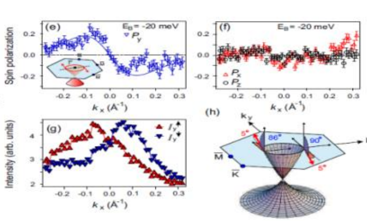
NATURE (2008) News&Views : Nature (2008)
Phys.Rev. B (09) Editor's Suggestion
SCIENCE (2009) News&Views : Science (2009)
NATURE PHYS (2009) News&Views : Nature Phys. (2009)

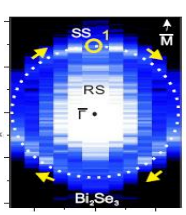


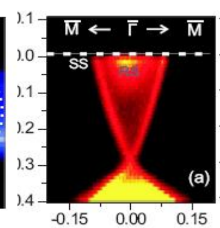
PHYSICS TODAY "Search&Discovery" April (2009)
See commentary by F. Wilczek in NATURE (2009)
also by B.I. Halperin at CMP Journal Club (2008)
NATURE (in rev.) (09) A tuneable Topological Insulator

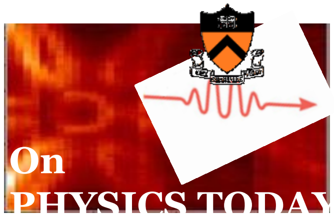
Topo Insulator is the realization of long-sought θ-vacuum/Axions (next talk by Moore).











Thanks !