Spin and angle-resolved photoemission spectroscopy on topological insulators

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Bi(114) surface:
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Justin Wells
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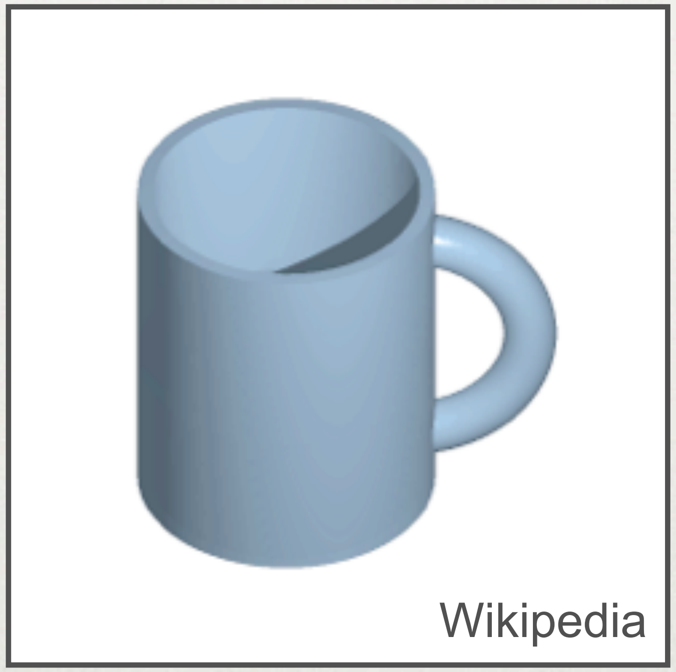
Outline

- Simple approach to topological insulators
- Introduction to SARPES
- Extraction of spin polarization vectors
- Topological insulators
  - $Bi_{1-x}Sb_x$, Bi_2Te_3
  - Bi(114)
- Summary

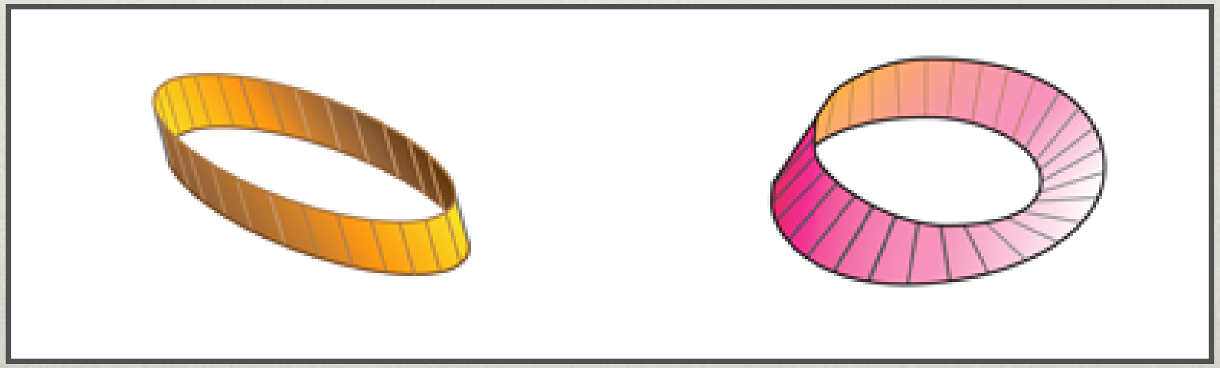
My knowledge of topology...

Homeomorphic objects are the same under continuous deformations

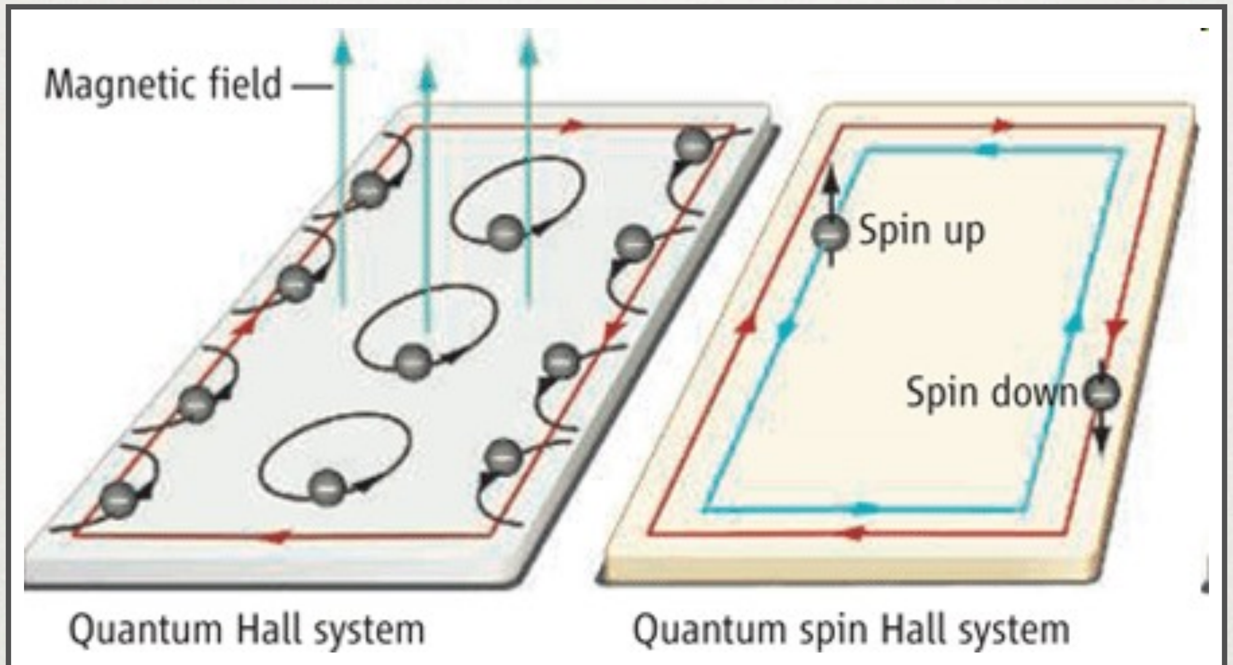
Same topology



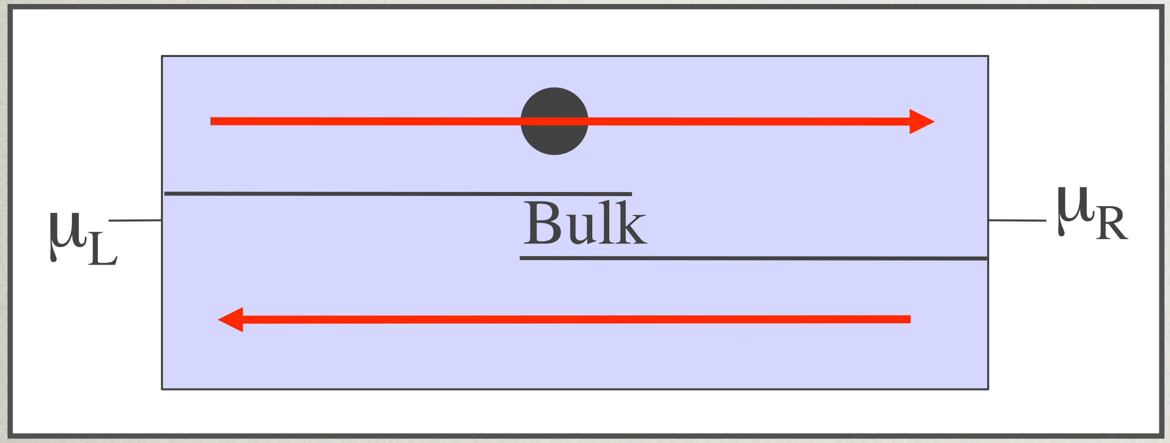
Different topology

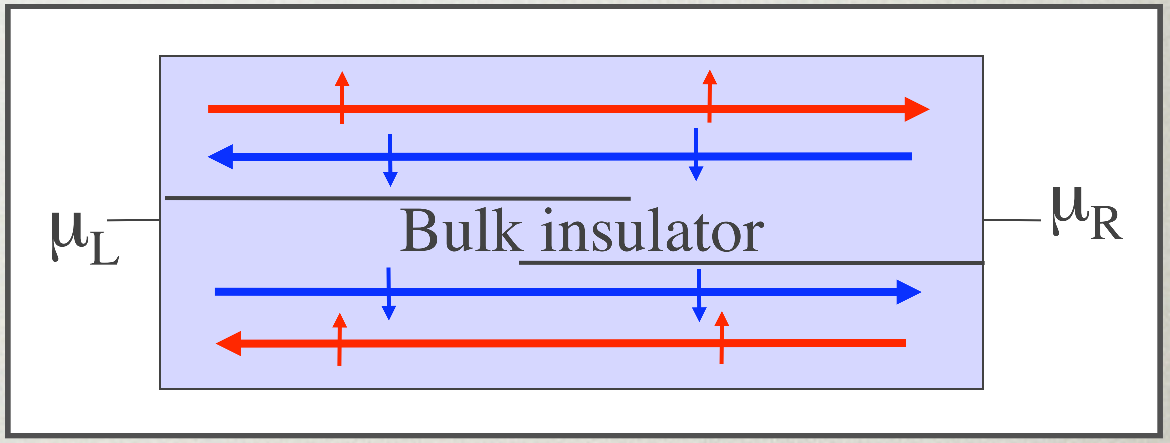


Quantum (spin) Hall effect: The experimentalist picture



N. Nagaosa, Science **318**, 758 (2007)

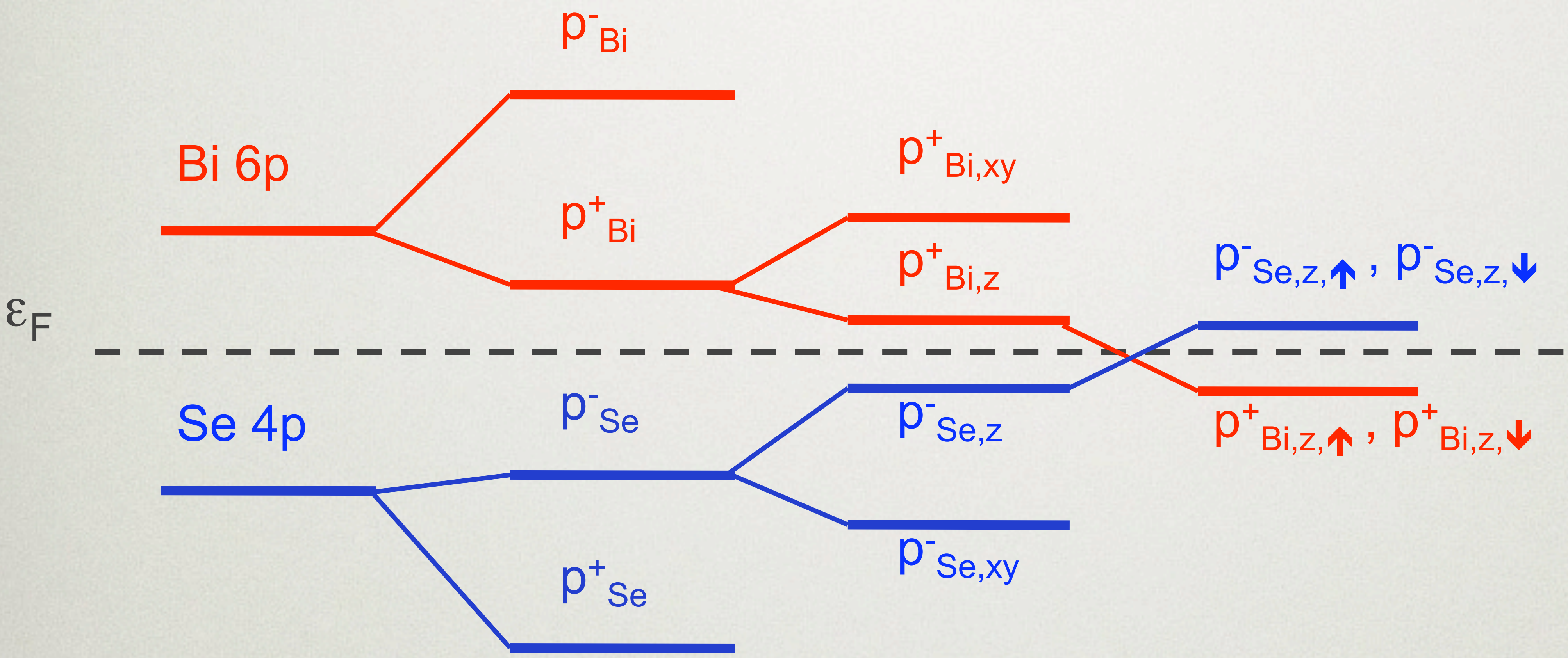




2D: Quantum spin Hall effect
3D: Topological magneto-electric effect

TOPOLOGICAL INSULATORS: TOPOLOGY

Example: Bi_2Se_3

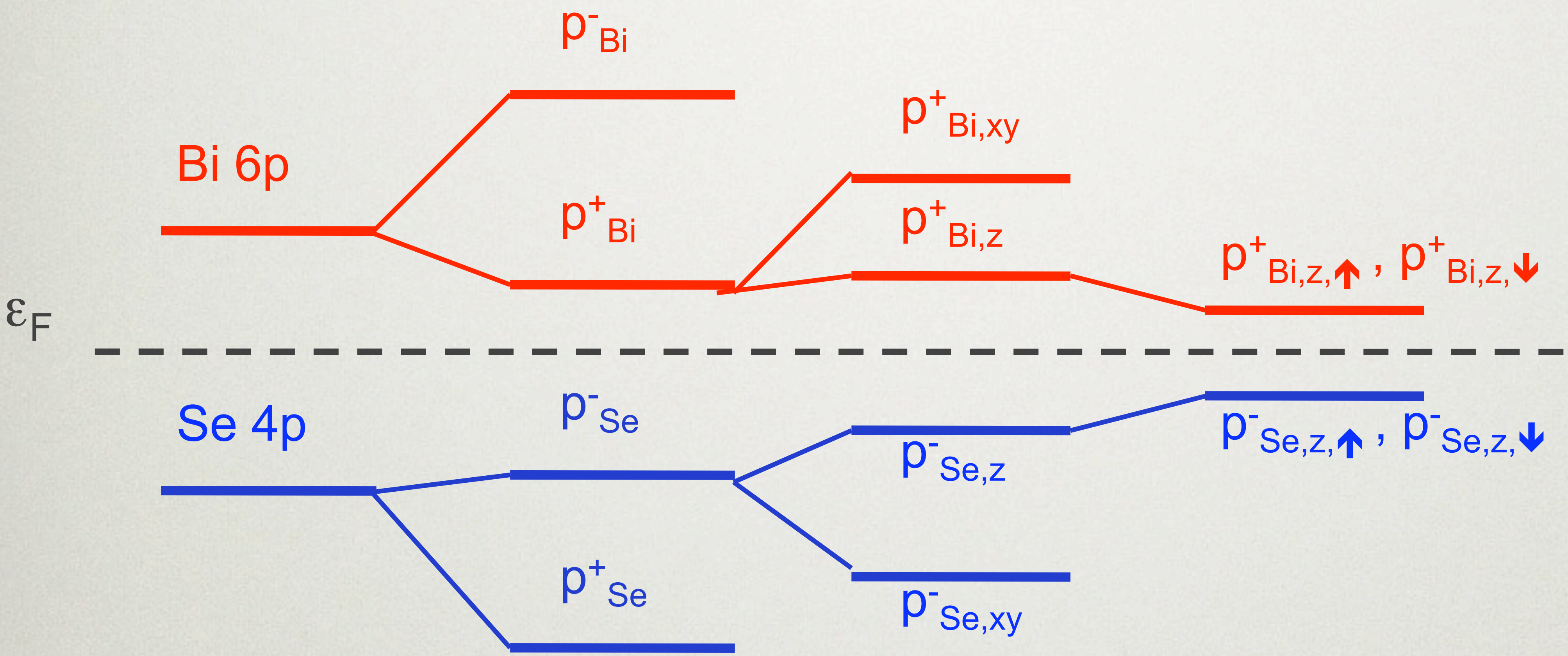


- Chemical bonds, parity with respect to crystal inversion center
- Crystal field, band structure, k=dependent splitting (here Γ point, TRIM)
- Spin orbit interaction, spin degeneracy remains

Following H. Zhang et al.,
Nature Physics 5, 438 (2009)

TOPOLOGICAL INSULATORS: Topology

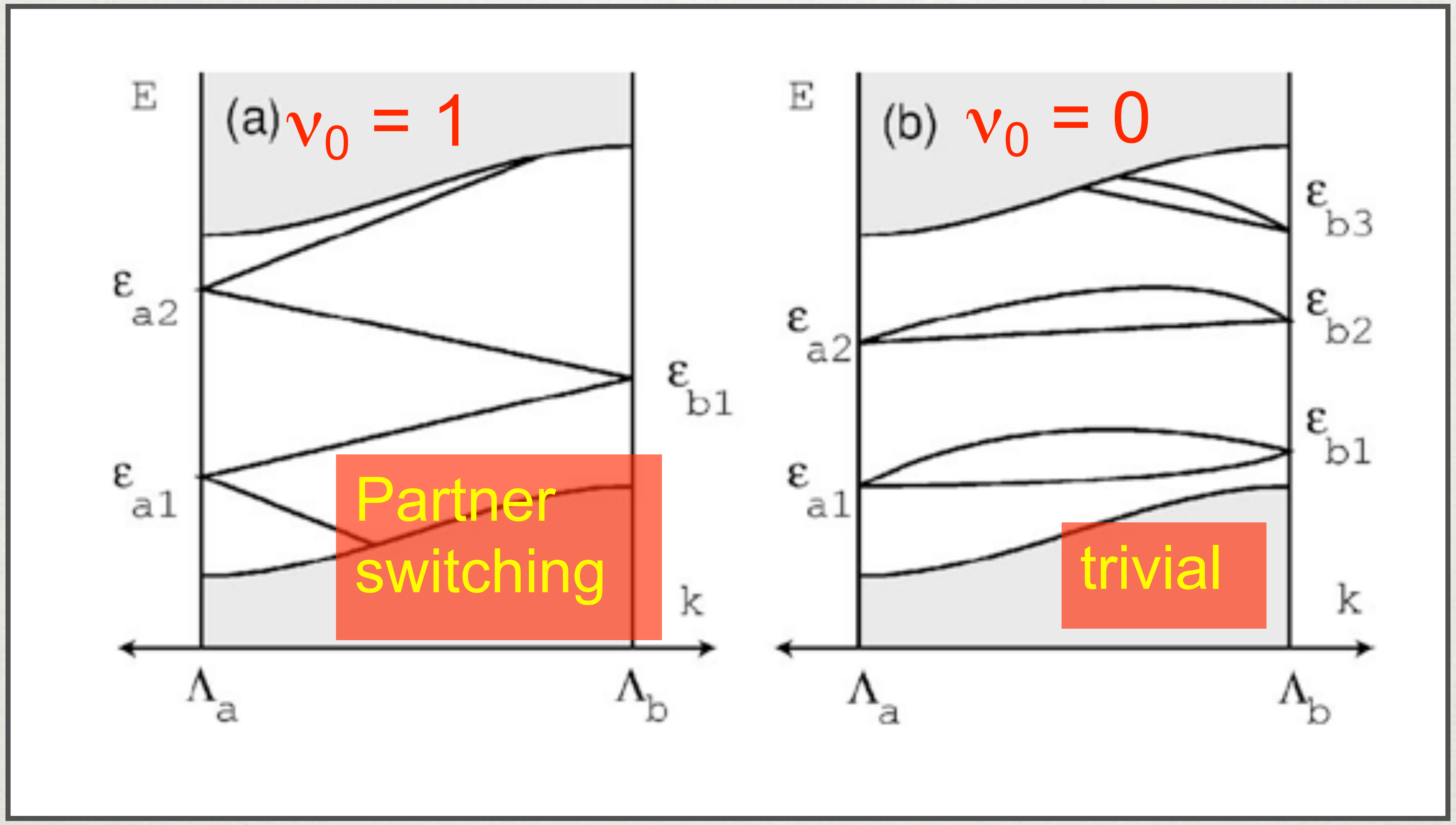
Example: Bi_2Se_3



- Chemical bonds, parity with respect to crystal inversion center
- Crystal field, band structure, k=dependent splitting (here L point, TRIM)
- Spin orbit interaction, spin degeneracy remains

Following H. Zhang et al., Nature Physics 5, 438 (2009)

Topological invariant ν_0



The Z_2 topological invariant ν_0 determines whether the surface states are trivial or non-trivial.

Parity product of all occupied states at each TRIM:

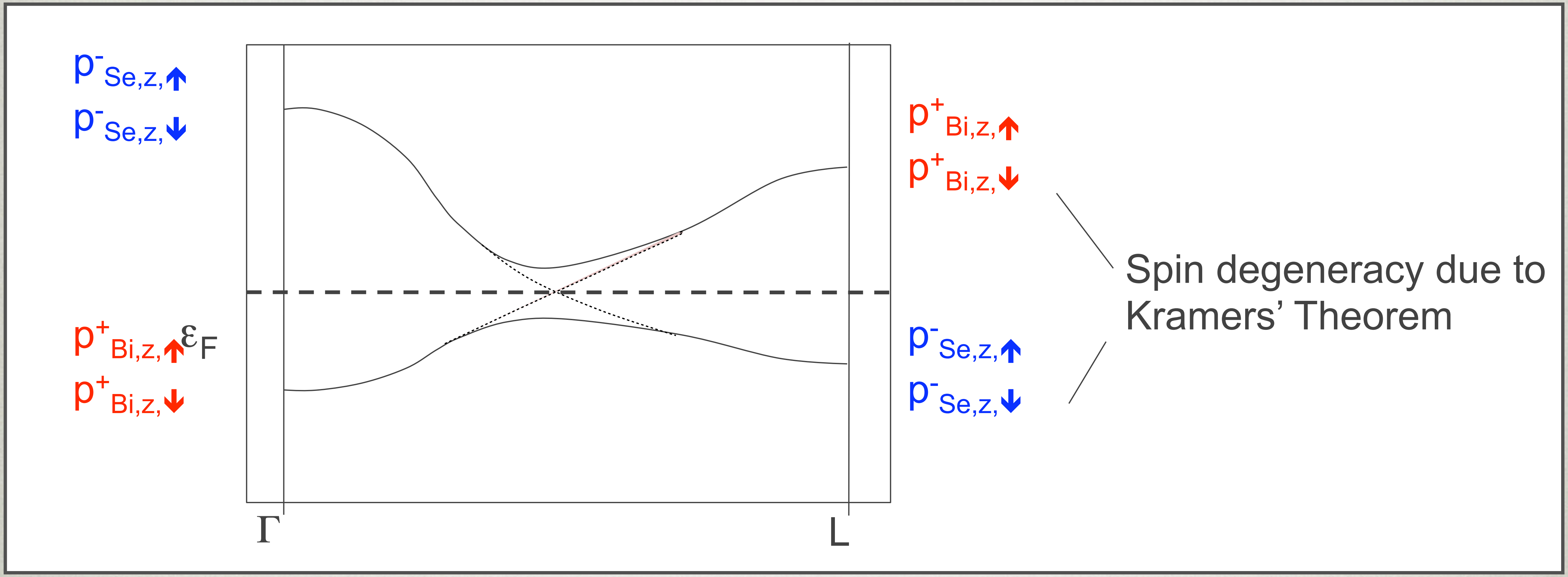
$$\delta_i = \prod_{m=1}^{N} \xi_{2m}(\Gamma_i).$$

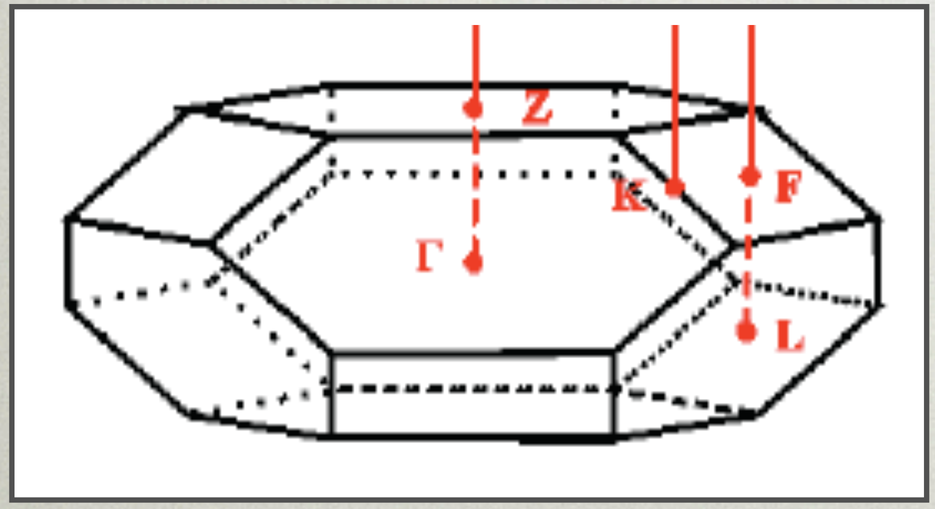
Product over all TRIMs:

$$(-1)^{\nu_0} = \prod_{i=1}^{8} \delta_i.$$

L. Fu, C. L. Kane, PRB 76, 045302 (2007)

Spin-orbit induced bulk band gap





Strong spin-orbit coupling

Avoided crossing
=> spin-orbit induced
inverted parity band gap

Following H. Zhang et al.,
Nature Physics 5, 438 (2009)

TOPOLOGICAL INSULATORS:
SURFACE STATES, TRIM

Existence of surface states due to topology:

Surface states split off inside band gap

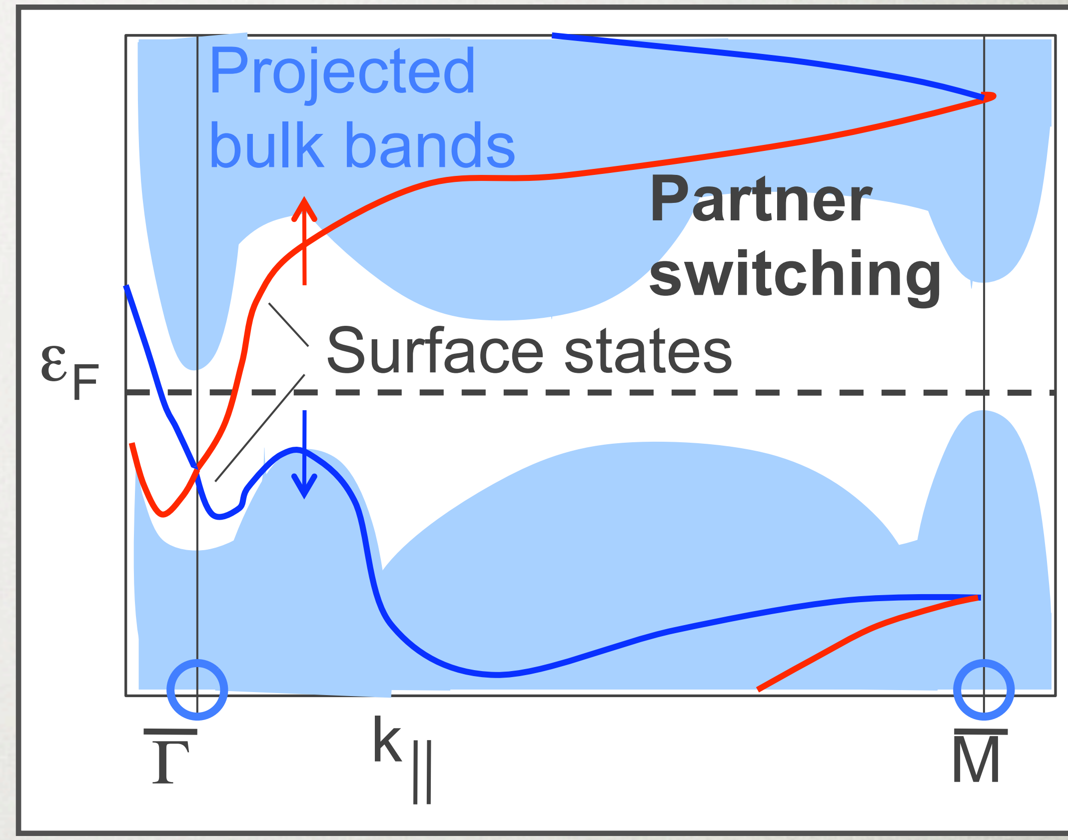
Spin degeneracy lifted due to broken inversion symmetry…

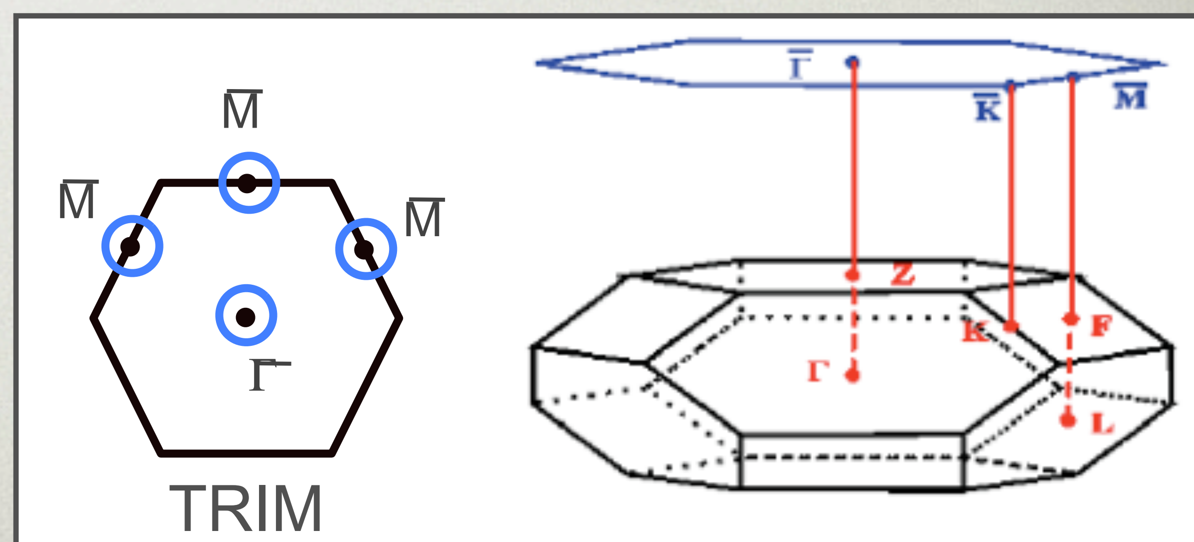
…but spin degeneracy protected at time-reversal invariant momenta (TRIM, k_T) !

Translational symmetry:
$\varepsilon(-k_T,\uparrow) = \varepsilon(-k_T+G,\uparrow) = \varepsilon(k_T,\uparrow)$

Time reversal symmetry:
$\varepsilon(k,\uparrow) = \varepsilon(-k,\downarrow)$ for all k

Inverted parity band gap
=> Topological insulator!
=> Partner switching
=> Odd number of Fermi level crossings



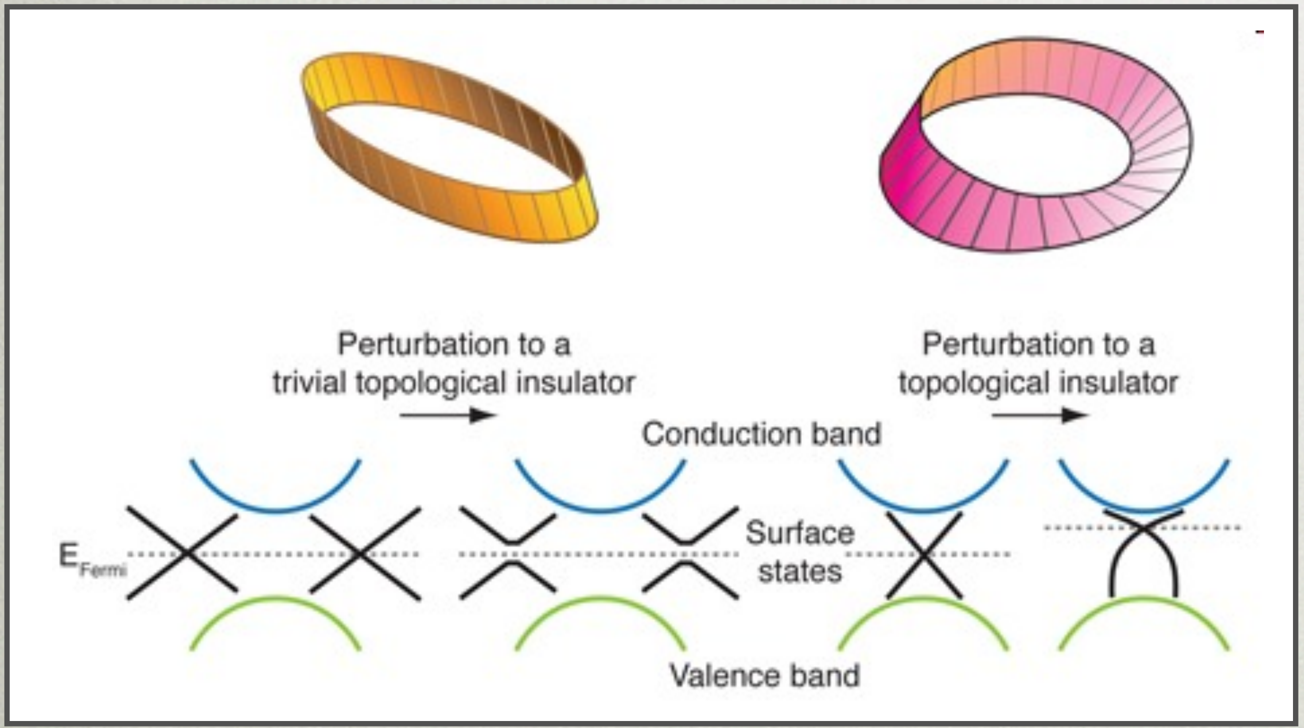


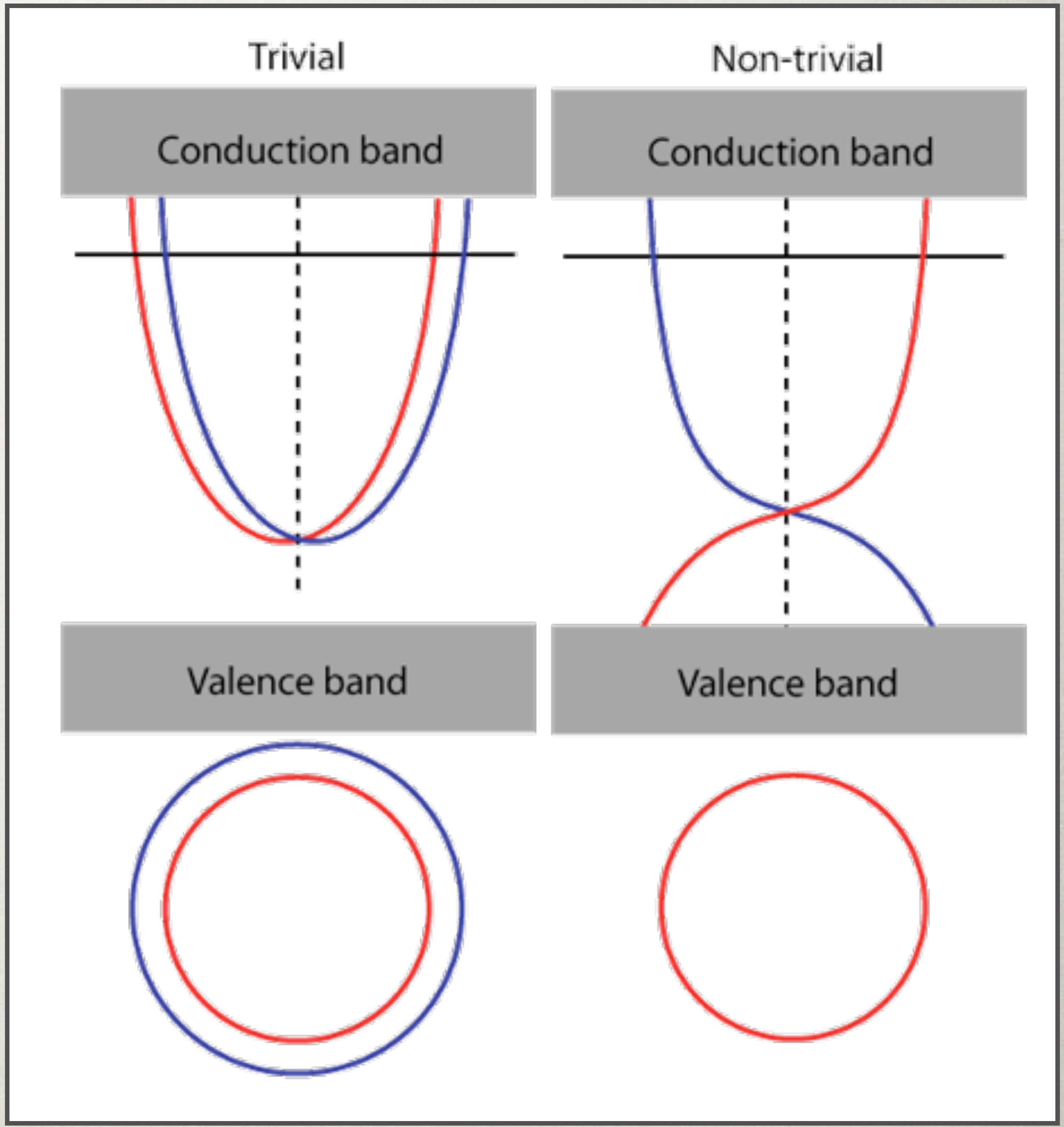
Surface states: perturbations

Topological insulator (non-trivial):

Odd number of Fermi level crossings of its surface states (partner switching) between two TRIM => detection by SARPES

Surface states protected against (non-magnetic) perturbations

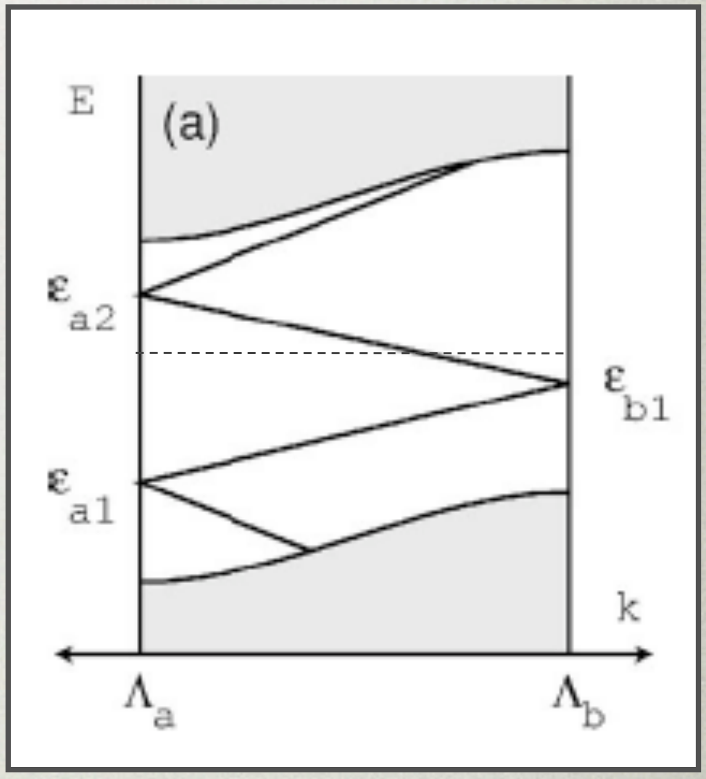




S.-C. Zhang, Physics **1**, 6 (2008)

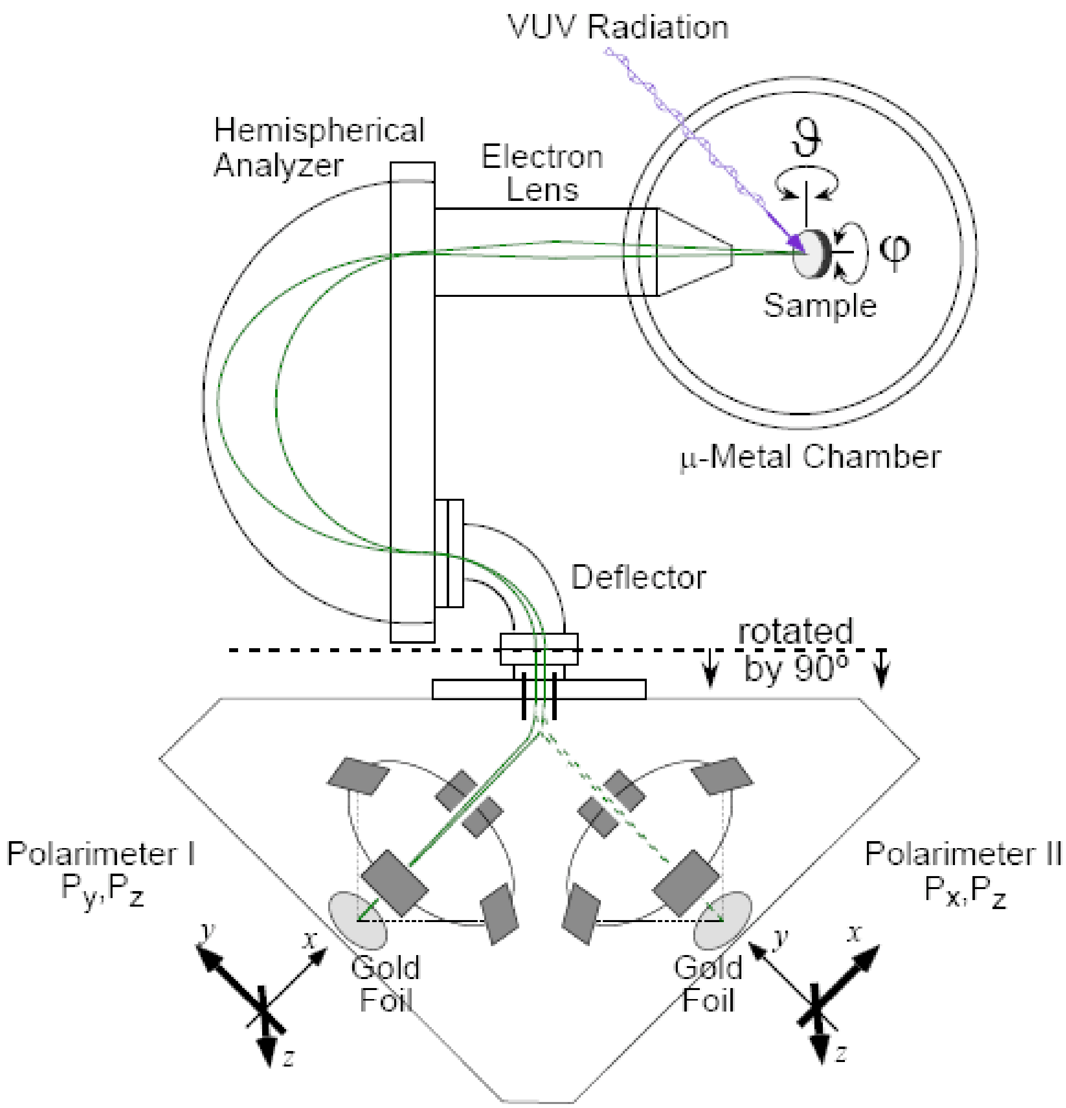
The experiment:
What are we looking for?

- Demonstrate the existence of a bulk band gap (insulator)
- Identify surface states
- Count the number of non-degenerate Fermi surface contours surrounding time reversal invariant points within the surface Brillouin zone
- Demonstrate the non-degeneracy by measuring spin polarization
- Extra bonus: measure spin texture => spin helicity



Spin- and angle-resolved photoemission spectroscopy

COPHEE



Hoesch et al.,
J. Electron Spectrosc. Relat. Phenom. 124, 263 (2002)

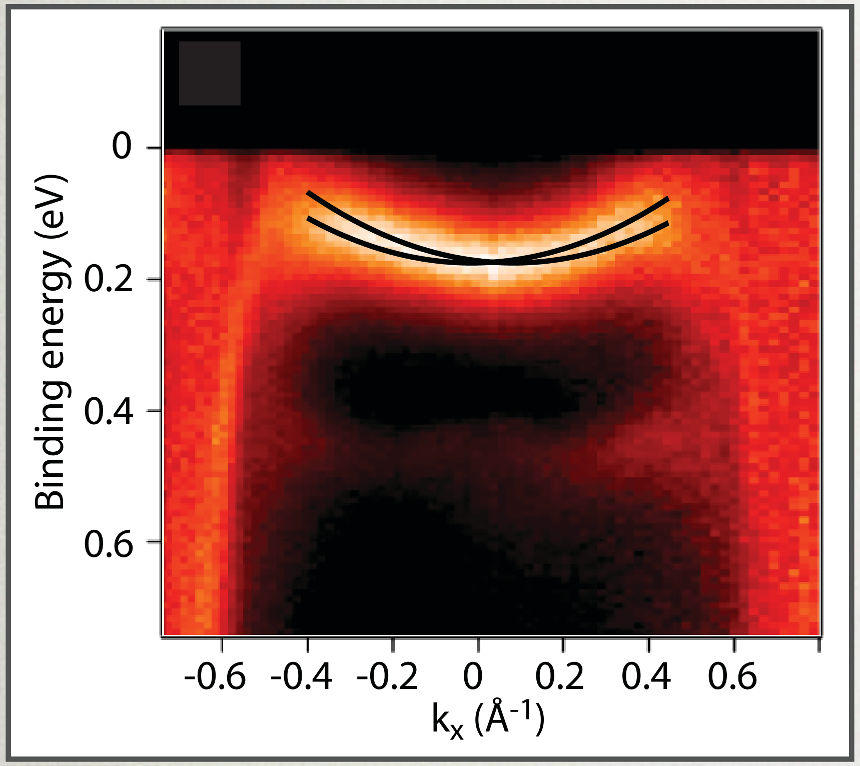
- Two orthogonal Mott scatterers with 4 detectors each
- Determine in-plane spin polarization components and out-of-plane spin component (3D)
- Access to "all quantum numbers" of the electron
- Asymmetry

$$A_\alpha = (N_l - N_r)/(N_l + N_r)$$

- Polarization

$$P_\alpha = A_\alpha / S$$

RESOLVING POWER: Pb/Si(111) QWS



Too small Rashba-type spin splitting to resolve with ARPES (~15 meV)

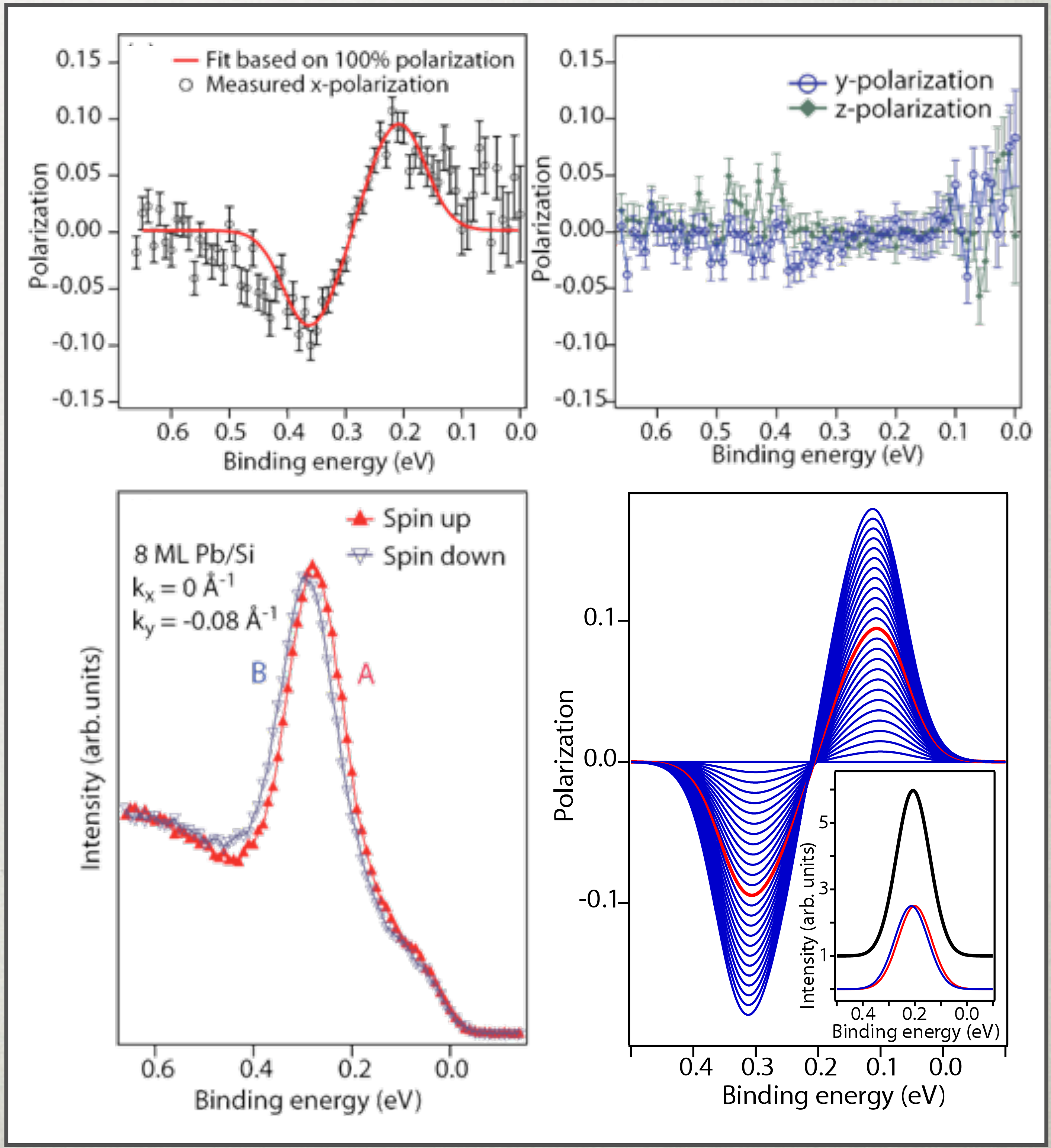
Clear polarization in x-direction

No polarization in y and z

Spin direction reversed compared to Au(111)

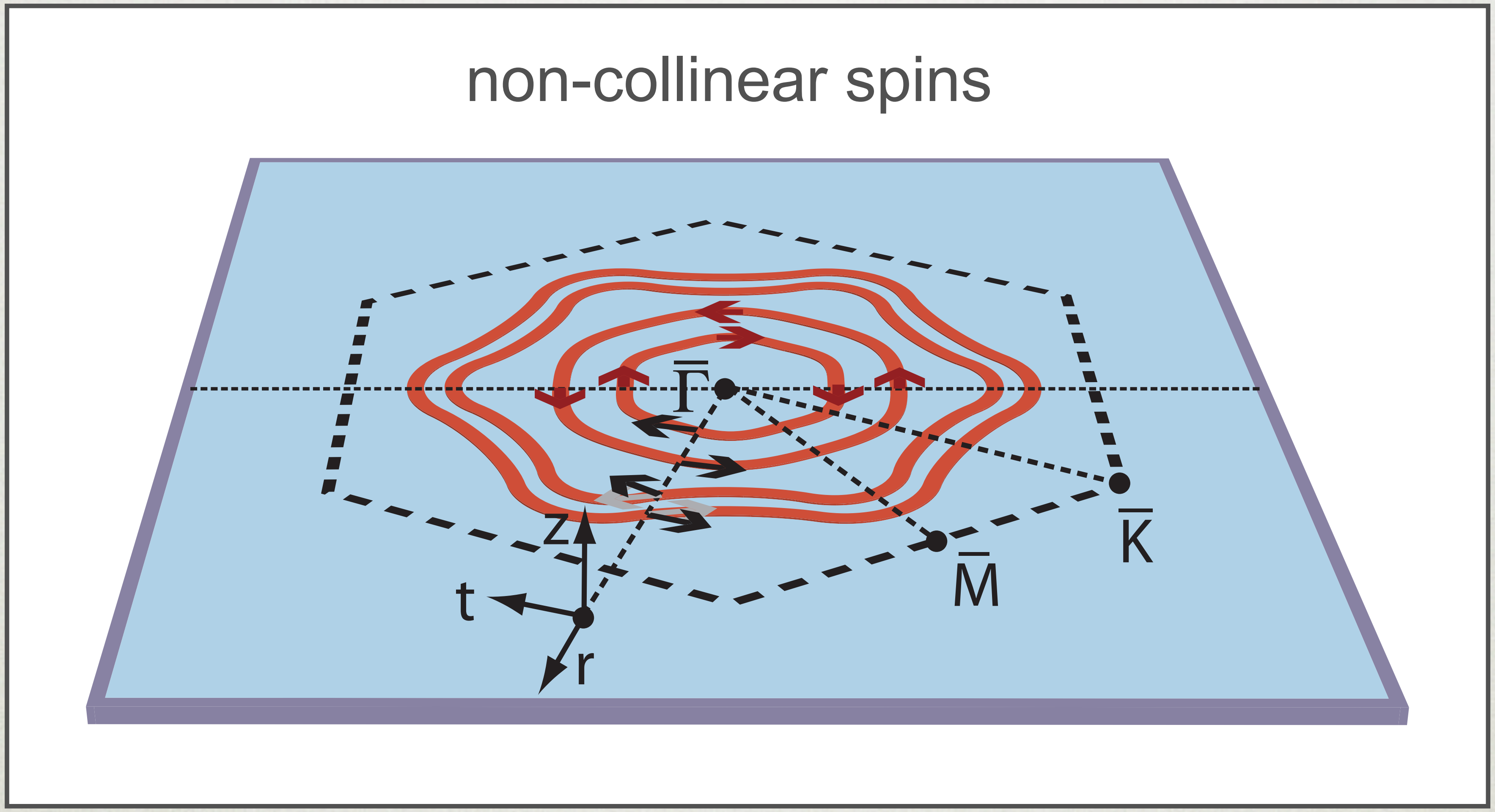
Resolving power of ~5 meV

due to spin tag



J. H. Dil et al., PRL 101 (2008) 165431.

3D spin polarimetry provides more information...

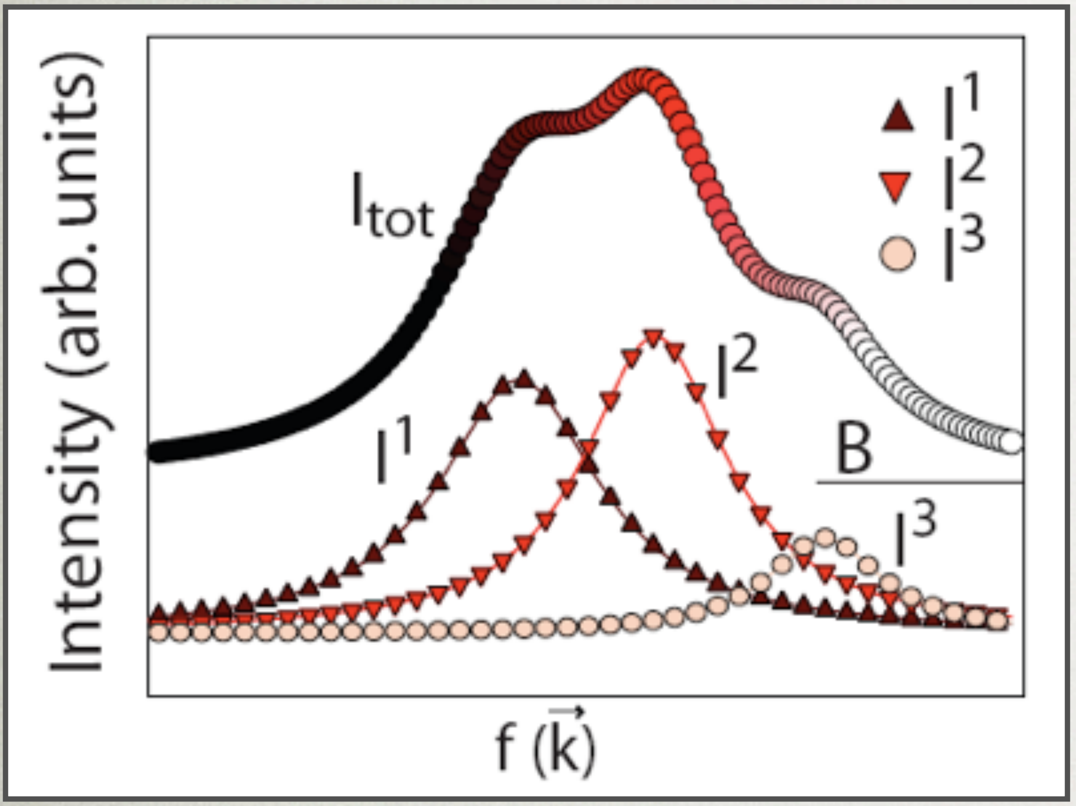


...when using a sophisticated method.

Two-step fitting routine allows us to extract the spin polarization vectors of each electronic state

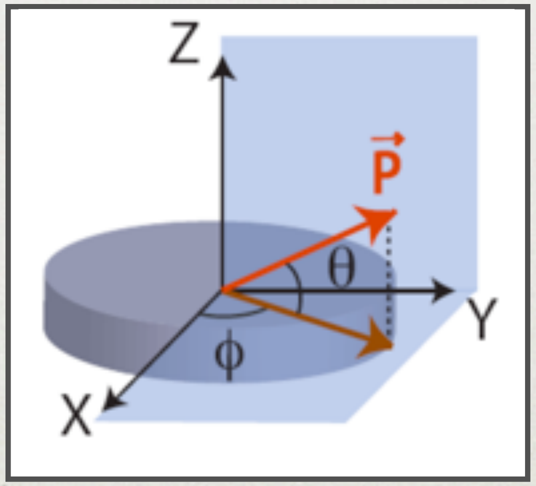
F. Meier et al., PRB 77 (2008) 165431.

Two-step fitting routine

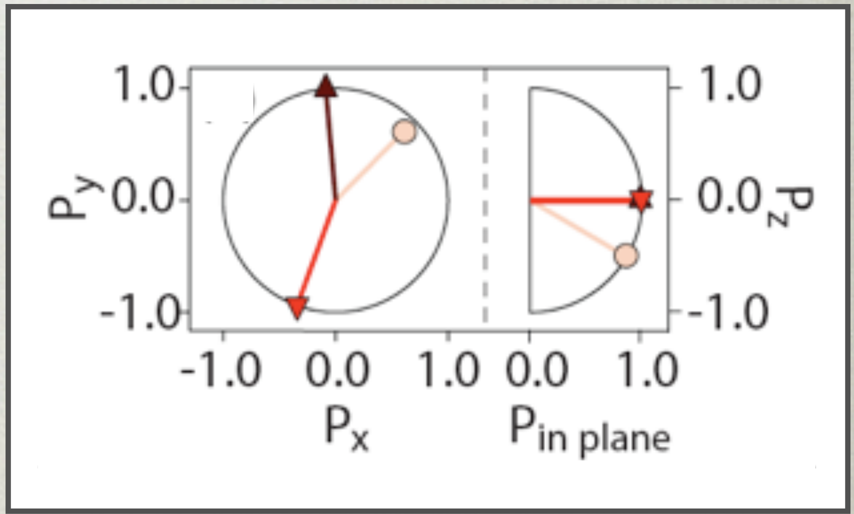


1st step:
Fit the intensity data as usual

$$I = \sum_i I_i + B$$



2nd step:
Fit spin polarization data



-Define spin polarization vector for each peak

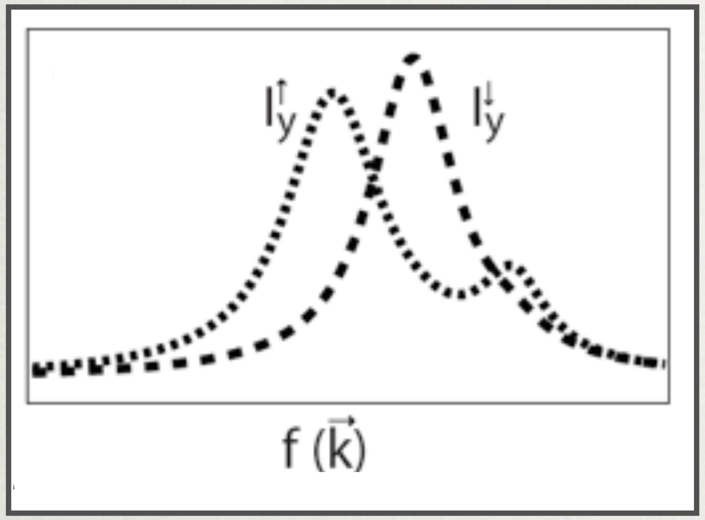
$$\vec{P}_i = c_i \cdot (\cos\theta_i \cos\phi_i, \cos\theta_i \sin\phi_i, \sin\theta_i)$$

$$0 \leq c_i \leq 1$$

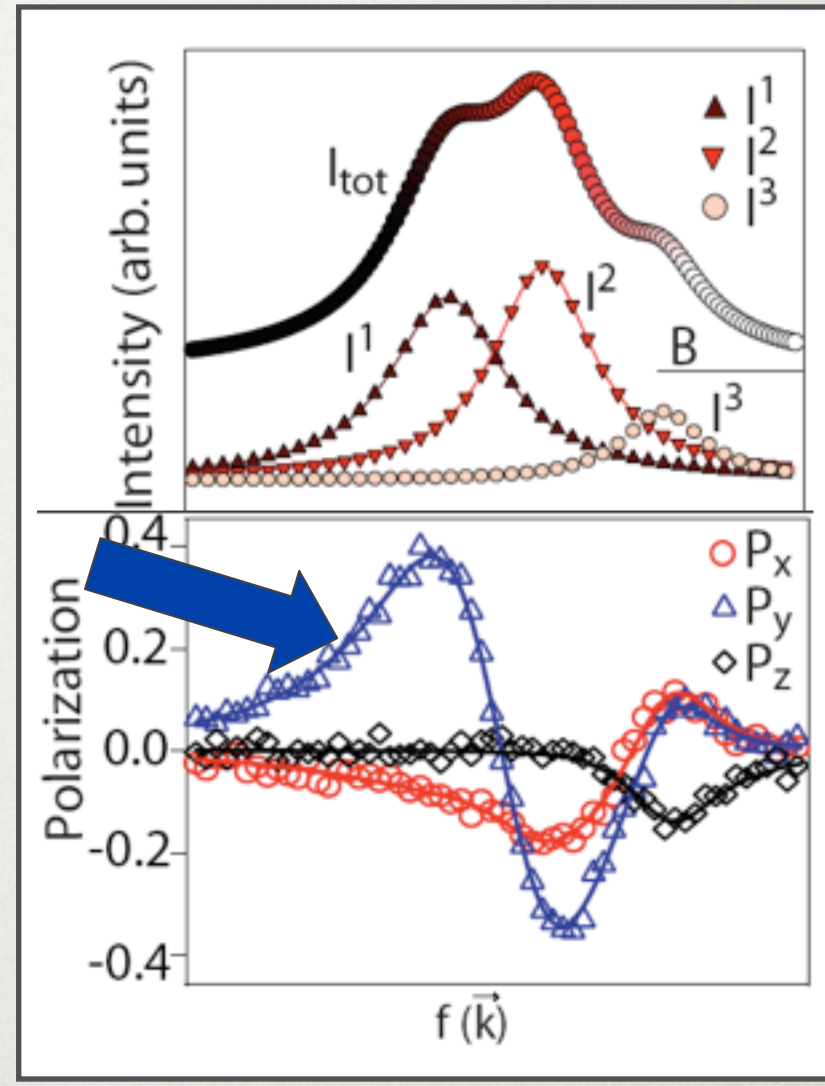
F. Meier et al., PRB 77 (2008) 165431.

Two-step fitting routine

-Calculate spin polarization curves
(e.g. along the y component)



$$P_y(E) = \frac{I_y^{\uparrow}(E) - I_y^{\downarrow}(E)}{I_y^{\uparrow}(E) + I_y^{\downarrow}(E)}$$

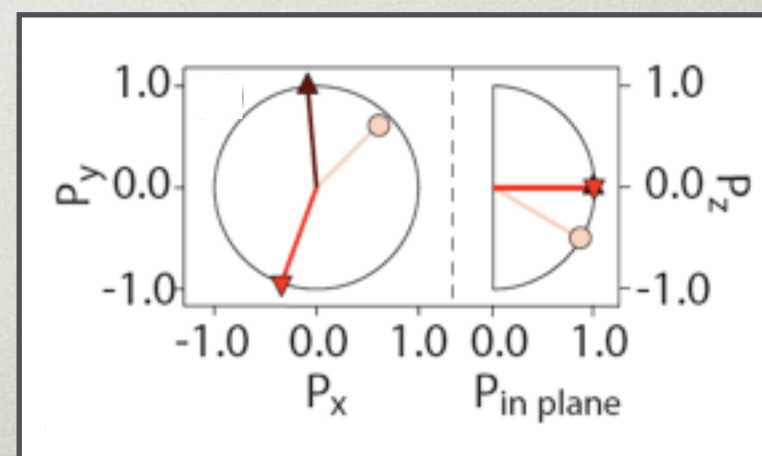


... and compare to data. Fitting parameters: θ_i, ϕ_i and c_i !

Obtain spin polarization vectors of the measured states.

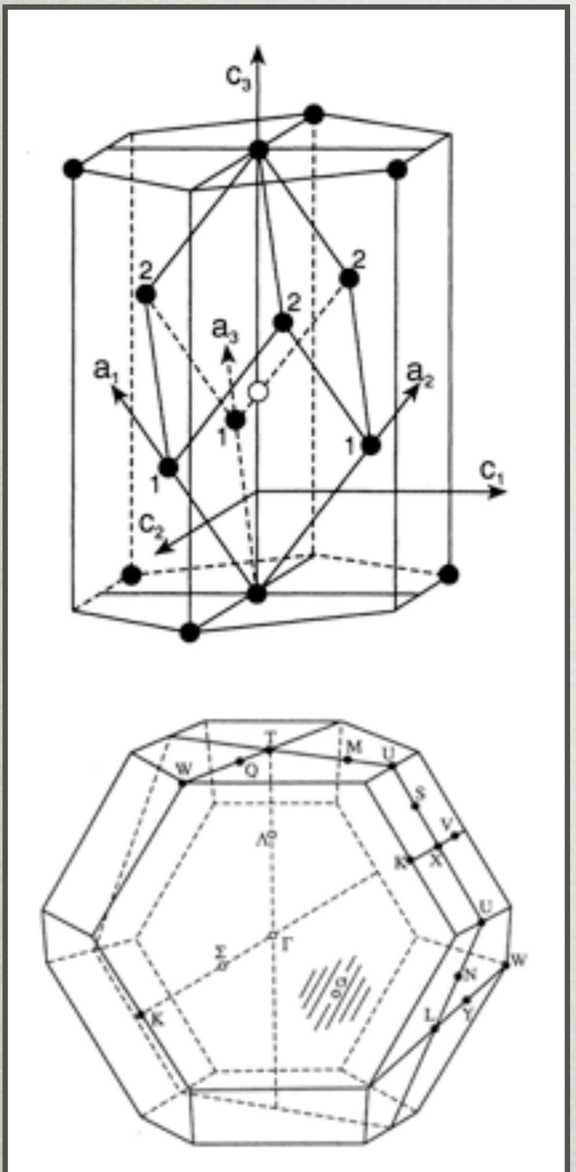
$$\vec{P}_i = c_i \cdot (\cos\theta_i \cos\phi_i, \cos\theta_i \sin\phi_i, \sin\theta_i)$$

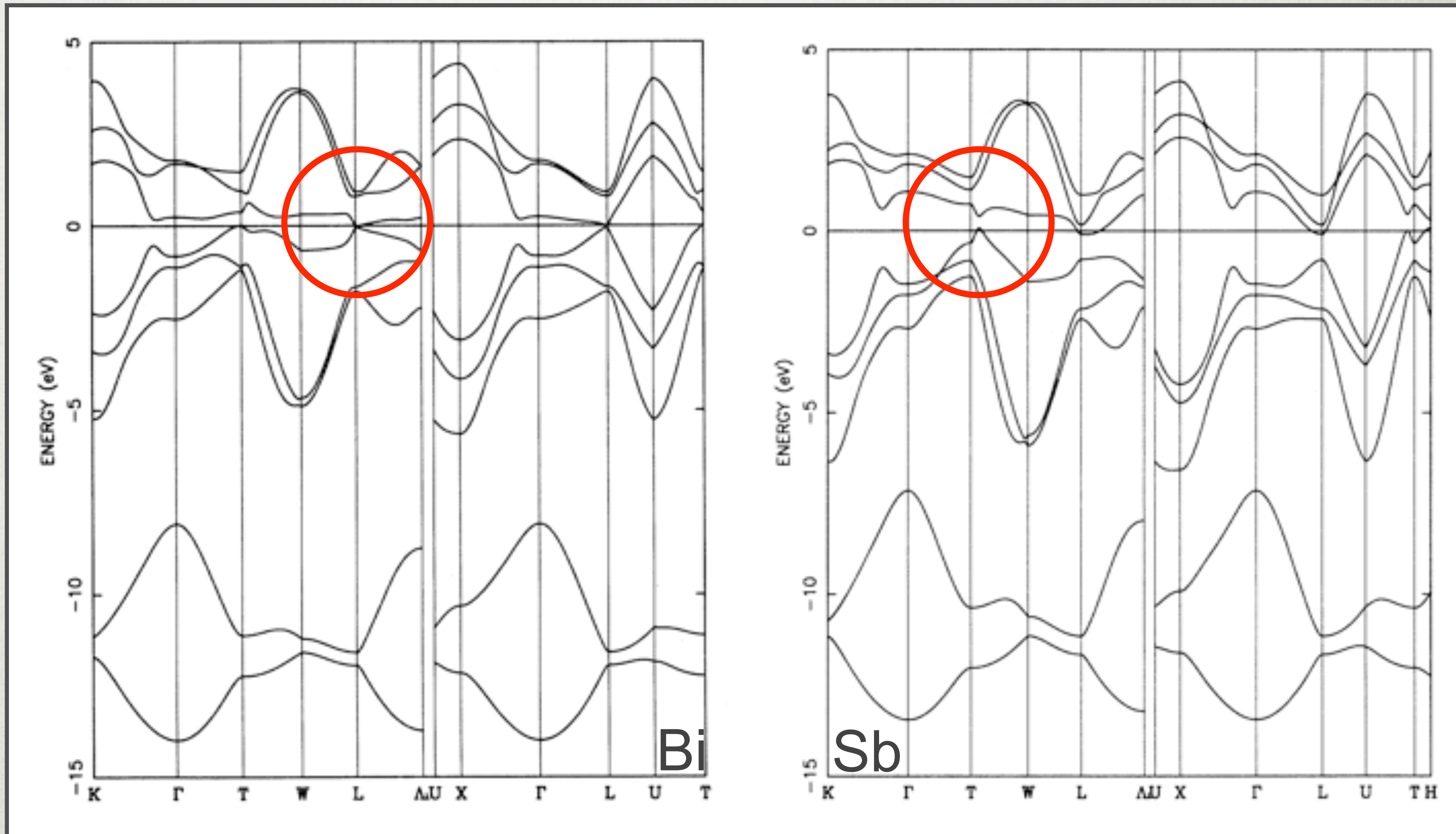
$$0 \leq c_i \leq 1$$



The band structures of Bi and Sb

Structure:
Rhombohedral A7
(distorted cubic)



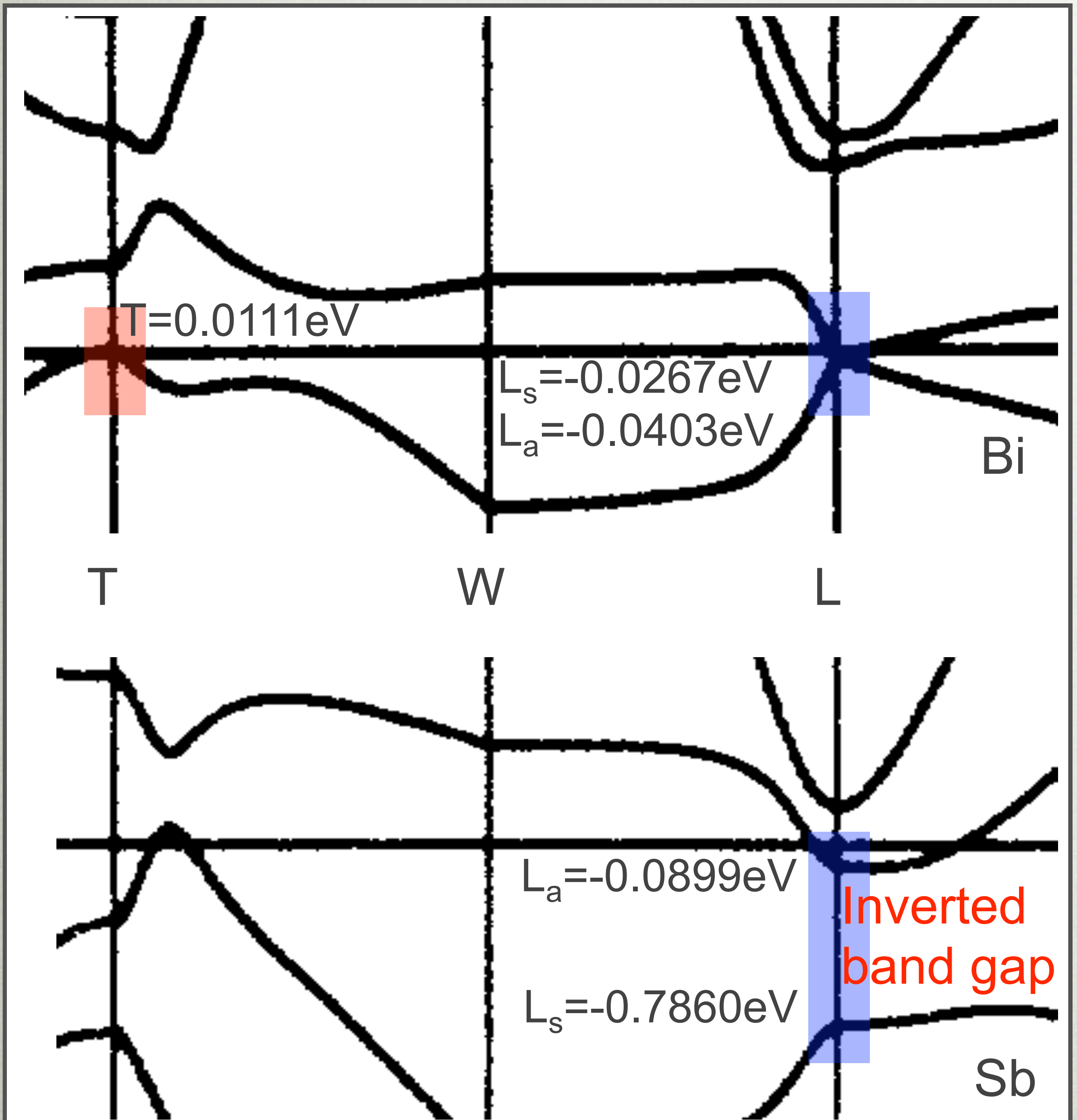


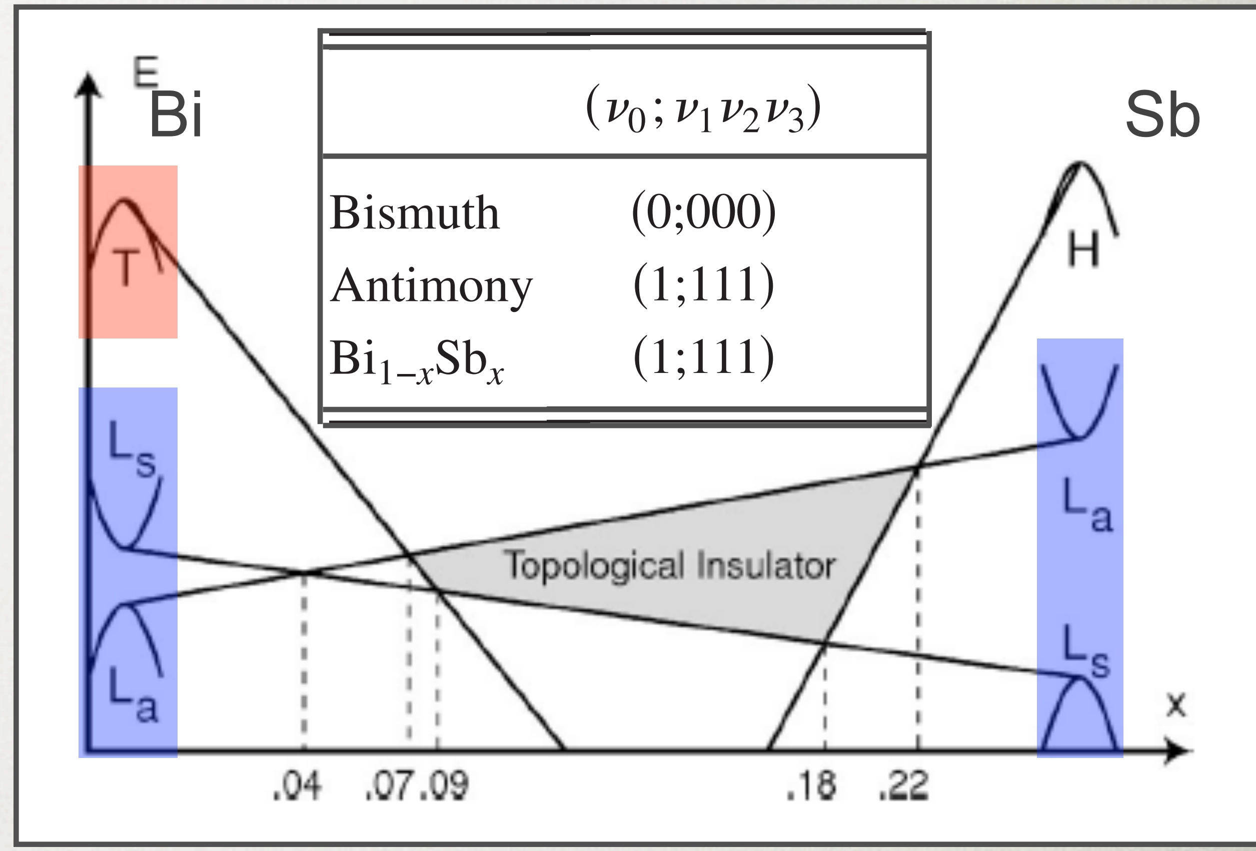
3rd neighbor tight binding model
including spin-orbit interaction

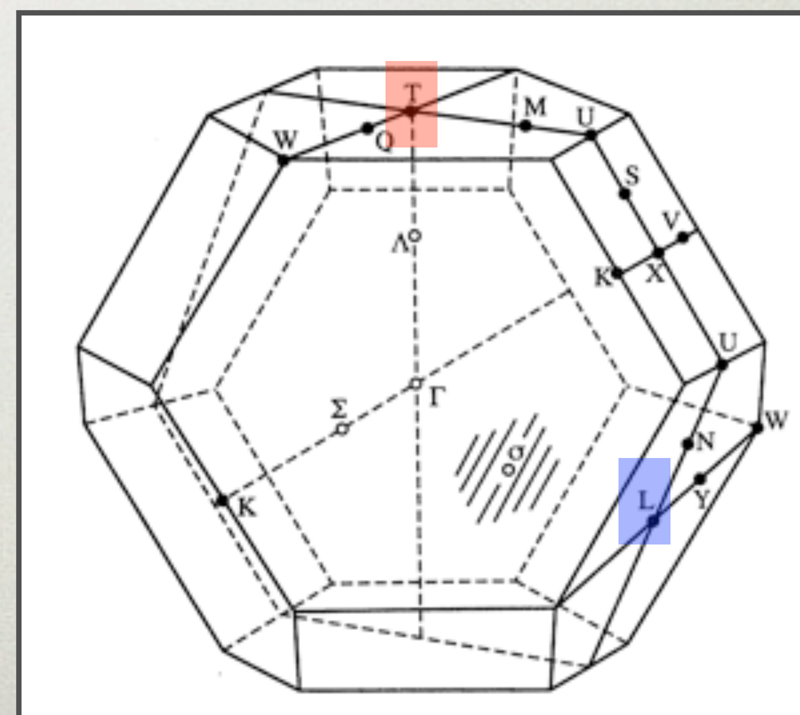
Spin-orbit induced
band gaps

Yi Liu and R. E. Allen, PRB 52, 1566 (1995)

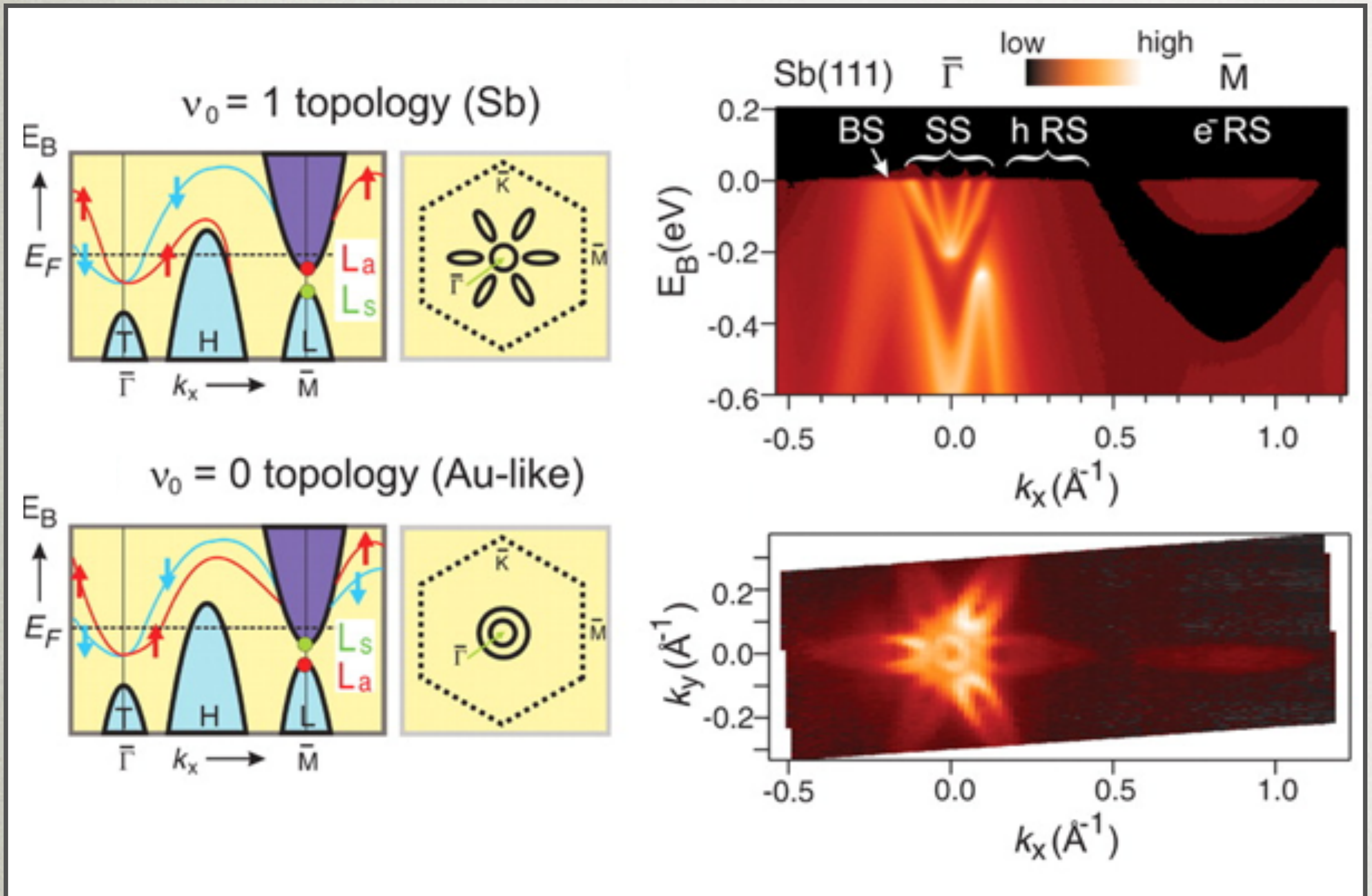
Z_2 TOPOLOGICAL NUMBERS

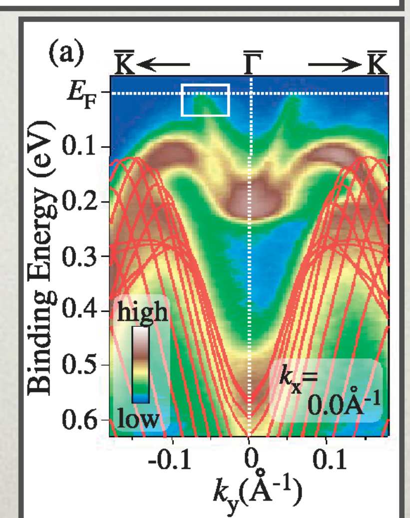


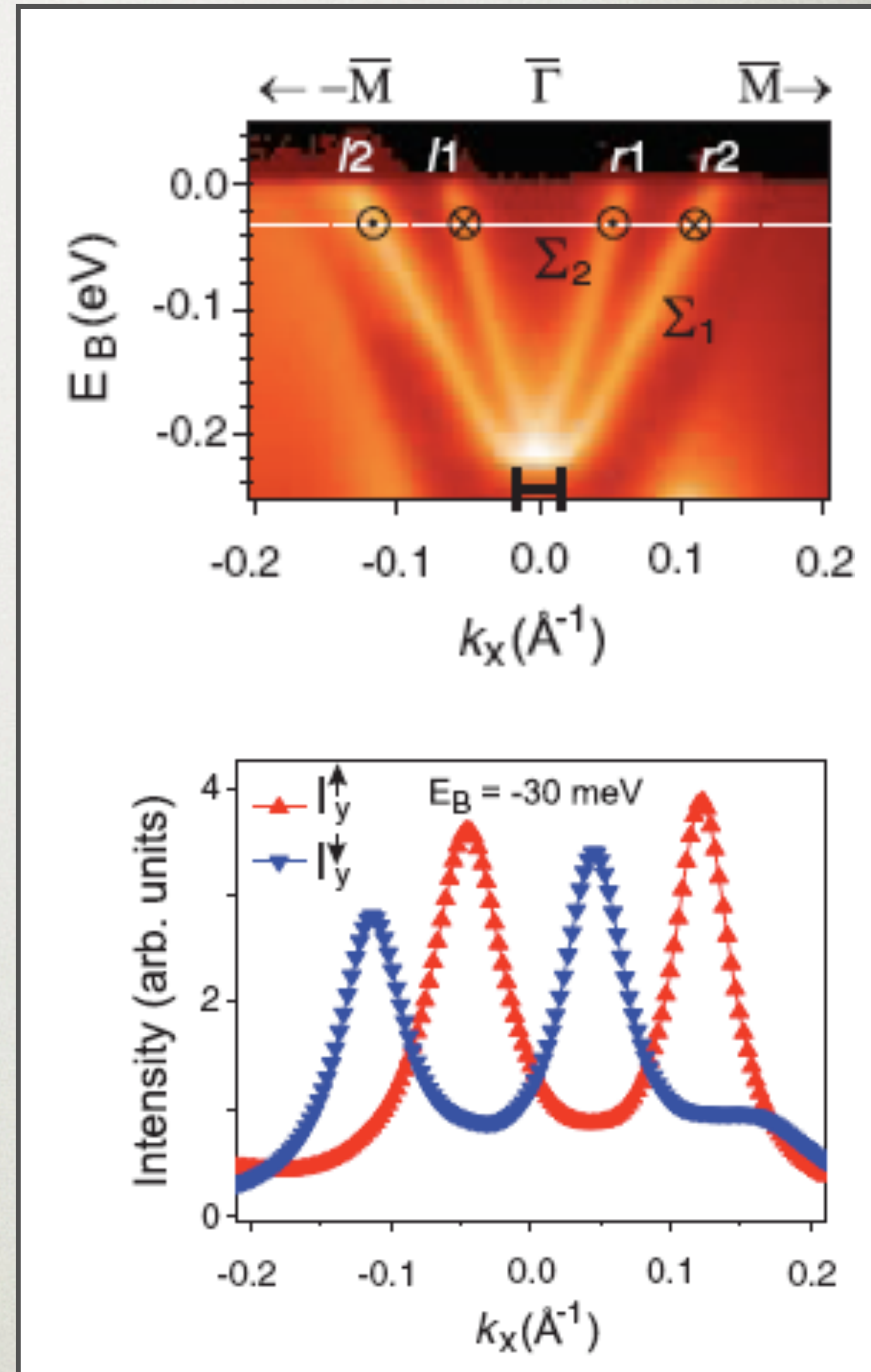




The parent compound: Sb(111)







-Correct topology (3 Fermi level crossings)

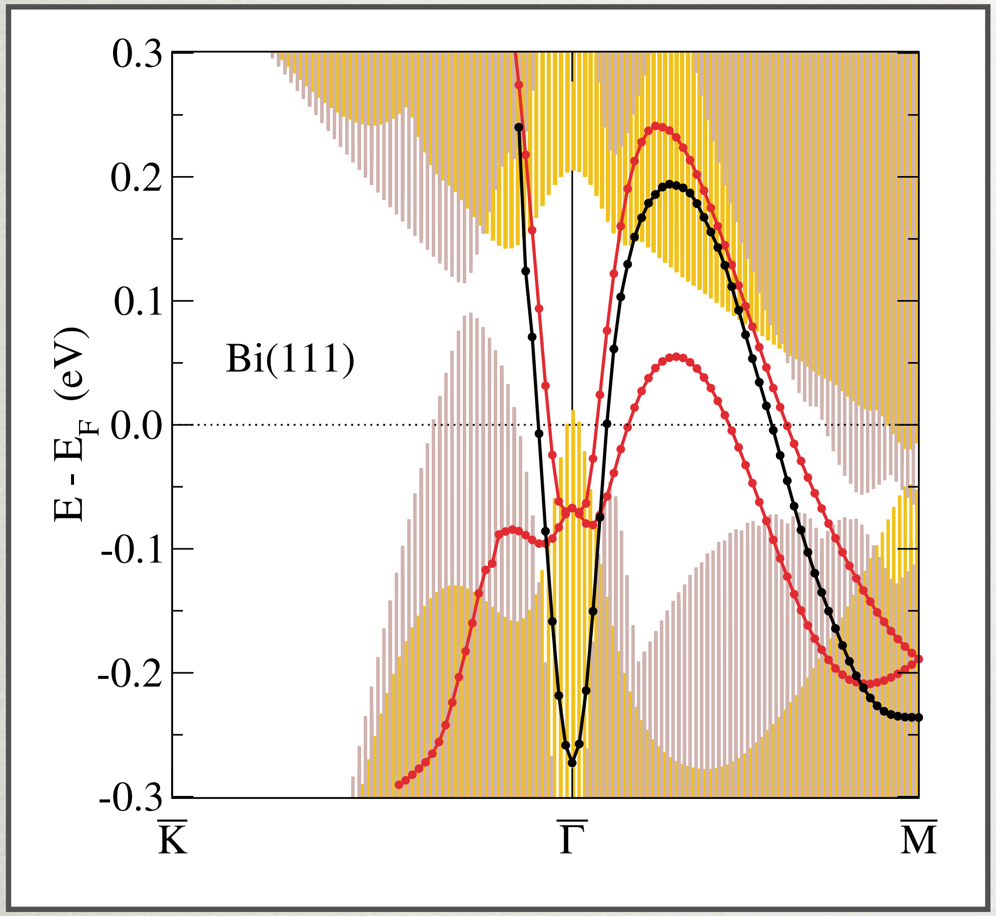
-Very large spin-splitting for relatively low Z

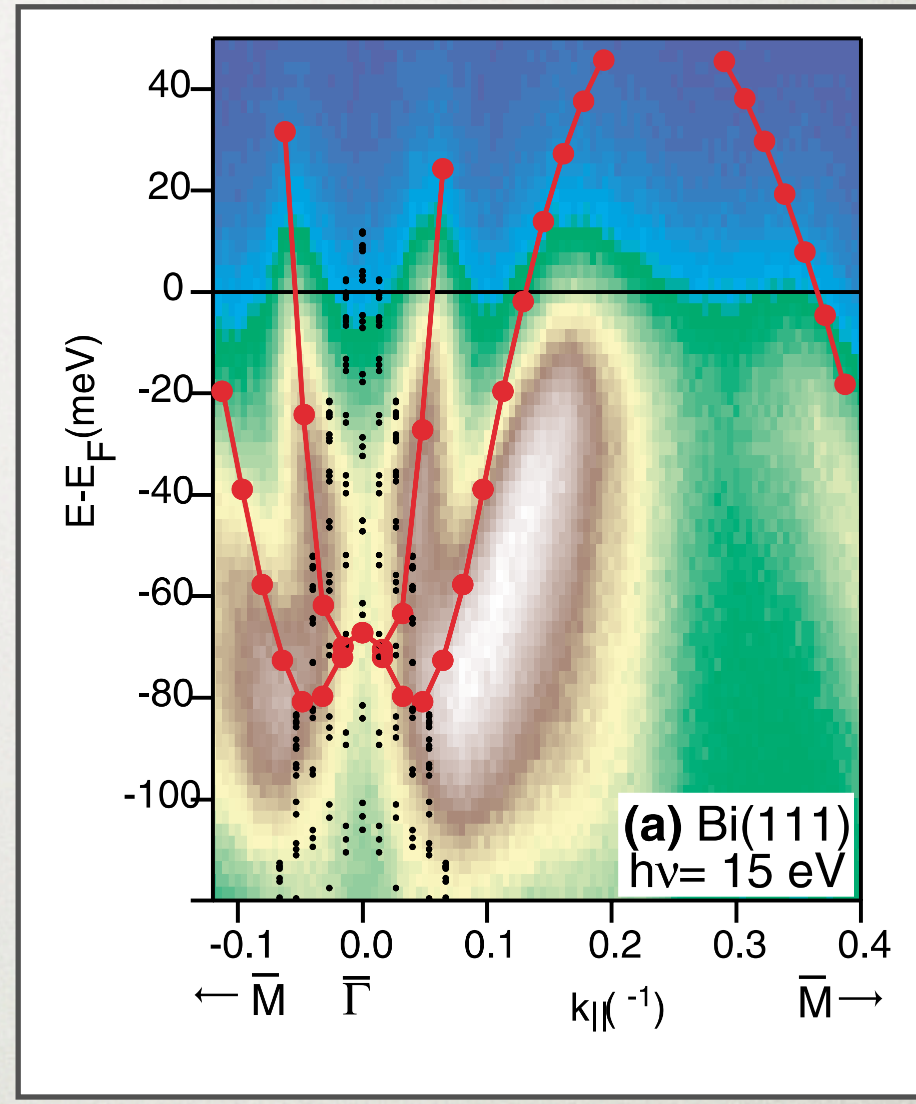
-Semi metal

Sugawara *et al.*, PRL 96 (2006) 046411.

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

Bi(111): surface states





-Trivial topology

-Surface states are spin split

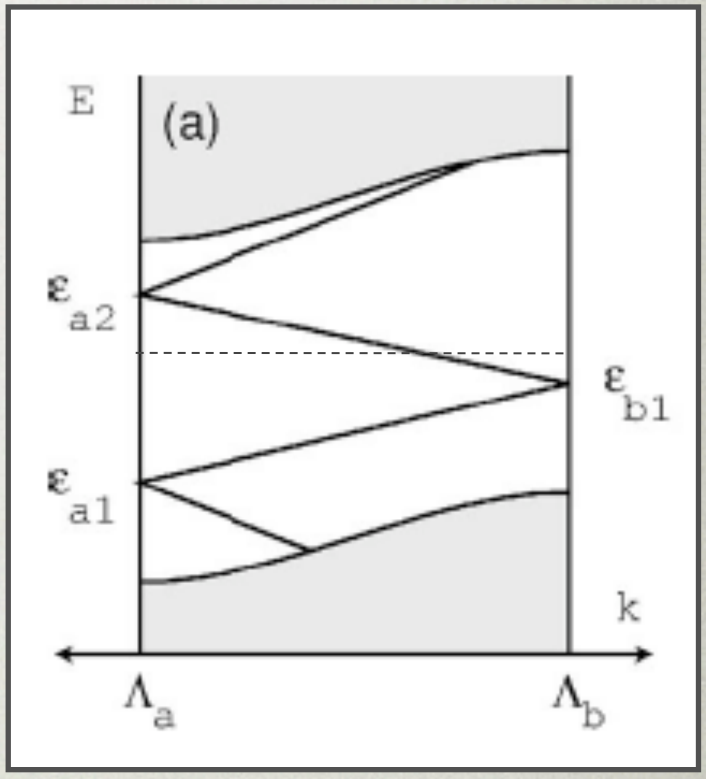
T. Hirahara *et al.*, PRB 76 (2007) 153305.

Y. Koroteev *et al.*, PRL 93 (2004) 046403.

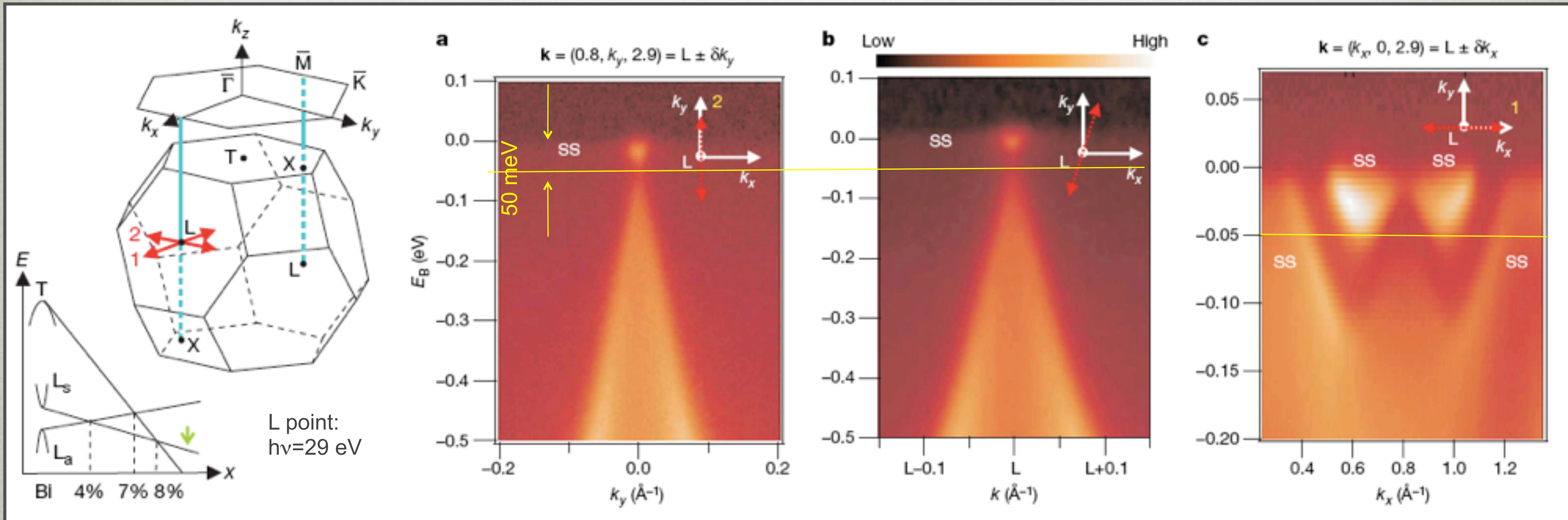
The experiment:
What are we looking for?

- Demonstrate the existence of a bulk band gap (insulator) (by transport or ARPES)
- Identify surface states (ARPES)
- Count the number of non-degenerate Fermi surface contours surrounding time reversal invariant points within the surface Brillouin zone (by SARPES)
- Demonstrate the non-degeneracy by measuring spin polarization (by SARPES)
- Extra bonus: measure spin texture

=> spin helicity (by SARPES)

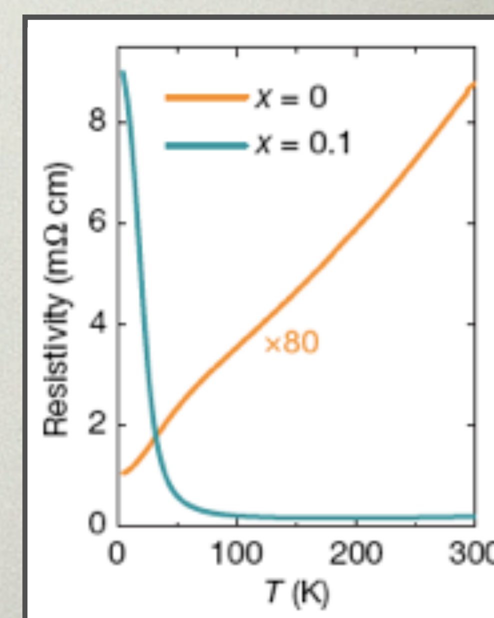


Bulk band gap in $Bi_{0.9}Sb_{0.1}$



ARPES: Look for band extrema at/near high-symmetry points in the bulk BZ
… first needs a clear identification of bulk / surface states
… exploit similarities with well known bands from the Bi(111) case

More directly: transport measurements !
- clearly semiconducting behavior
- fit yields E_g = 7.6 meV
  (impurity bands, disorder)



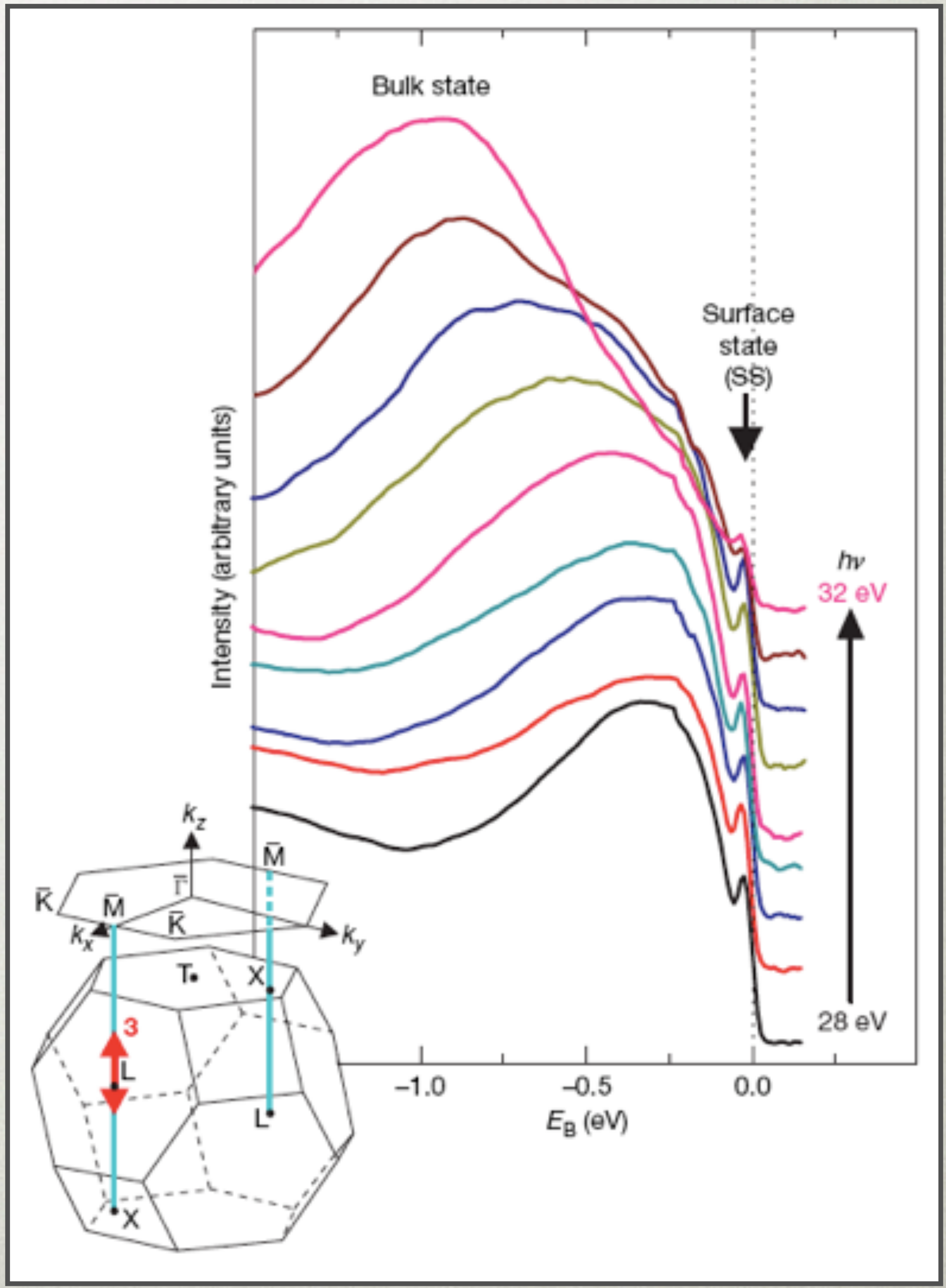
D. Hsieh *et al.*, Nature **452** (2008).

Identification of surface states in $Bi_{0.9}Sb_{0.1}$

Photon energy dependent ARPES:

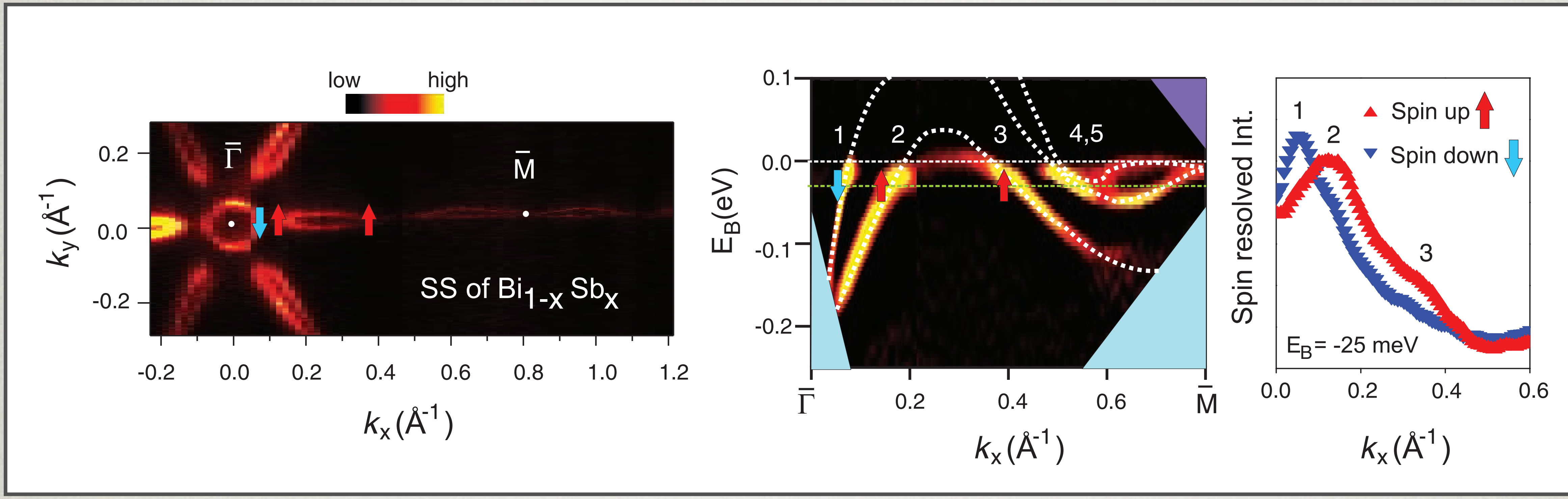
bulk states disperse with k_z, are broad

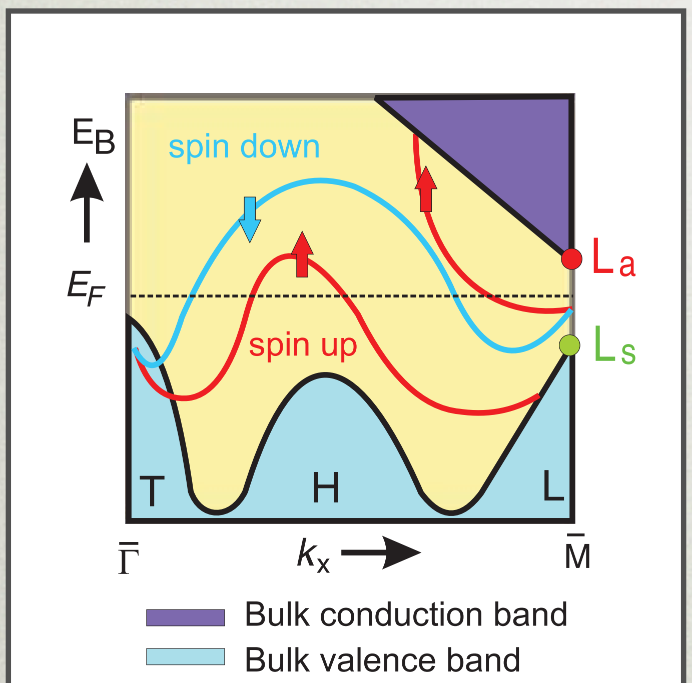
surface states do not disperse with k_z

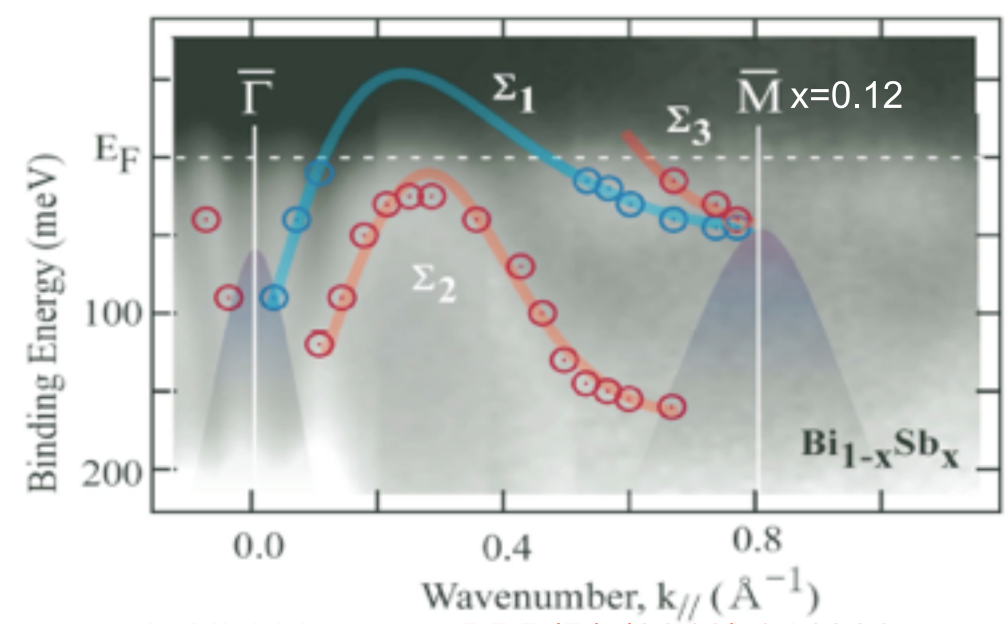


D. Hsieh *et al.*, Nature **452** (2008).

First 3D topological insulator: $Bi_{0.9}Sb_{0.1}$







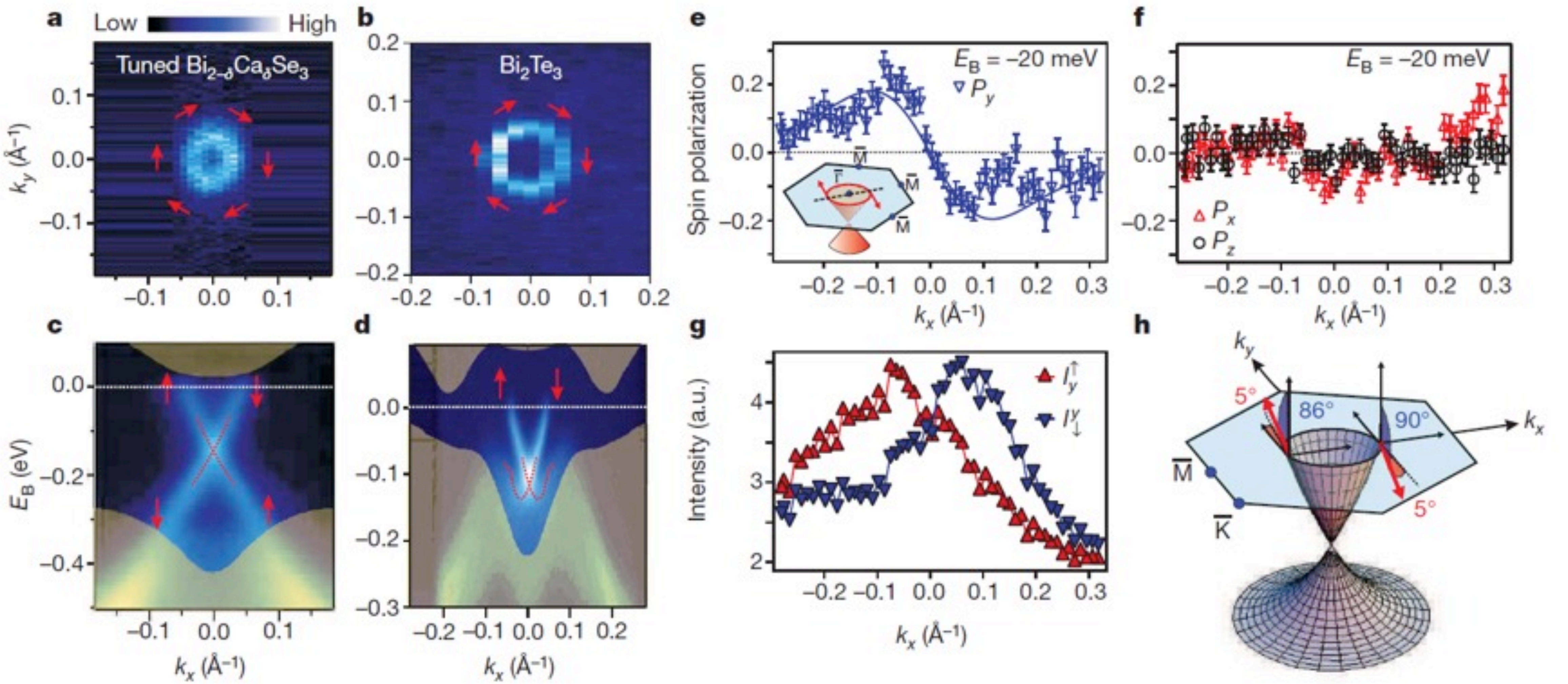
A. Nishide *et al.*, PRB(R) (2010) 041309

-small band gap (~50 meV)

-5 Fermi level crossings

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

Bi2Se3, Bi2Te3: next generation topological insulators



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

left-handed spin helicity

J. Black et al., J. Phys. Chem. Solids 2, 240 (1957)

-Larger energy gaps: -Bi_2Se_3 350 meV

-Bi_2Te_3 180 meV

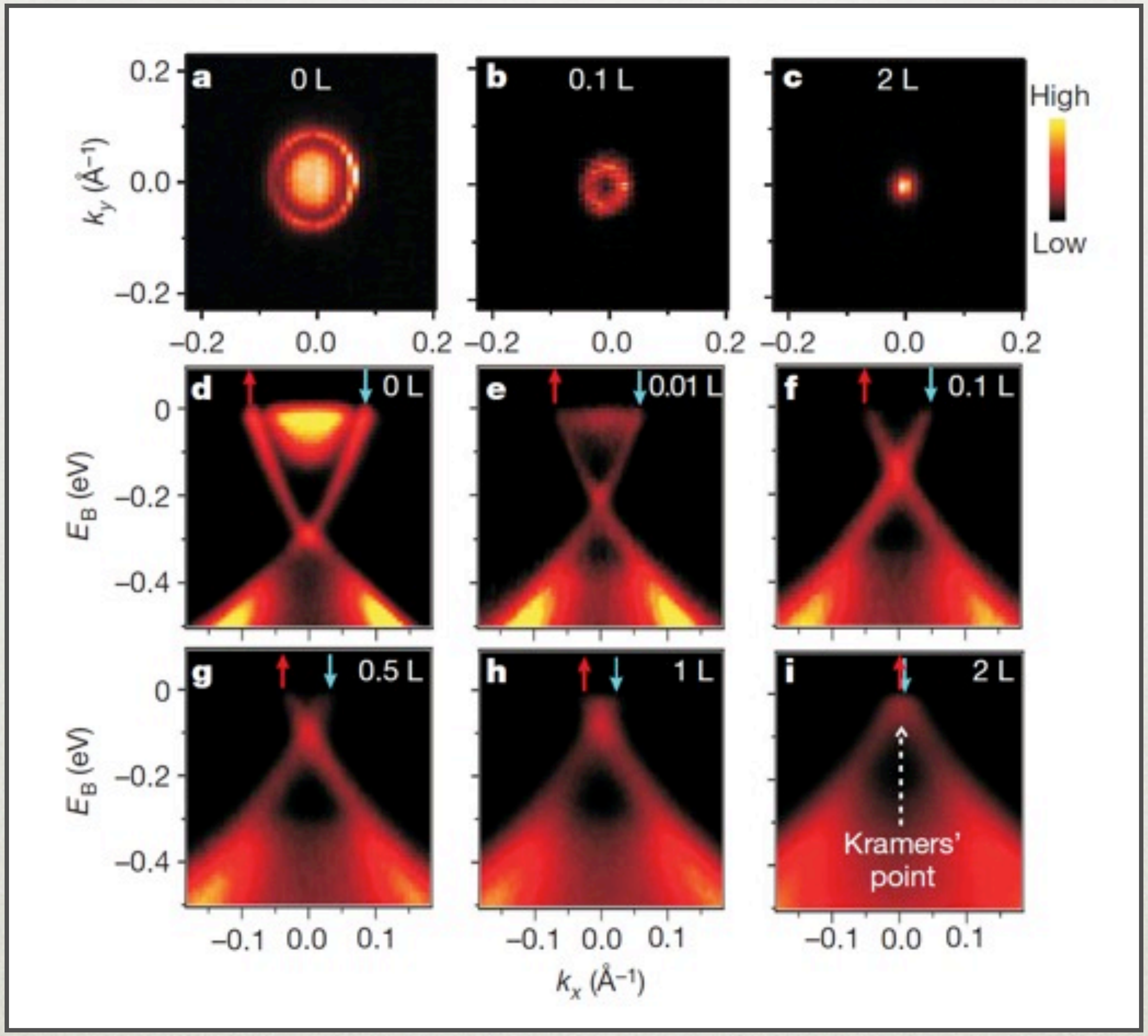
G. A. Thomas et al., PRB 46, 1553 (1992)

-Room temperature topological insulators

-Only a single,non-degenerate surface state

H. Zhang et al., Nature Physics 5, 438 (2009)

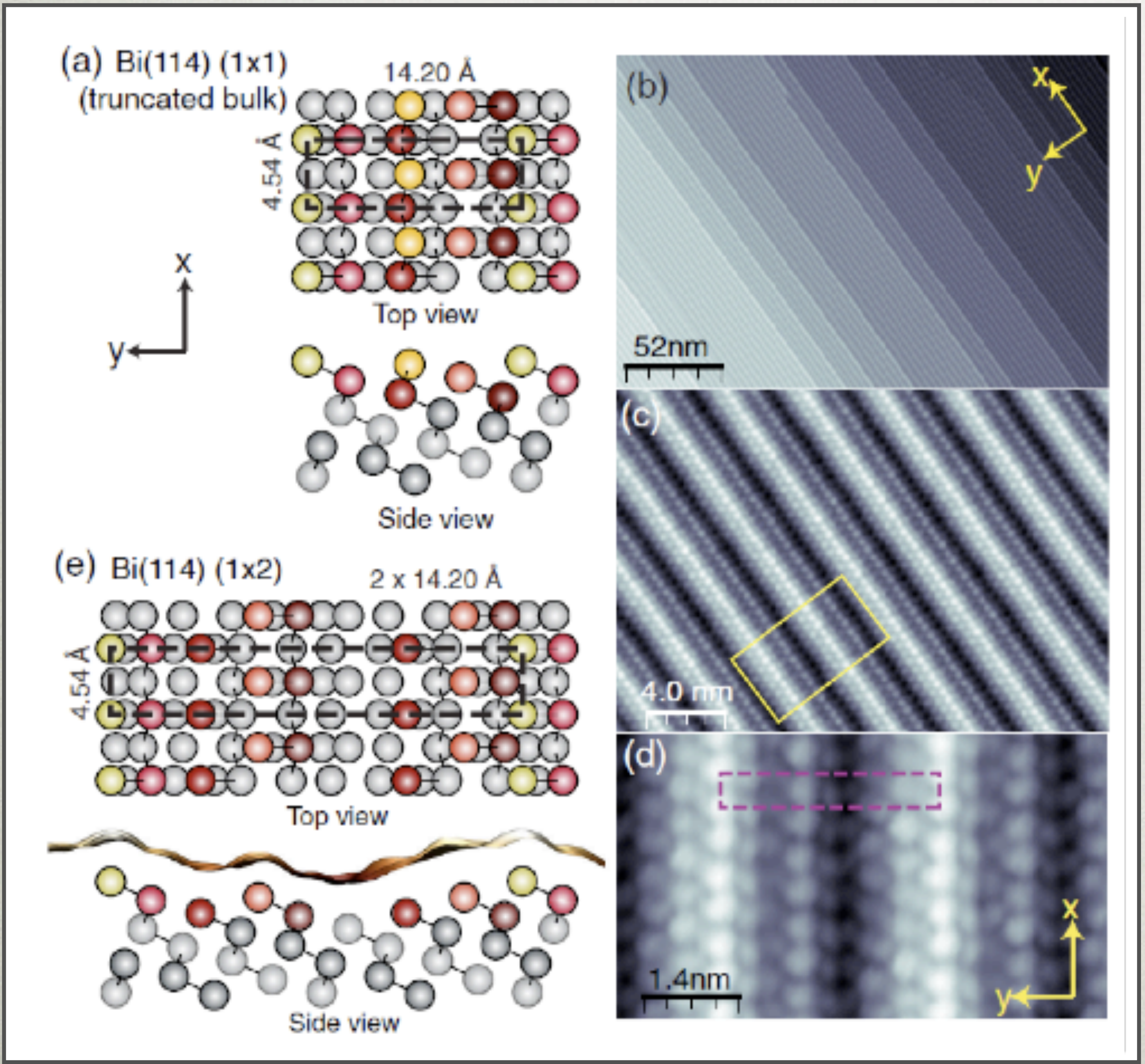
Aligning the Kramers point



Surface doping with NO_2 aligns the crossing point (Kramers, Dirac point) to the E_F
=> Spin polarised Dirac Fermions at zone centre

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

Bi(114): A one-dimensional quantum spin hall system?



Extremely miscut surface of Bi(111): 56°

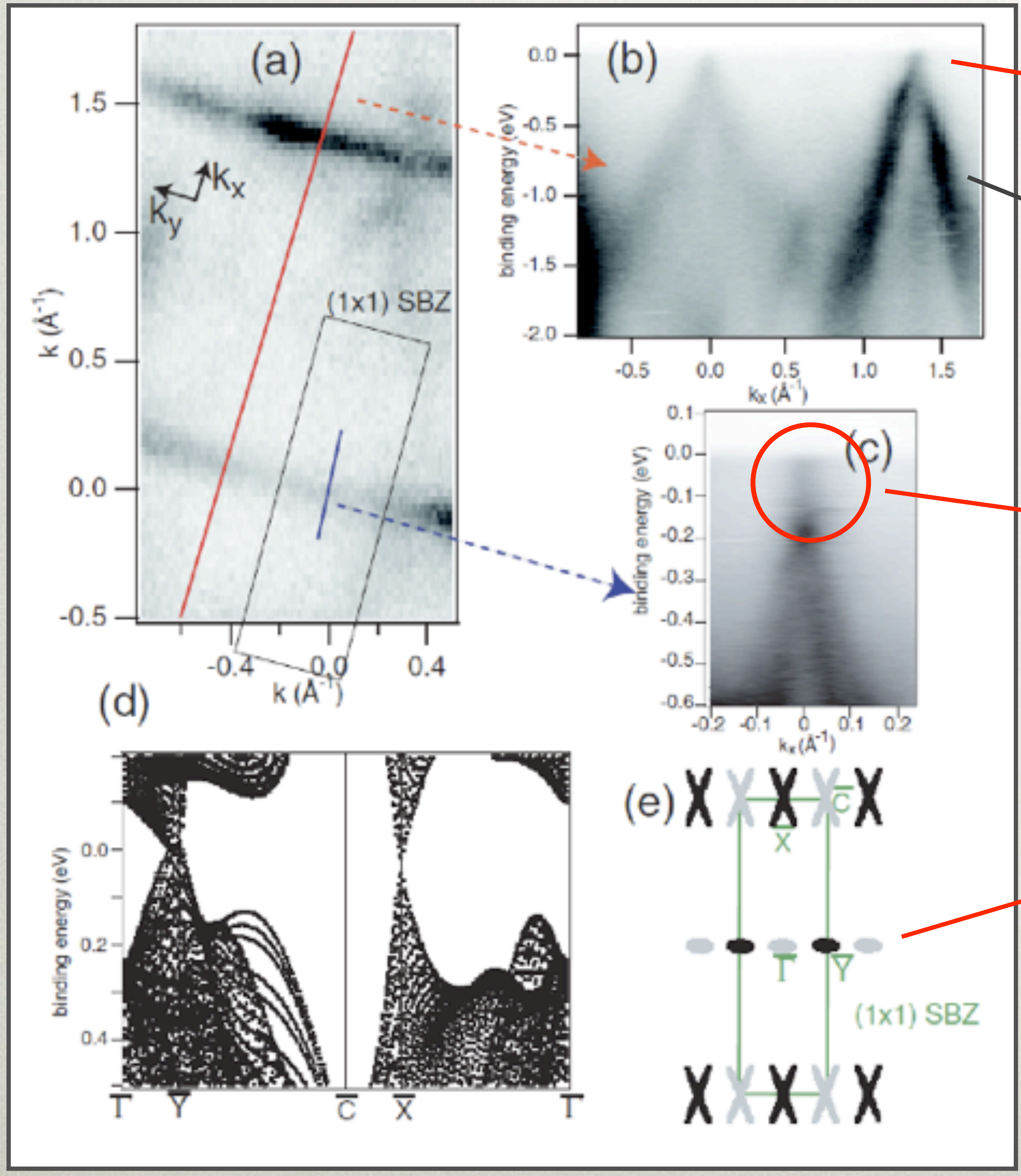
STM and LEED show 1D crystal structure

Missing row reconstruction in y-direction

In STM at 5K pairing of atoms in x-direction (Peirls transition?)

J. W. Wells *et al*. PRL **102** (2009) 096802

Bi(114): A one-dimensional quantum spin hall system?



Surface state

Bulk states
(not fully gapped)

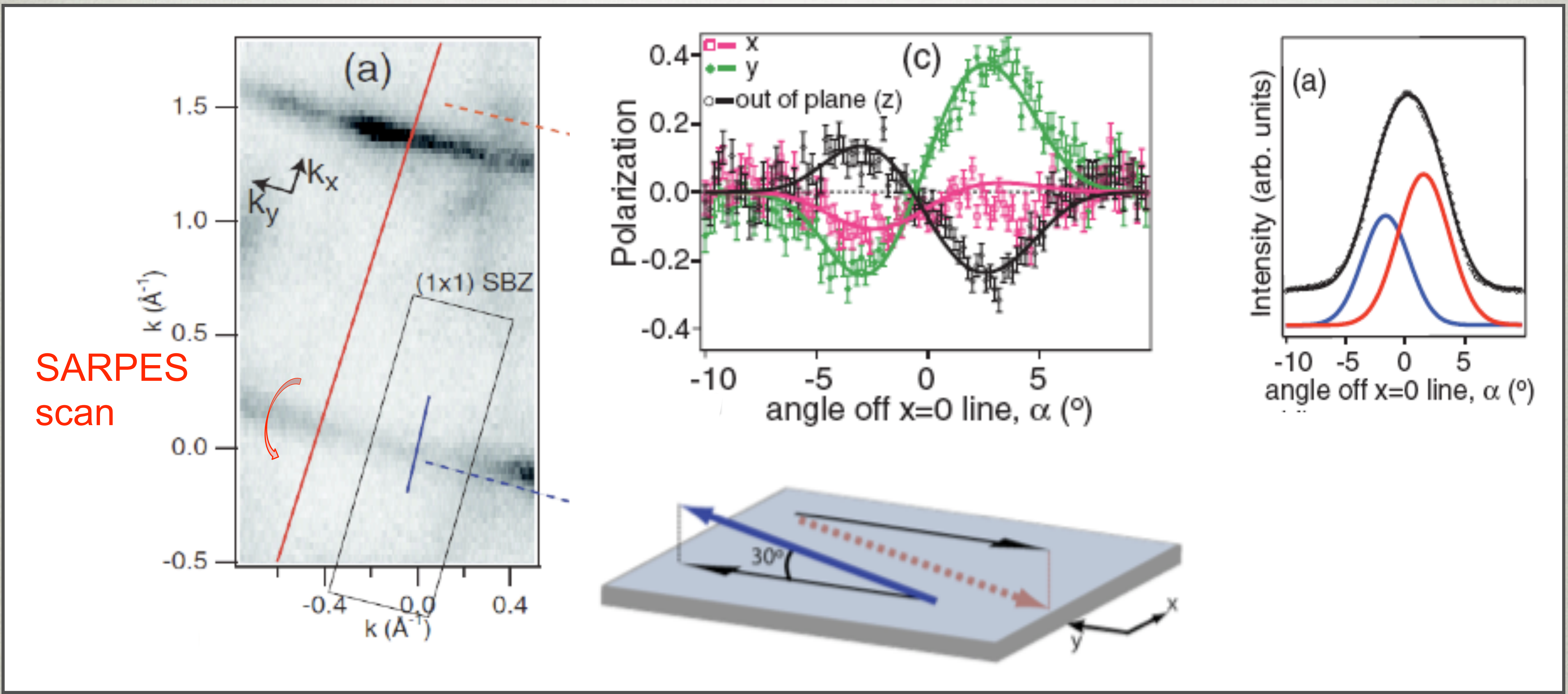
1D surface state
with very small k_F
(dispersion not resolved)

Bulk states at E_F

State oscillates between
being a surface state
and a surface resonance

J. W. Wells *et al.* PRL **102** (2009) 096802

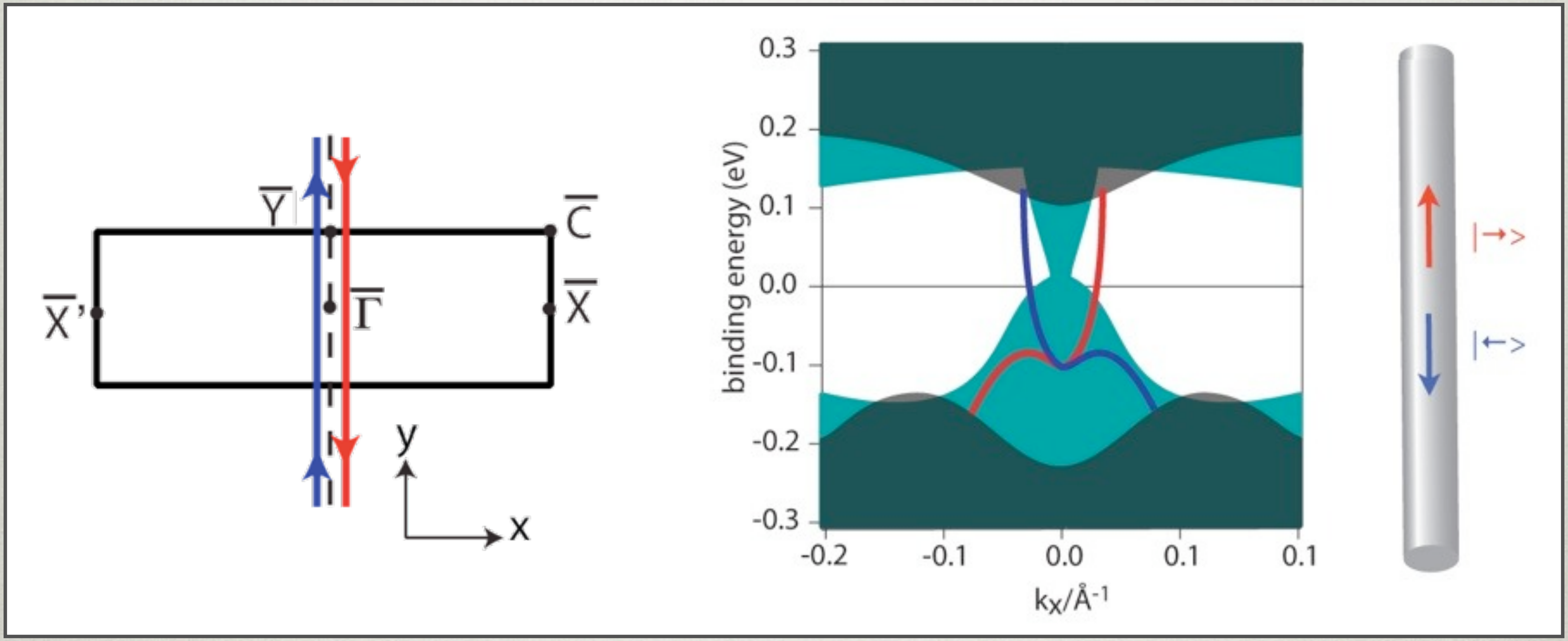
SARPES: Spin structure of the surface states



- We measure a spin-split band, split across the SBZ center line
- Spin polarization vectors are almost parallel to the Fermi surface
- We observe the same vectors at several places along the line

 J. W. Wells *et al.* PRL **102** (2009) 096802

Exotic spin texture arising from these data



Only one Fermi crossing between two time-reversal invariant momenta (Γ-X)

$Bi_{0.9}Sb_{0.1}$(114): 1D quantum spin Hall phase ?

New concept: 1D edge states on a 3D topological insulator ?

(instead of (n-1)D on nD)

 J. W. Wells *et al.* PRL **102** (2009) 096802

Conclusions

- SARPES is a powerful tool for the investigation of the surface spin structure
- (S)ARPES provides clear signatures for the topological magneto-electric effect of surface states on $Bi_{0.9}Sb_{0.1}$, Bi_2Se_3 and Bi_2Te_3.
  - odd number of Fermi level crossings between TRIMs
  - spin polarization, spin texture
- Bi(114): 1D quantum spin hall system?