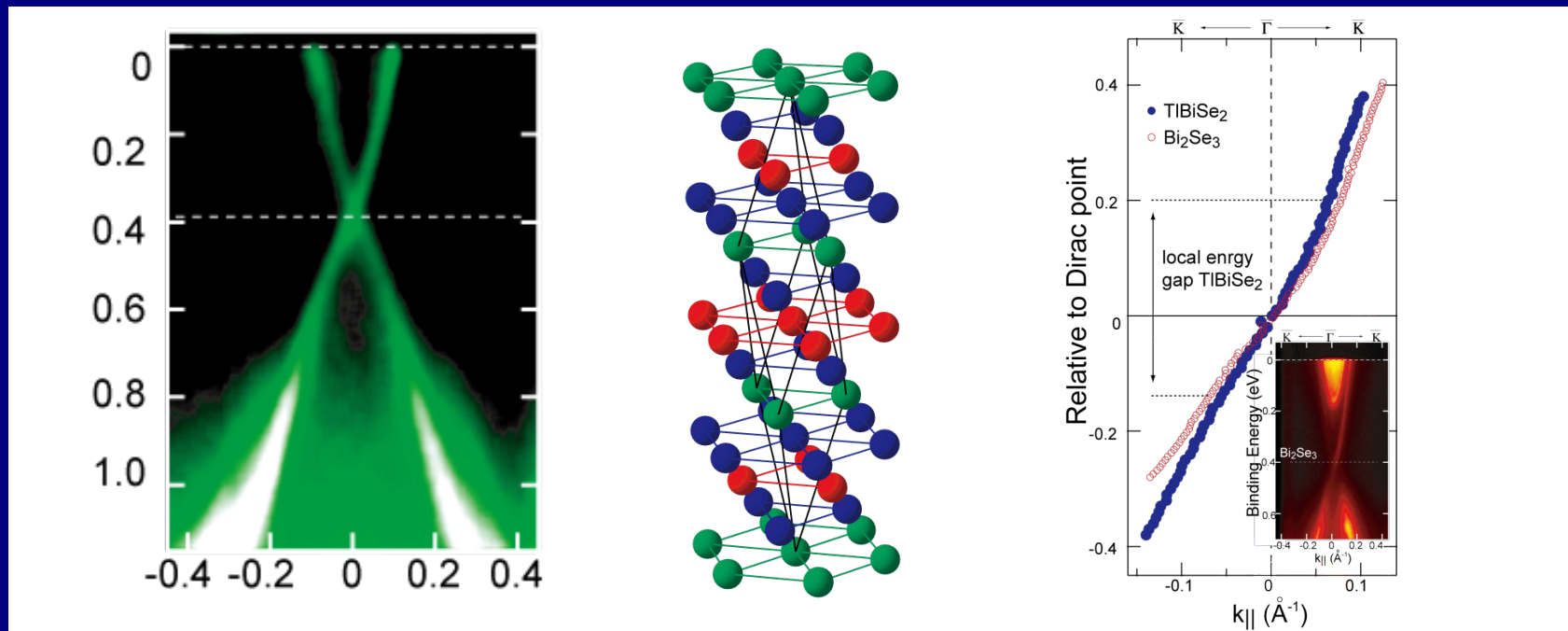


「東京大学アウトステーション (SPring-8 BL07LSU) での物性研究の新展開」

トポロジカル物質のスピンの分解ARPES

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広島大学大学院理学研究科



平成23年3月8日(火) 東京大学物性研究所 6階第一会議室

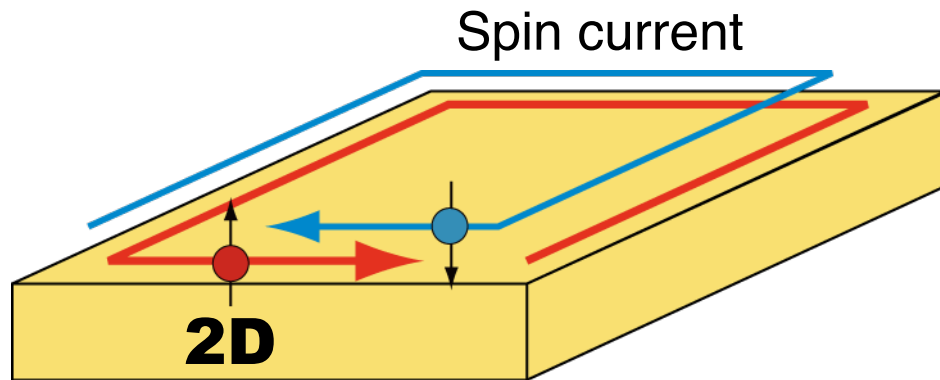
Topological insulators

Insulating bulk states

+ Odd number of gapless surface states

C. L. Kane and E. J. Mele, PRL (2005).

B. A. Bernevig and S. C. Zhang, PRL (2006).



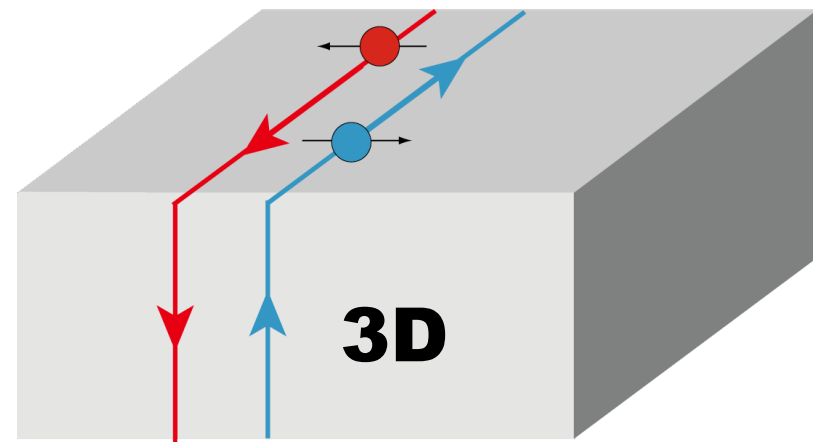
Bi ultrathin film

Theory: S. Murakami, PRL (06).

Quantum Well: CdTe/HgTe/CdTe

Theory: B. A. Bernevig et al., Science (2006).

Exp.: L. M. König et al., Science (2007).



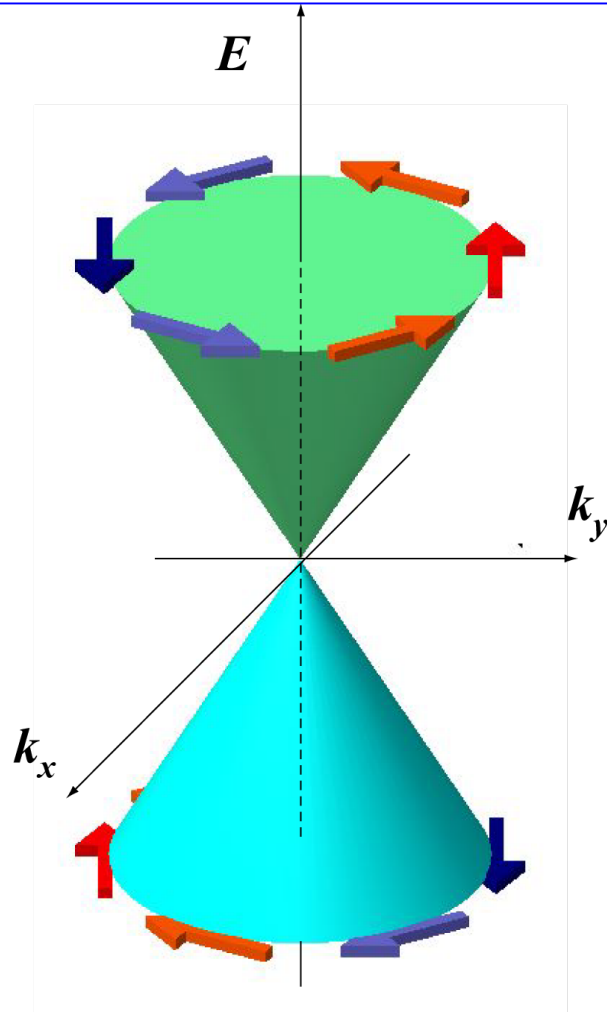
$\text{Bi}_{0.9}\text{Sb}_{0.1}$

Theory: L. Fu et al., PRL (2007).

Exp.: D. Hsieh et al., Nature (2008).

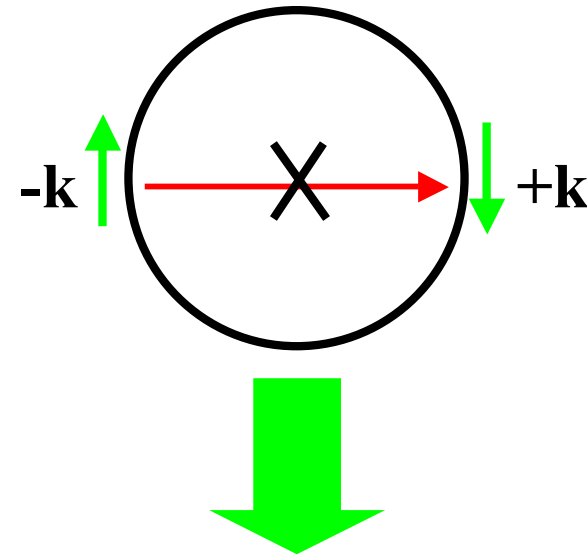
What are attractive points?

Massless electron



Spin is 'locked' with momenta.

Forbidden backscattering

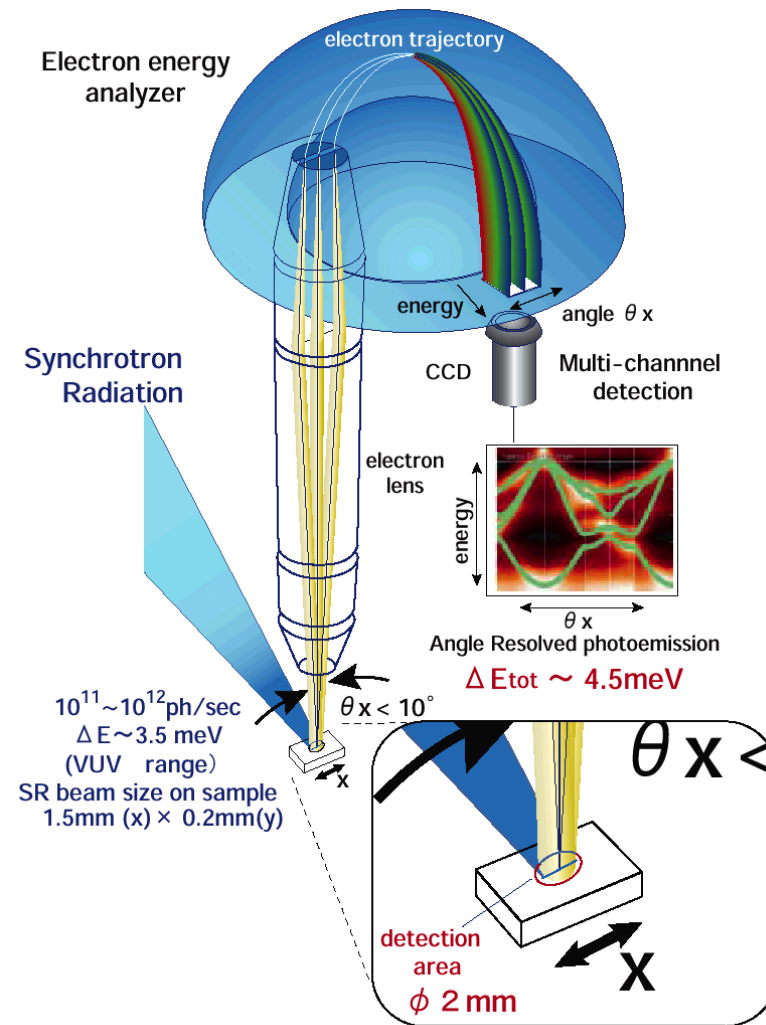
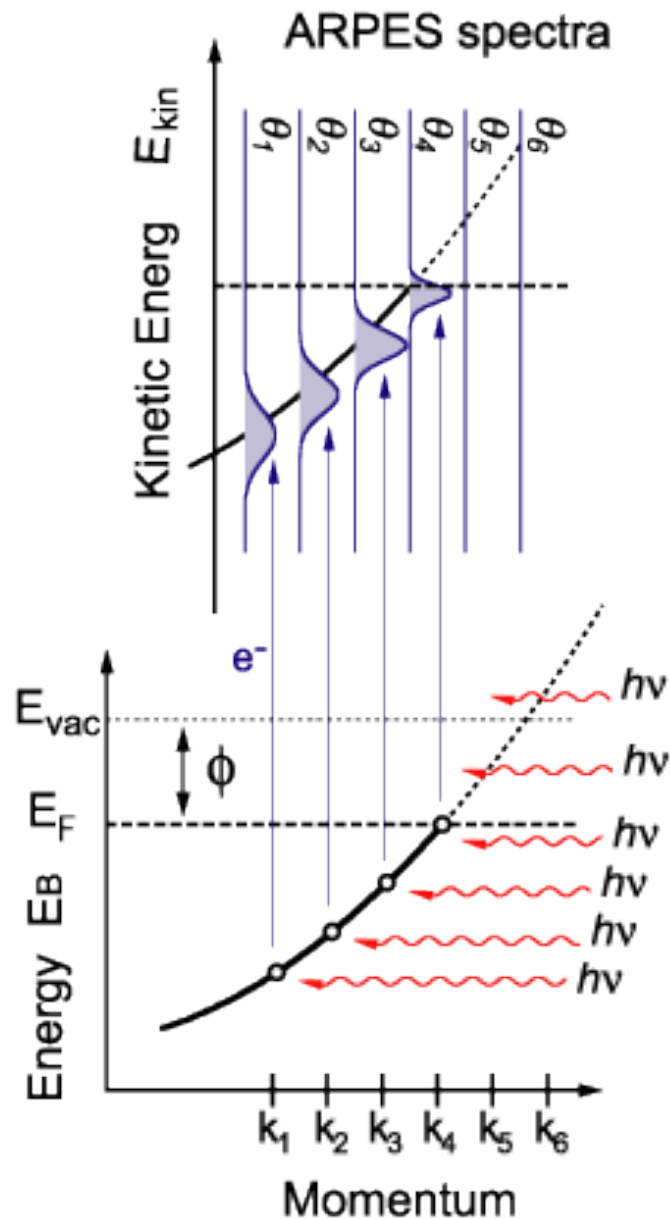


Surface electron transport

Dissipationless

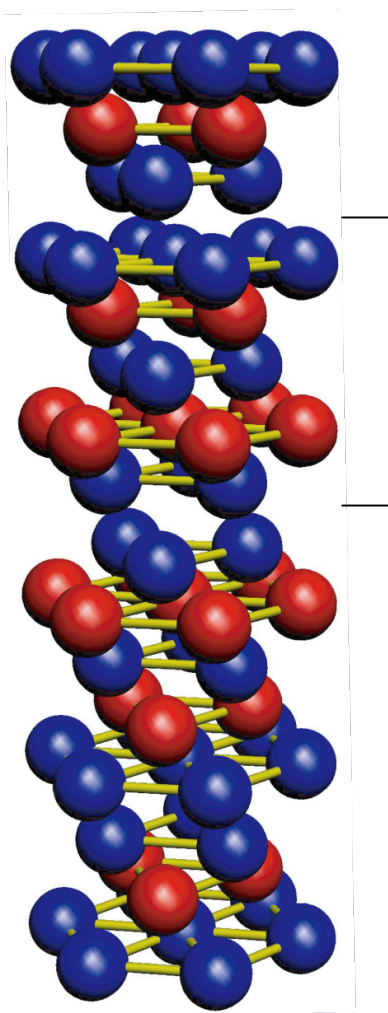
Ultra-high mobility

Angle-resolved photoelectron spectroscopy



- Multi-channel detection
- High energy and high angular resolution

Surface Dirac cones of Bi_2Y_3

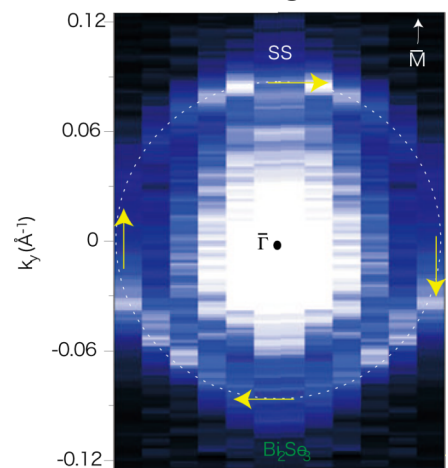


Quintuple layer

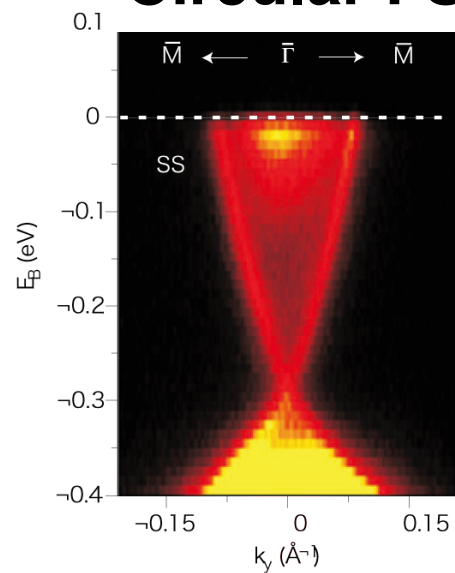


$\nu_0=1$
(non-trivial)

Bi_2Se_3

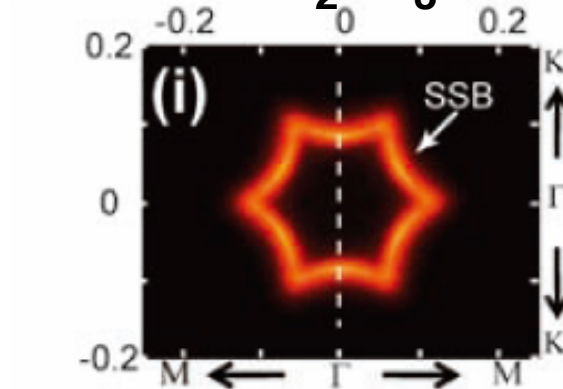


Circular FS

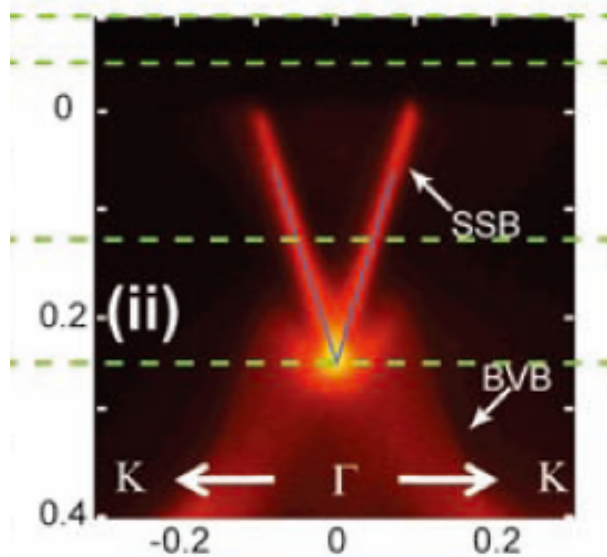


Y. Xia et al., (2009).

Bi_2Te_3



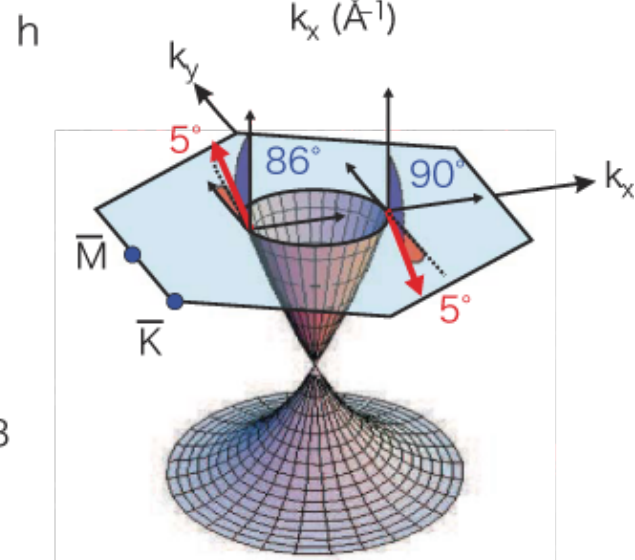
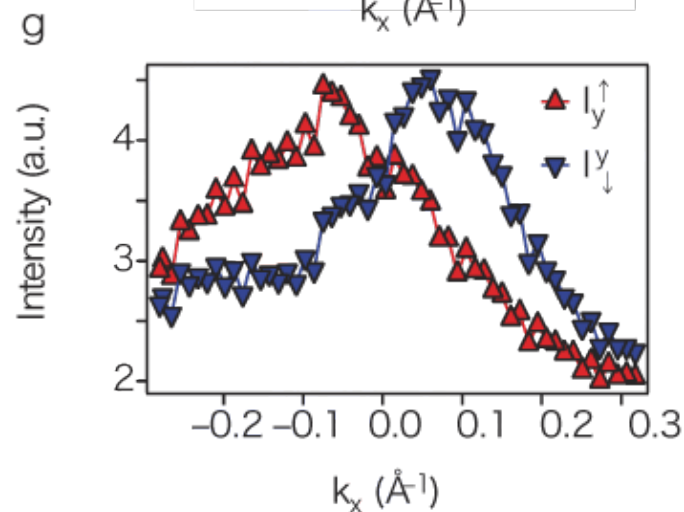
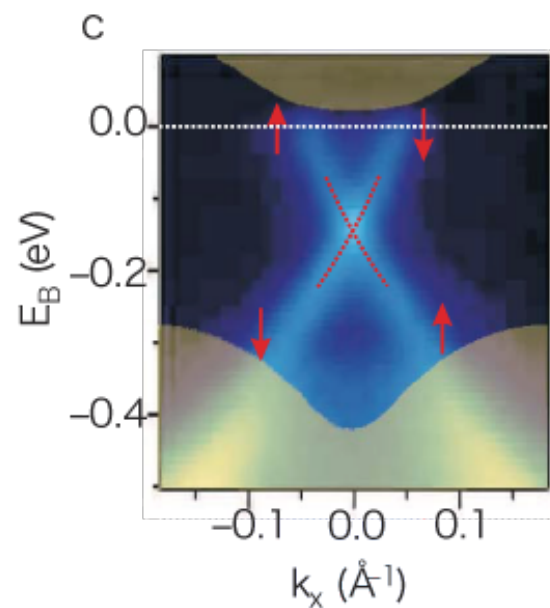
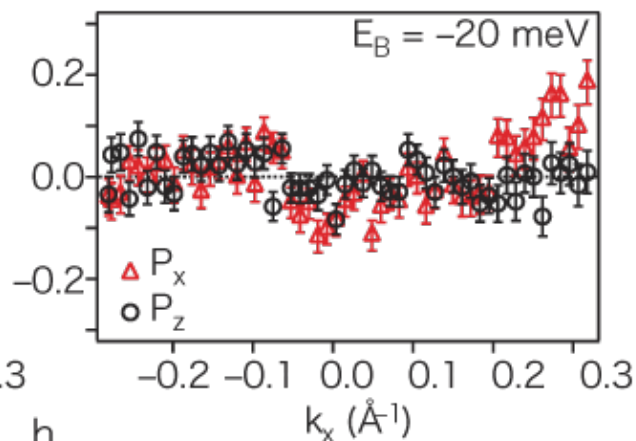
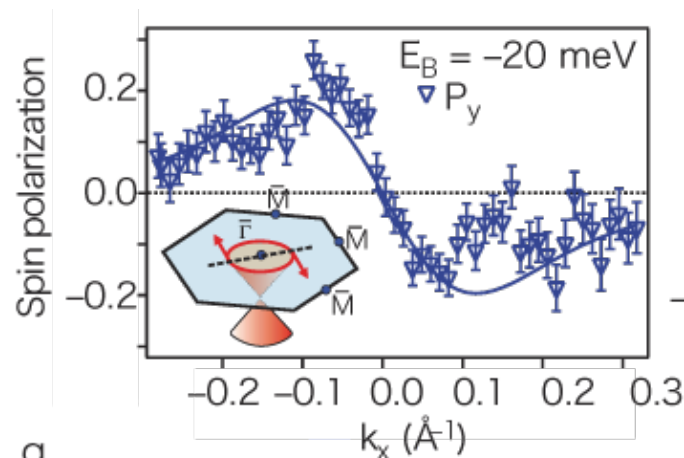
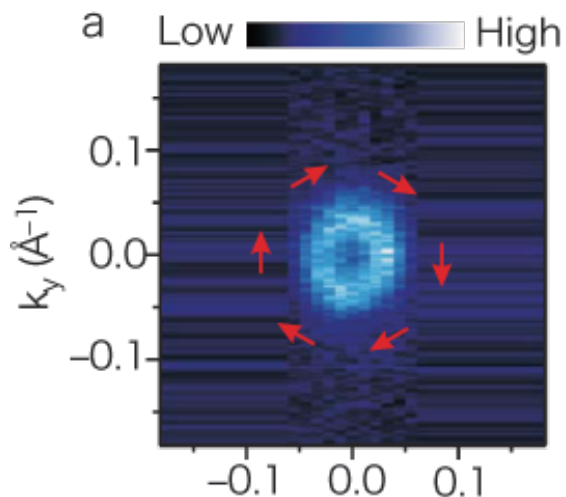
Warped FS



Y. Chen et al., (2009).

Pioneering work of spin ARPES (Bi_2Se_3)

D. Hsieh et al., Nature **460**, 1101 (2011).



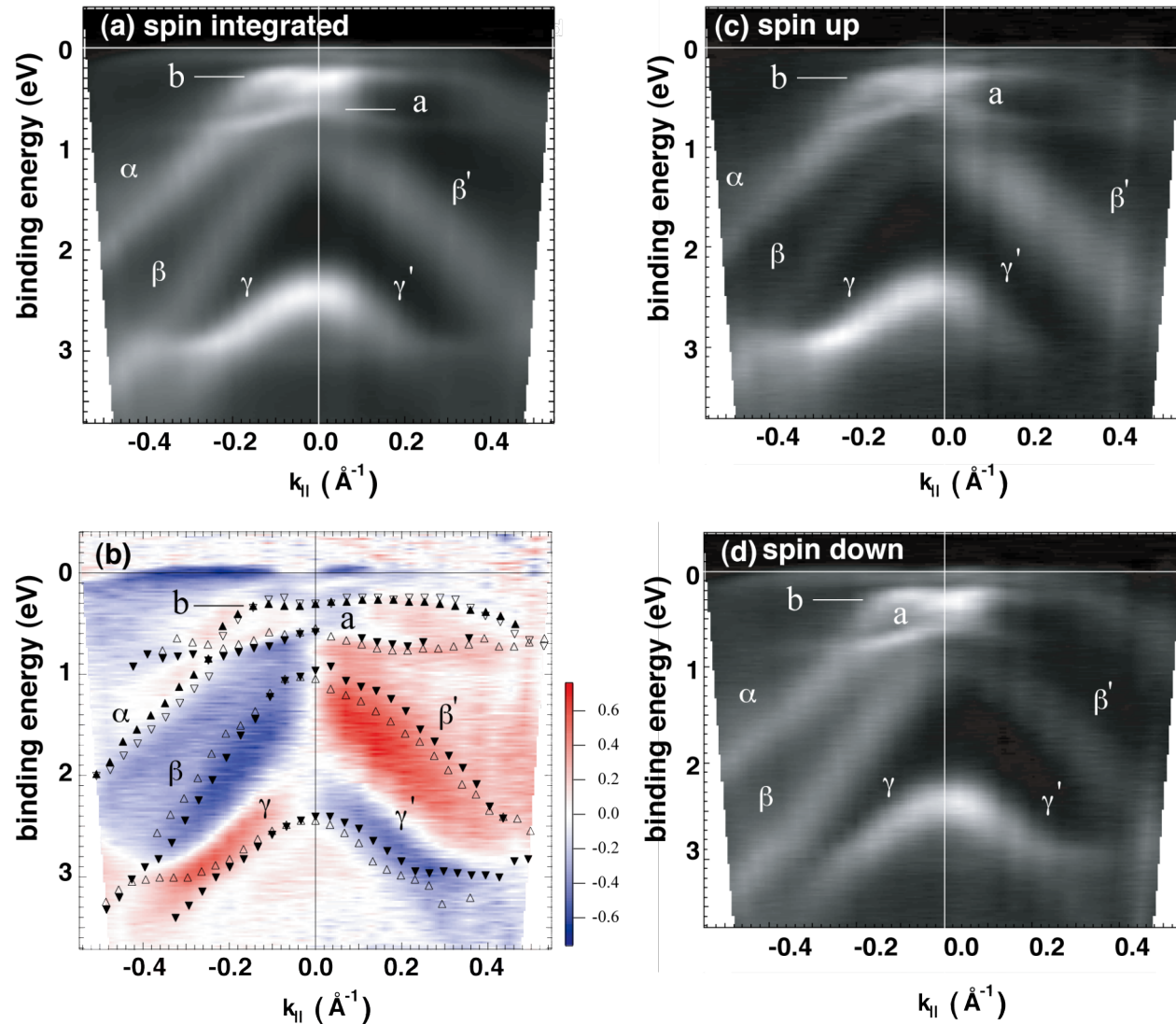
$\Delta E = 80$ meV, $\Delta k = 3\% \cdot \text{SBZ}$.

The observed spin pol. is as small as $\pm 20\%$ ($\ll 100\%$).

Strong Rashba Type Spin Polarization of Bulk Continuum States of Bi(111)



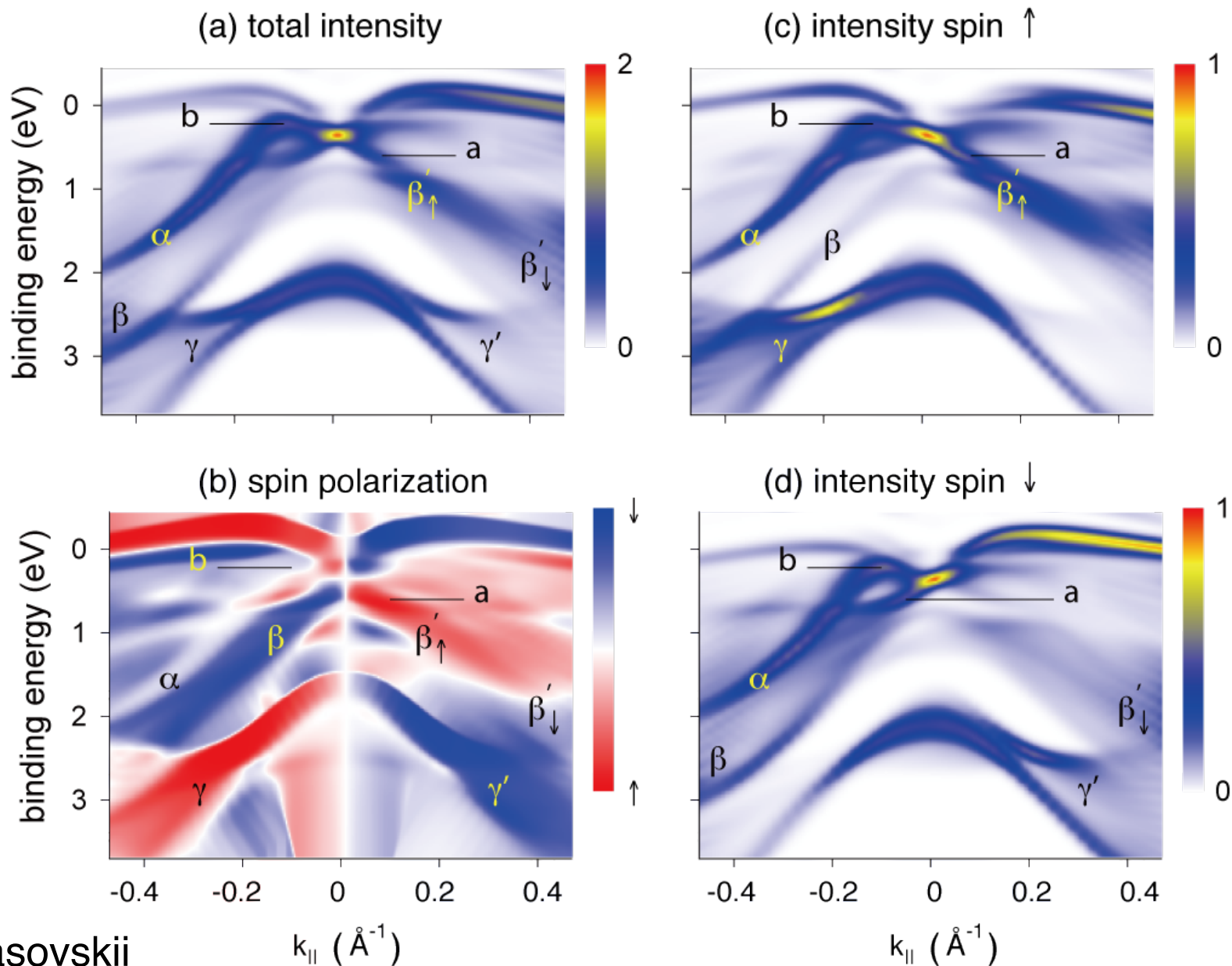
A. Kimura et al., Phys. Rev.Lett. 105, 076804 (2010).



One-step model photoemission calculation

16BL Bi slab

A. Kimura et al., Phys. Rev.Lett. **105**, 076804 (2010).



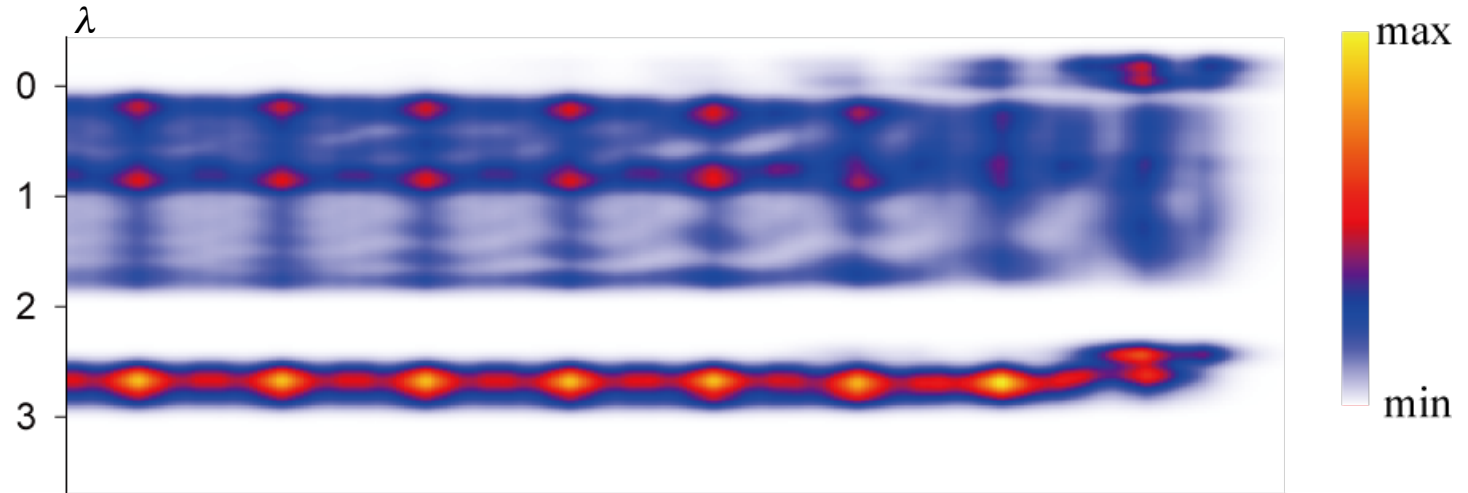
E. E. Krasovskii

Layer resolved charge and spin densities

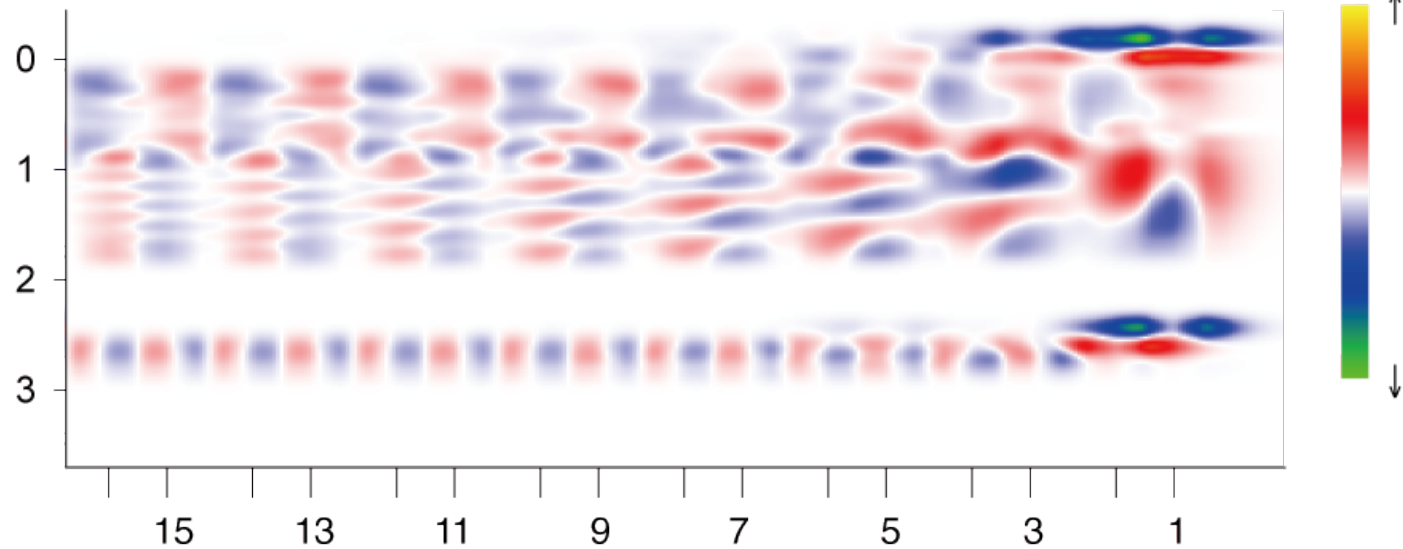
16BL Bi slab

$$\rho_{k_{\parallel}}^{\sigma}(z, E) = \int dr_{\parallel} \sum_{\lambda} |\psi_{\lambda k_{\parallel}}^{\sigma}(\mathbf{r})|^2 \delta(E_{\lambda k_{\parallel}} - E) \quad \text{A. Kimura et al., PRL (2010).}$$

Total DOS

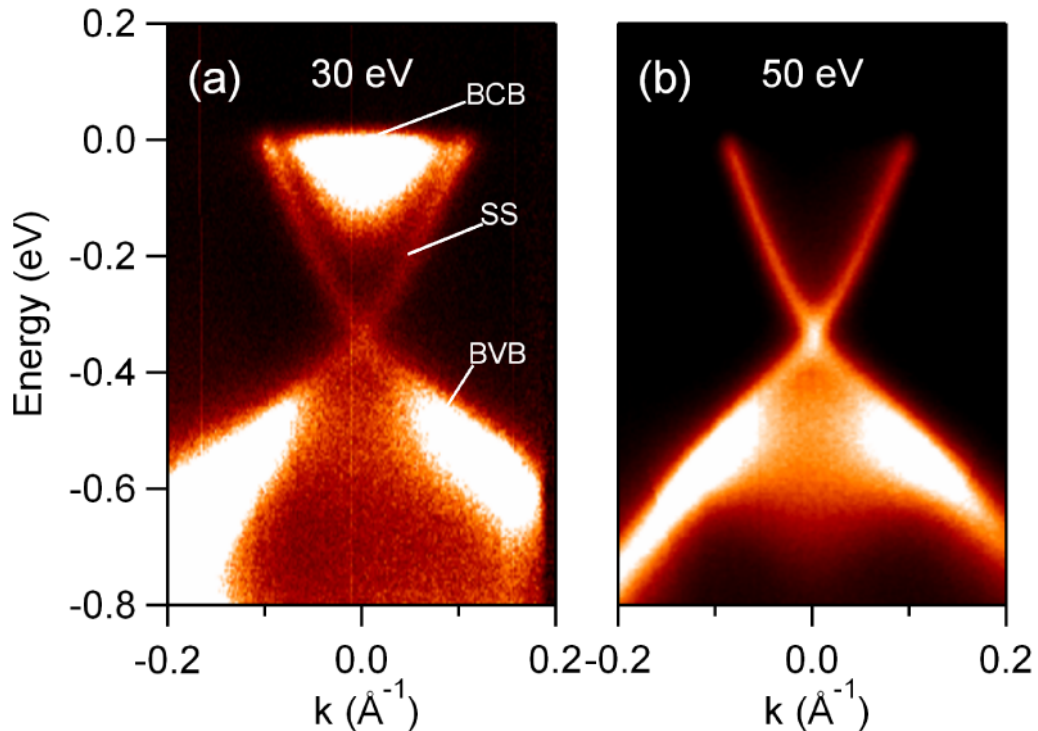


Spin density



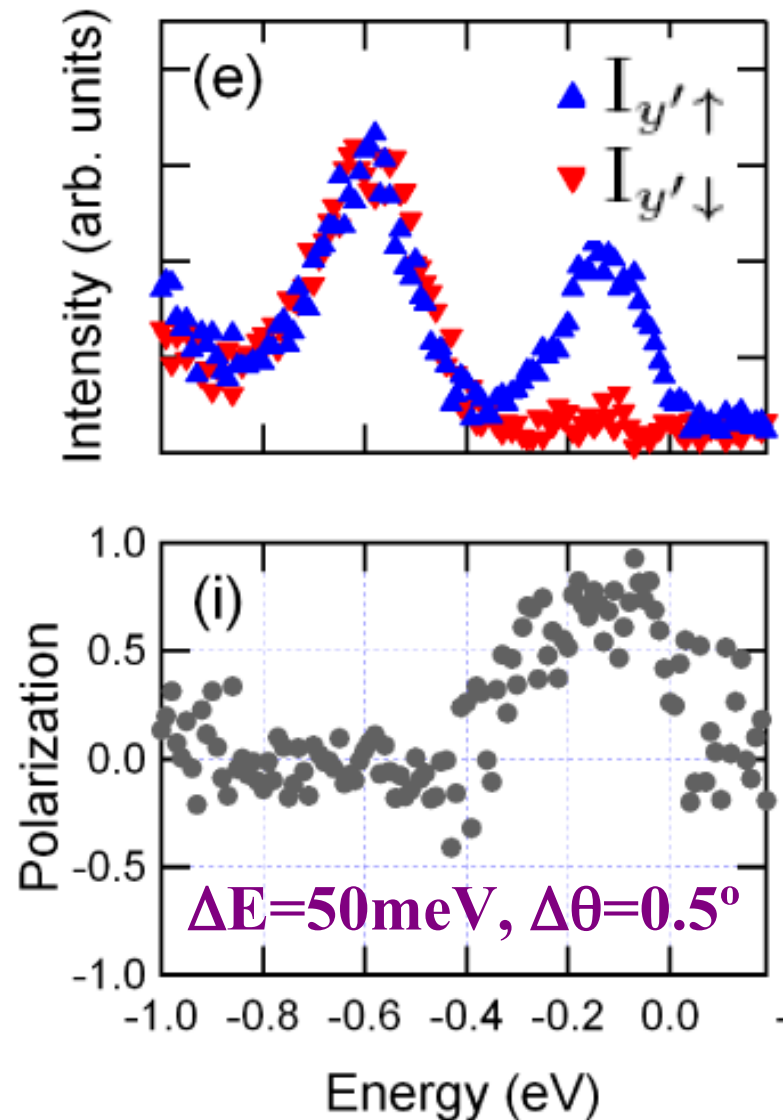
Suppression of bulk continuum signals

H. Pan et al., arXiv 1101.5615 (2011).



U5UA @ NSLS

Topological surface state is well separated from the bulk state at $h\nu=50\text{eV}$ (near Z point of BZ).



A high-degree of spin pol. ($\sim 75\%$) is observed.

Hiroshima Synchrotron Radiation Center



BL-1

- Linear undulator
- $h\nu = 26-300\text{eV}$
- VG-Scienta R4000

$$\Delta E = 4-6\text{meV},$$
$$\Delta\theta = 0.2^\circ - 0.3^\circ$$

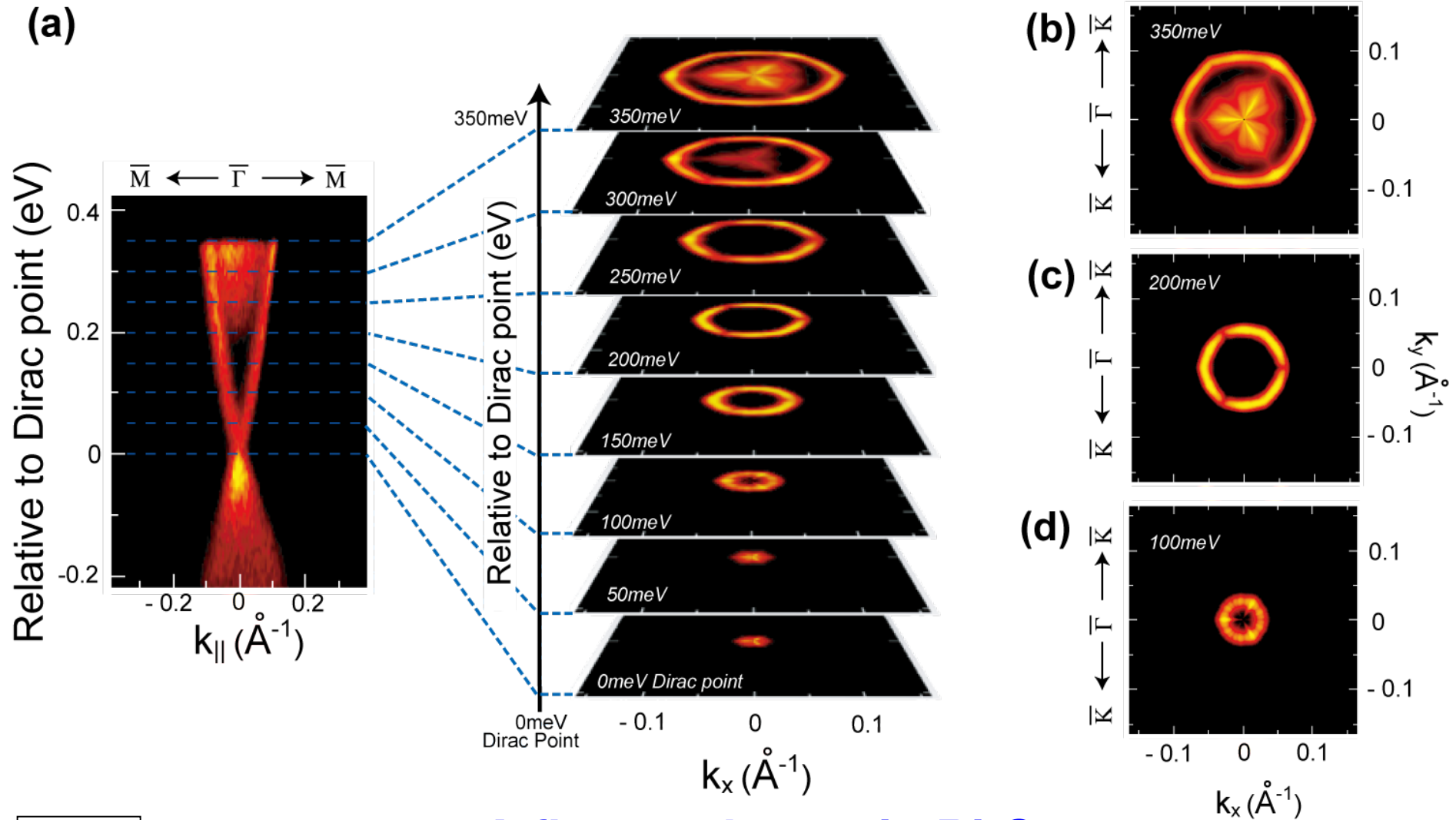
BL-9A

- Helical undulator
- $h\nu = 4-30\text{eV}$
- VG-Scienta R4000

Hexagonal Warped Iso-energy Surfaces of Bi_2Se_3



K. Kuroda et al., PRL 105, 076802 (2010).

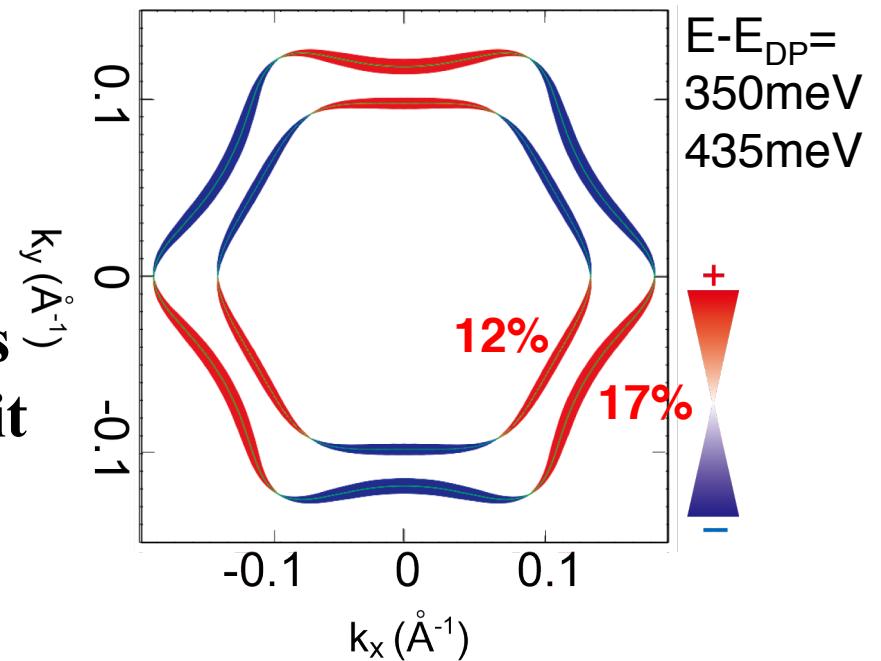
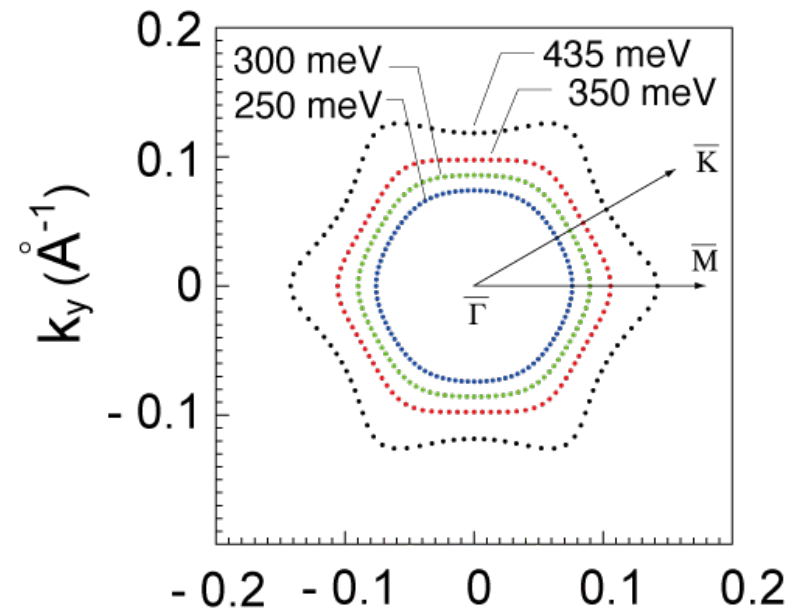
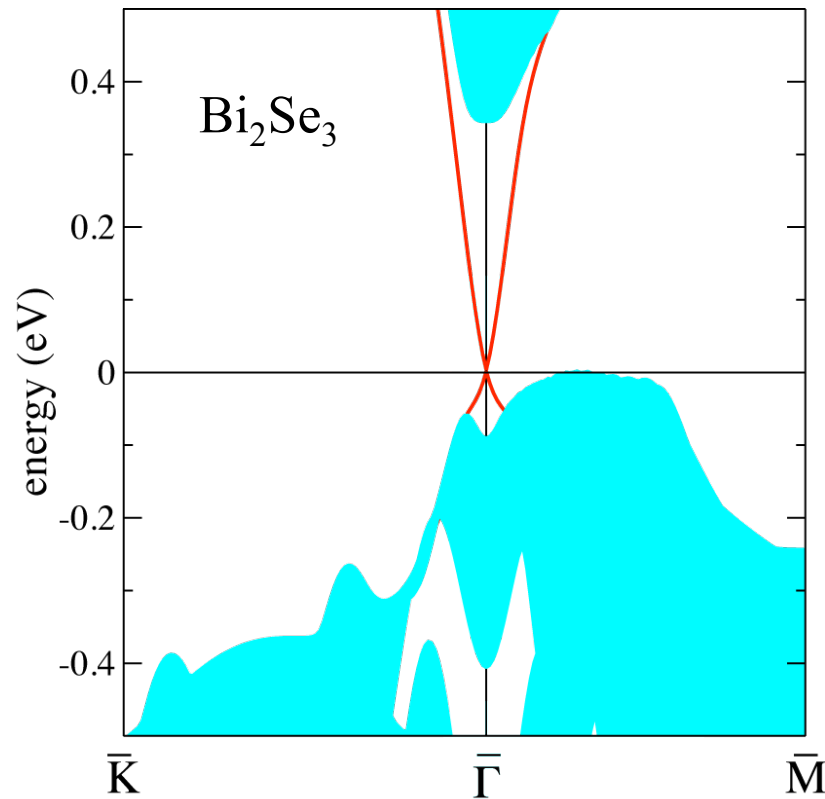


BL-1

A flattened cone in Bi_2Se_3 .

Predicted Fermi surface of Bi_2Se_3

E. E. Krasovskii



The out- of-plane spin pol. (12%) is maximal along Γ - \bar{K} direction, and it vanishes along Γ - \bar{M} line due to the mirror symmetry.

General discussion on spin direction

Around $\bar{\Gamma}$ point

Time reversal invariance

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

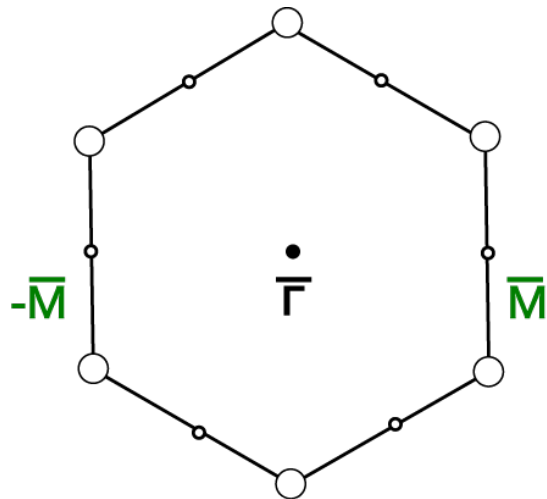
Bloch's theorem

$$E(\vec{k}, \uparrow) = E(\vec{k} + \bar{G}, \uparrow)$$

Around \bar{M} point

$$\bar{M} = \frac{\bar{G}}{2}$$

$$\bar{M} = -\bar{M} + \bar{G}$$



$$\begin{aligned} E(\vec{k} + \bar{M}, \uparrow) &= E(-\vec{k} - \bar{M}, \downarrow) \\ &= E(-\vec{k} - \bar{M} + \bar{G}, \downarrow) \\ &= E(-\vec{k} + \bar{M}, \downarrow) \end{aligned}$$

Time reversal invariance

No time reversal invariance for K point

TI / Si(111)-(1x1) : Spin-ARPES

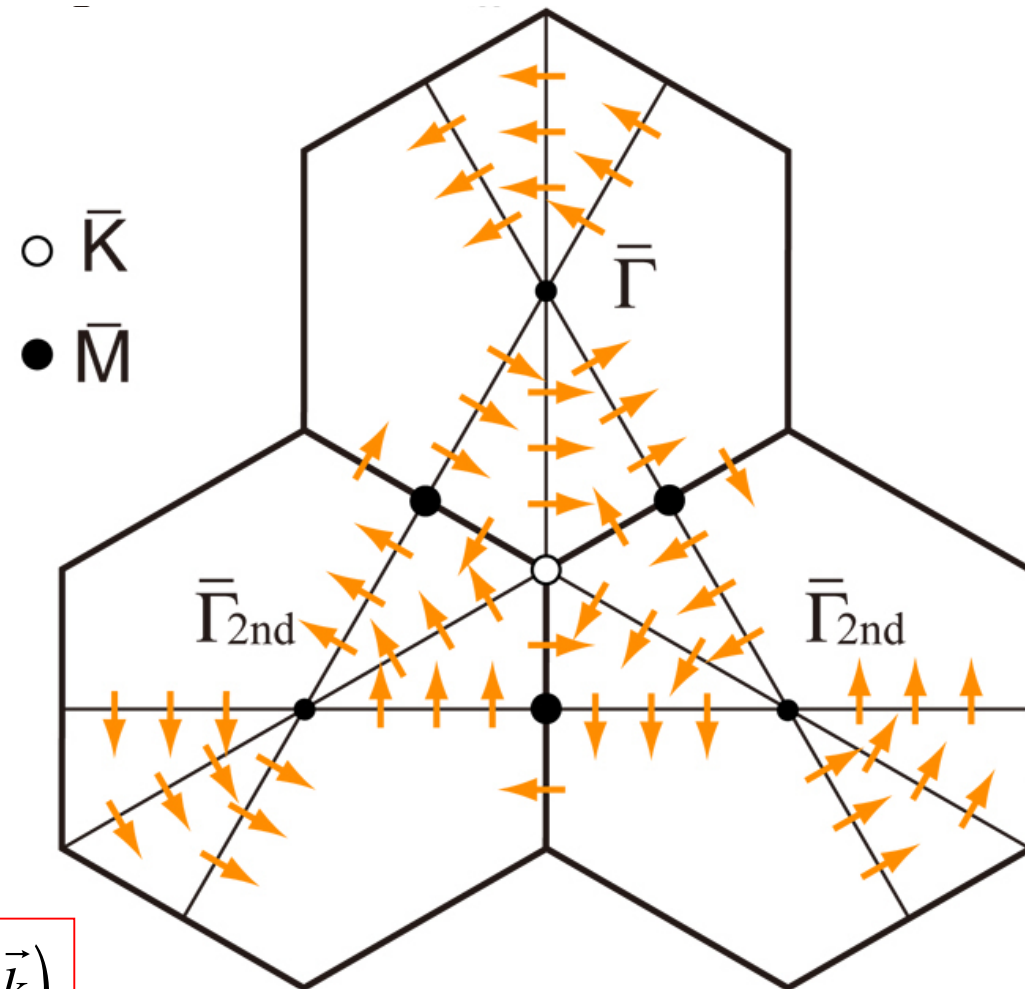
Around $\bar{\Gamma}$ point,

Vortical spin: **CCW**

Around \bar{M} point,

Vortical spin: **CW**

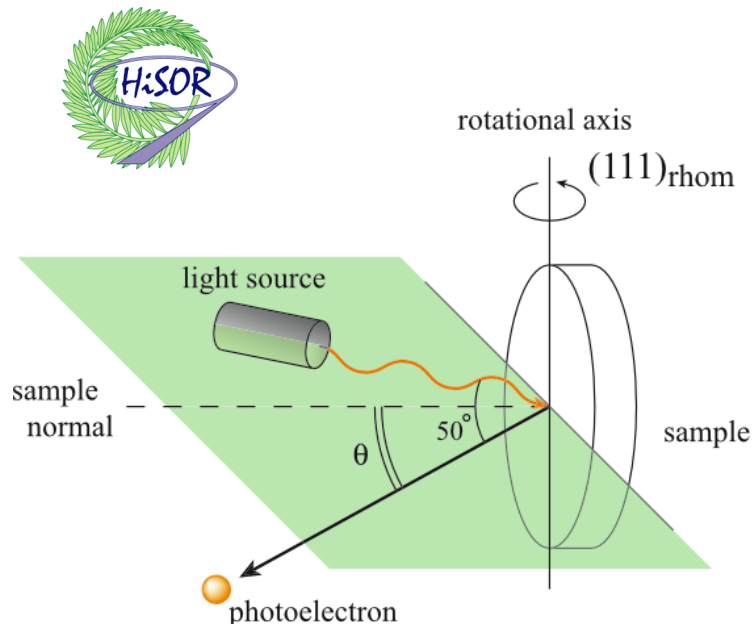
Spin direction is
indeterminable at \bar{K}



$$H_{SO}(\vec{k}) = \vec{\sigma} \cdot (\vec{\alpha}_n(\vec{k}) \times \vec{k}) + \vec{\sigma} \cdot \vec{B}_n(\vec{k})$$

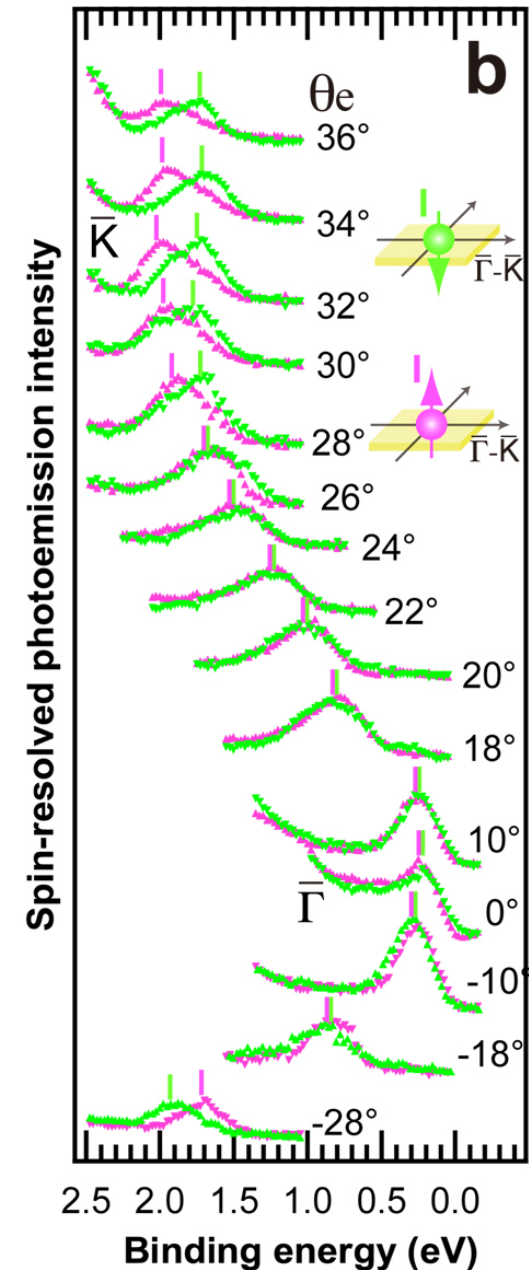
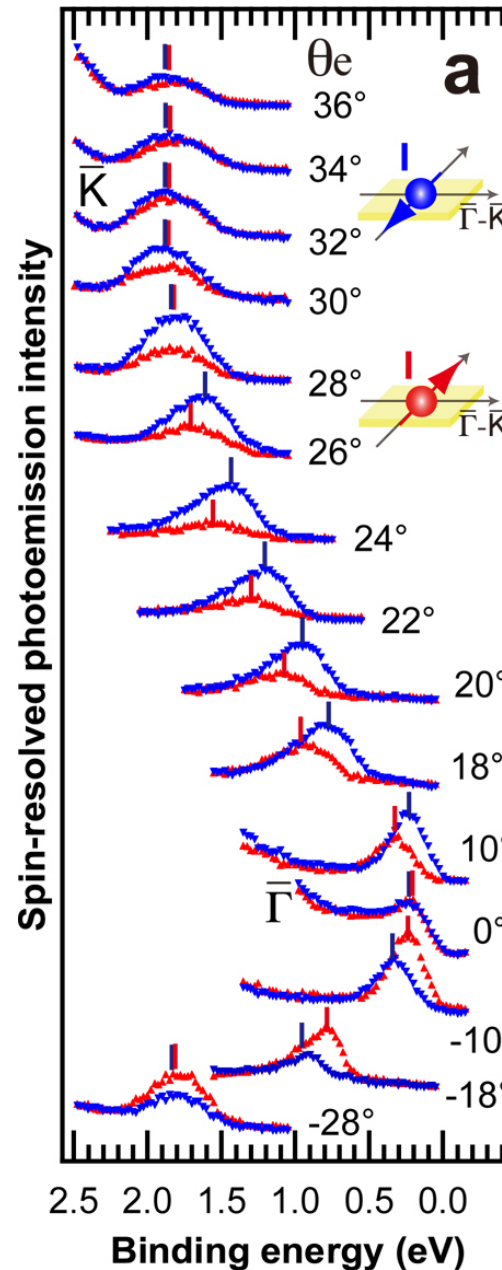
Spin "stands up" at \bar{K} point.

TI / Si(111)-(1x1) : Spin-ARPES



- $h\nu=21.2\text{eV}(\text{He}1\alpha)$
- $\Delta E = 200\text{meV} (E_p=10\text{eV})$
- $\Delta\theta = \pm 1^\circ$

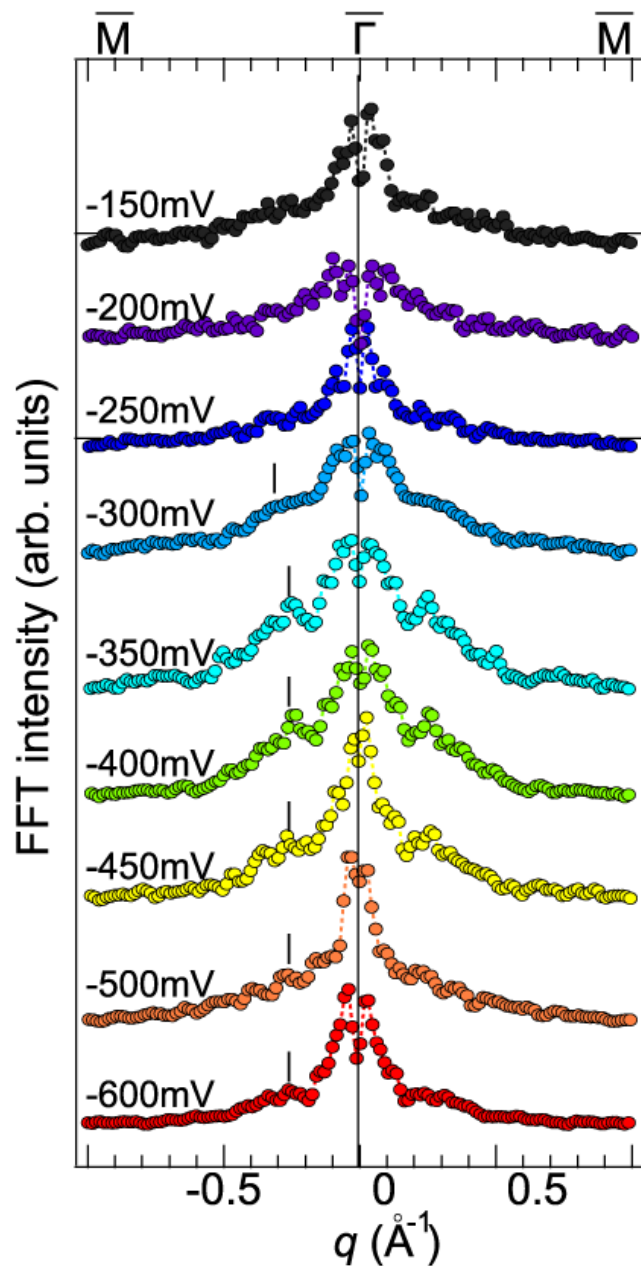
K. Sakamoto et al.,
PRL **102** (2009) 096805.



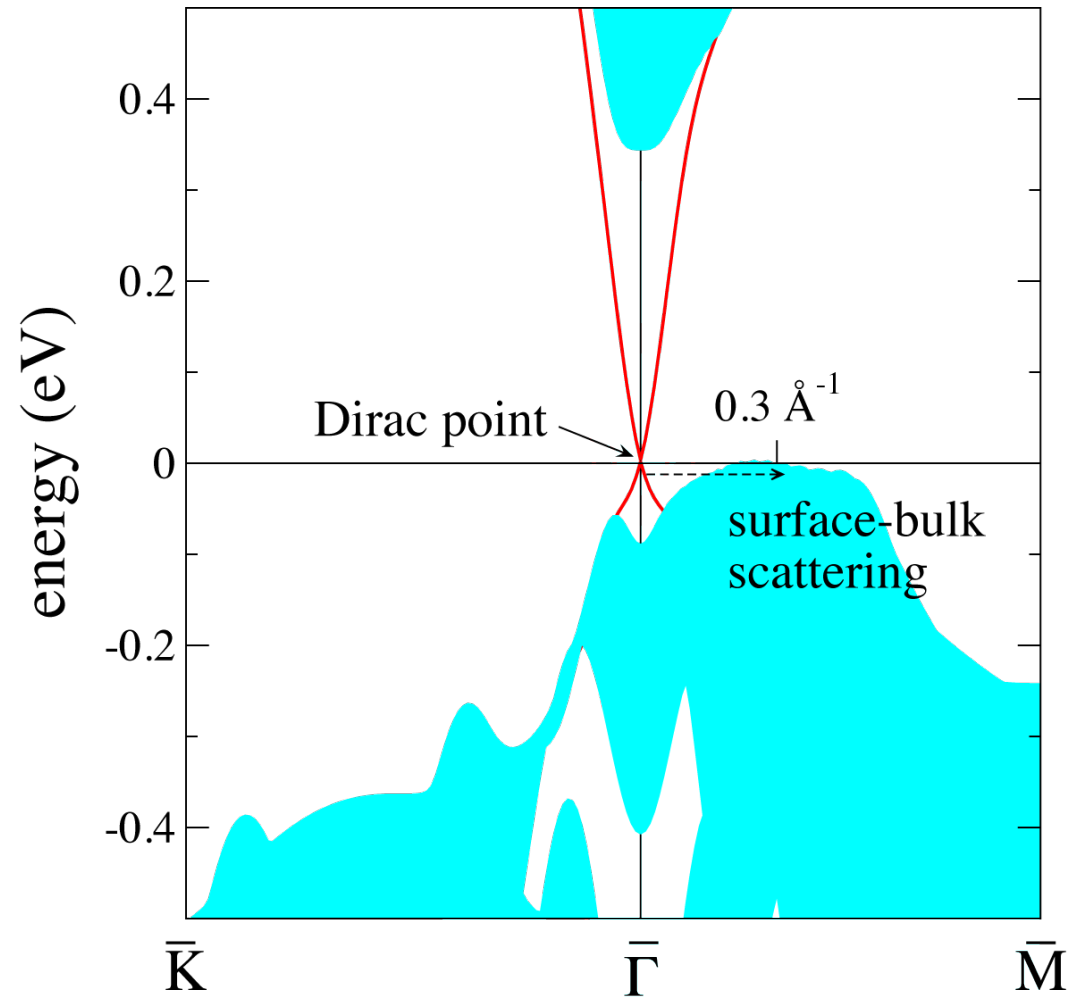
Unwanted feature?

S. Kim et. al., submitted.

LT-STM



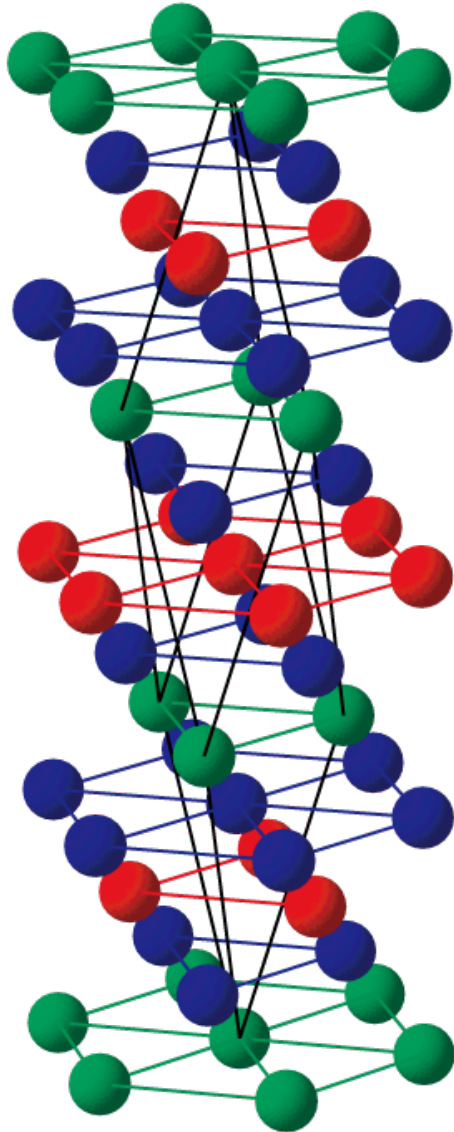
E. E. Krasovskii



Surface-bulk electron scattering channel possibly opens.

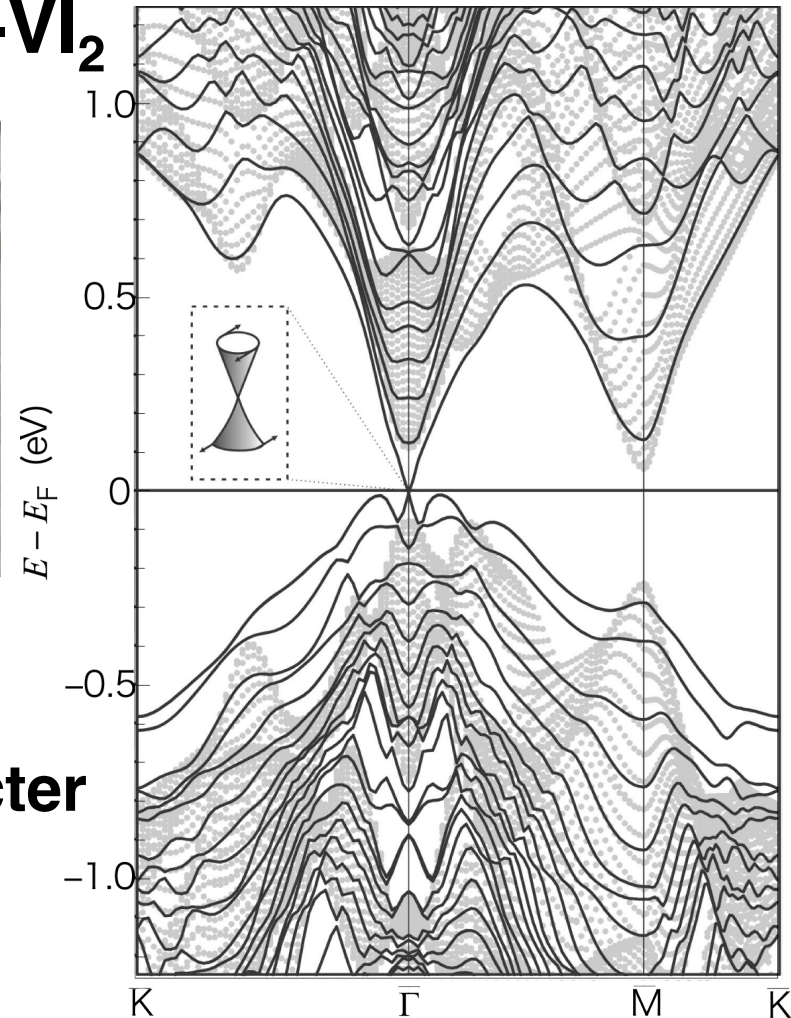
New Family of 3D Topological Insulator

Ternary Chalcogenides: TI-V-VI₂



High-quality
single crystal

Strong 3D character



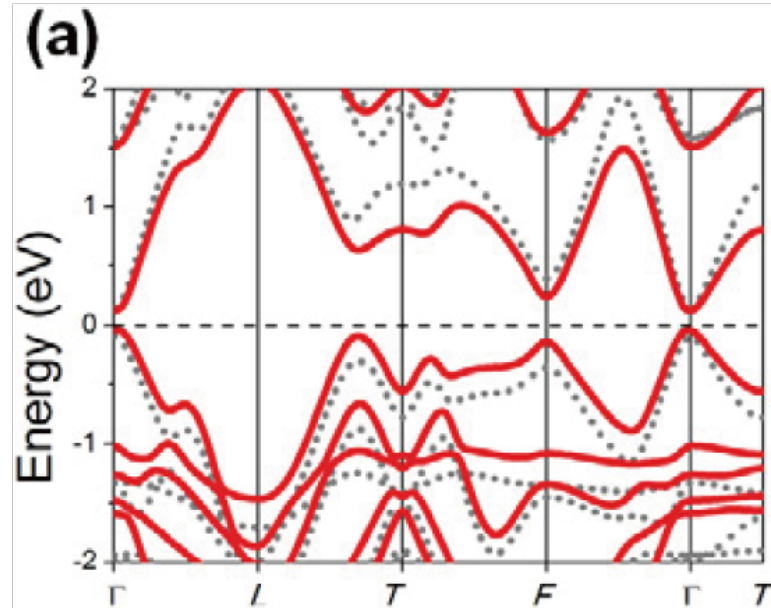
S. Eremeev et al., JETP Lett. 91, 594 (2010).

B. Yan et al., Europhys. Lett. (2010).

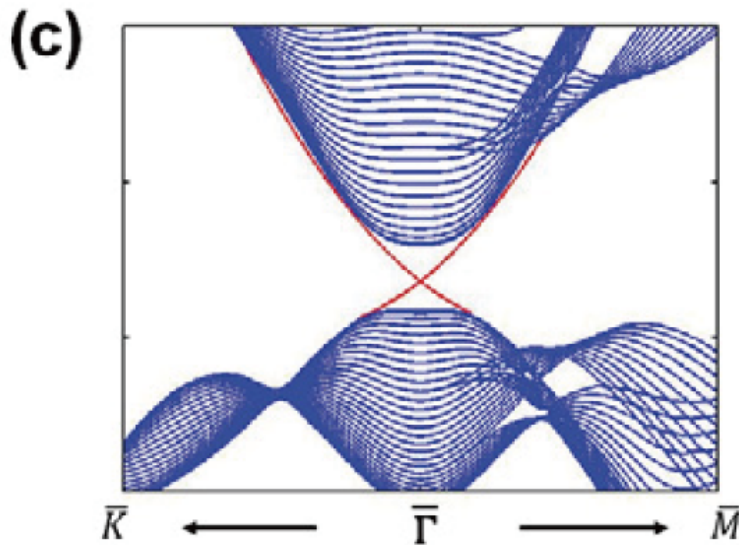
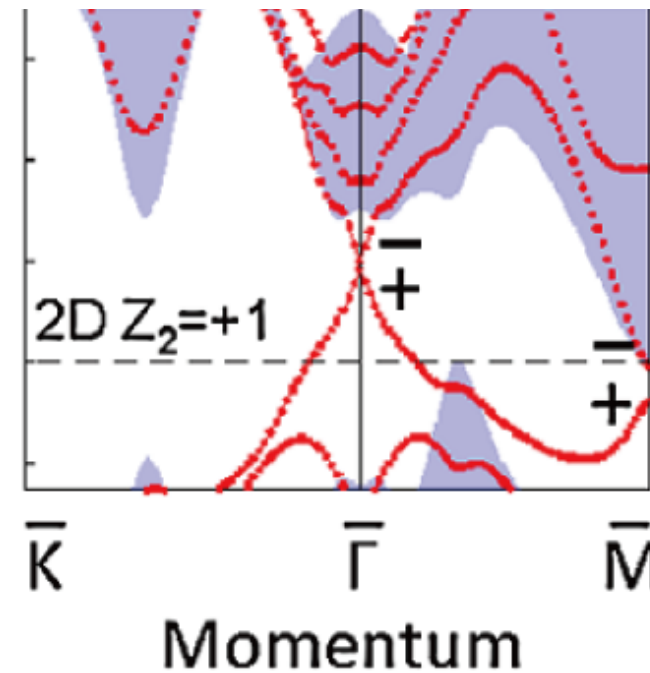
H. Lin et al., Phys. Rev. Lett. (2010).

Discrepancy in the theoretical bands

B. Yan et al., Europhys. Lett. (2010).



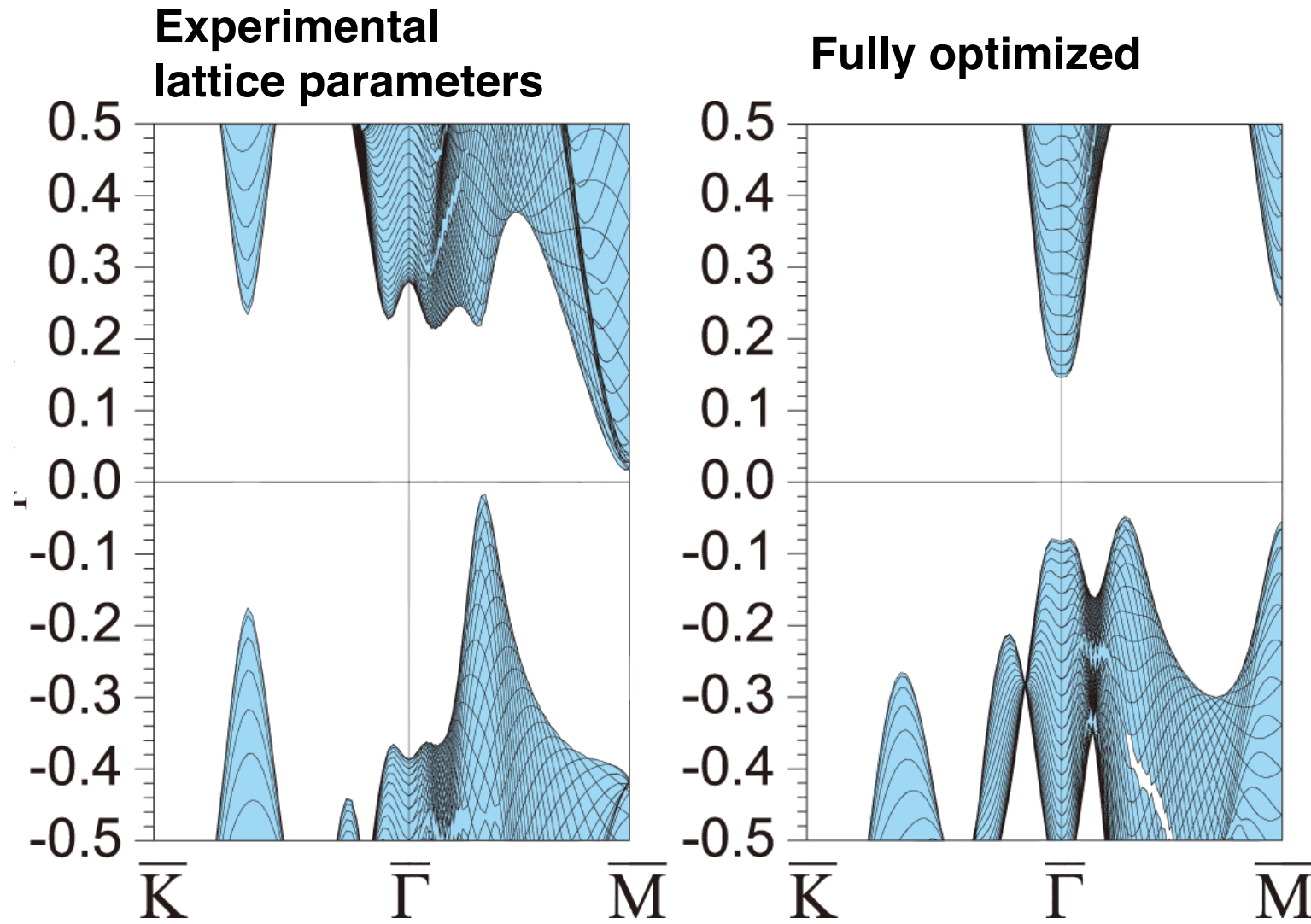
H. Lin et al., Phys. Rev. Lett. (2010).



Why?

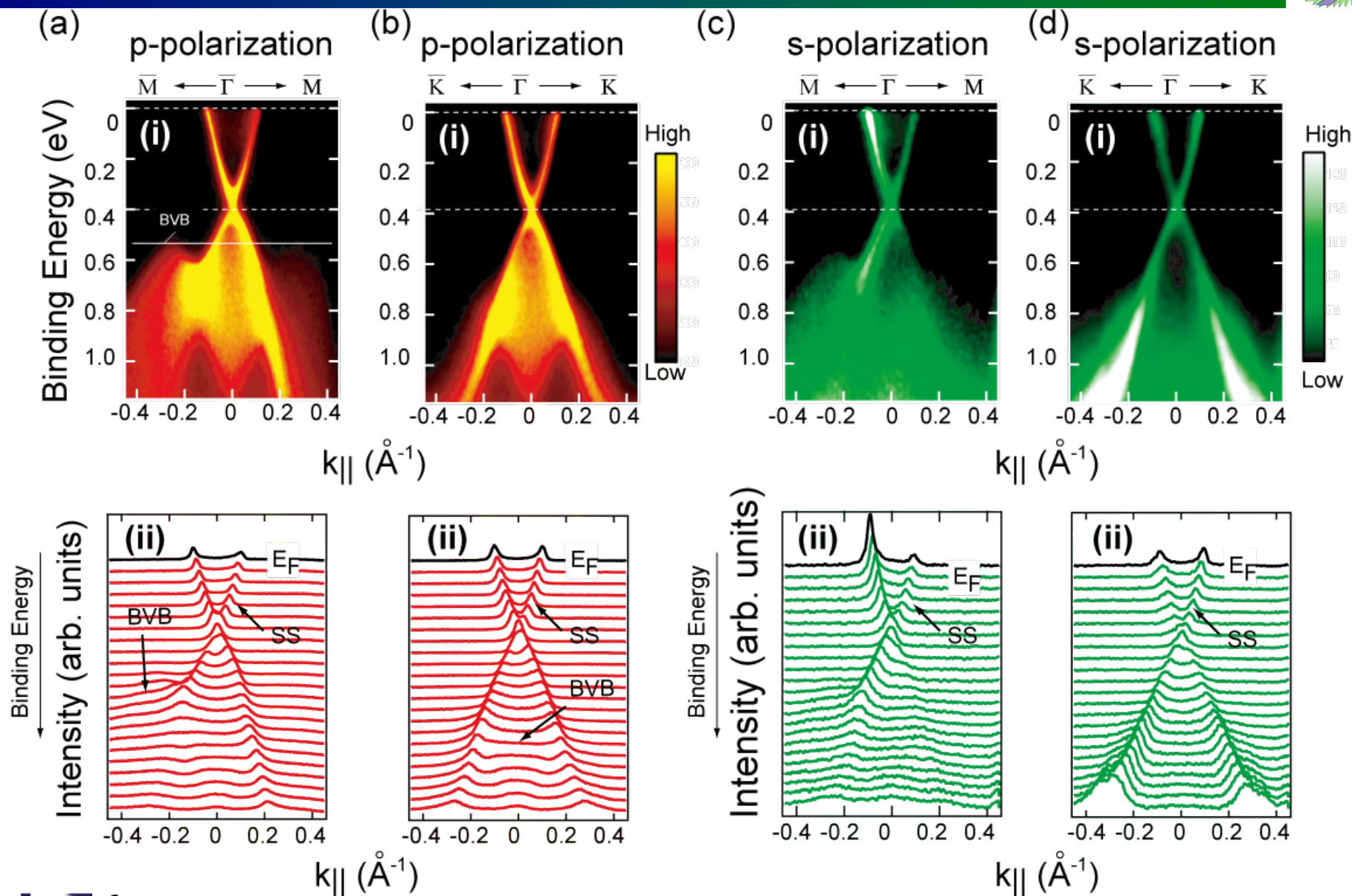
Theoretical k_{\parallel} projected bulk band

VASP code by S. V. Eremeev (Tomsk State Univ.)



Quite sensitive to the small changes in geometry.

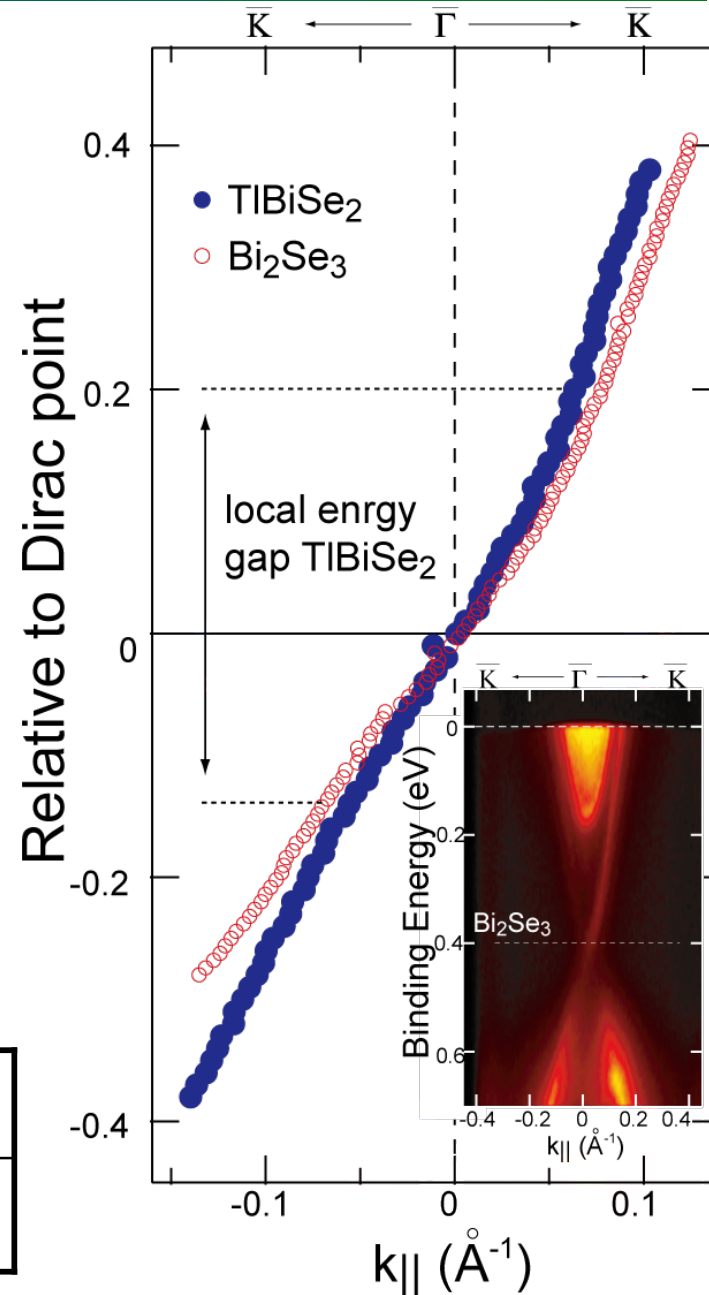
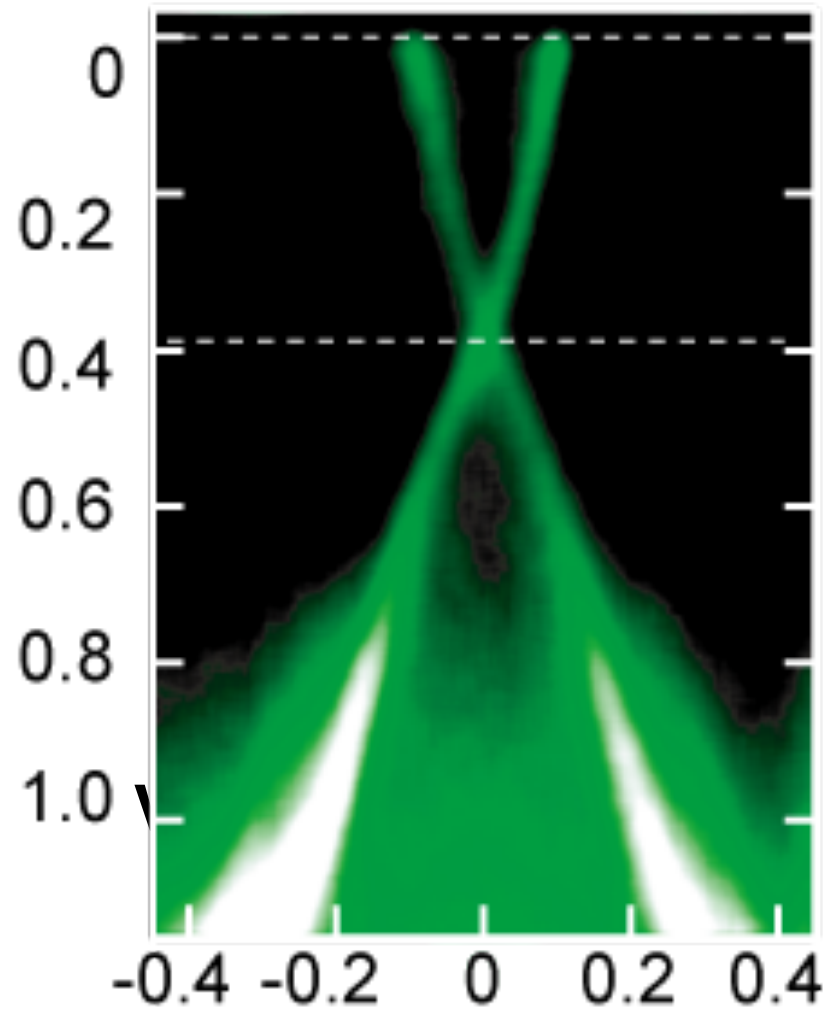
Surface energy dispersion of TlBiSe₂ BL-1



K. Kuroda et al., Phys. Rev. Lett. 105, 146801 (2010).

A more ideal Dirac cone of TIBiSe₂

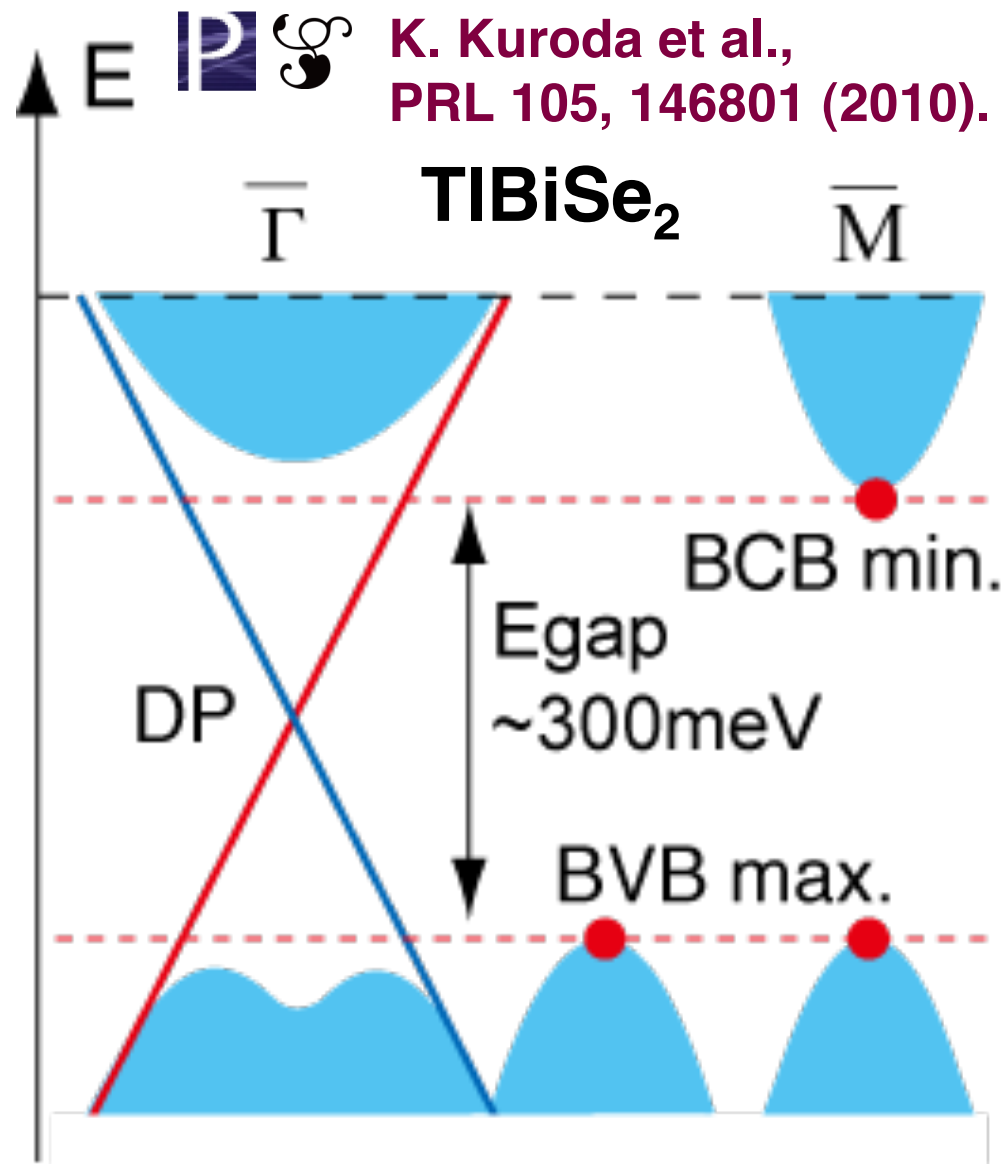
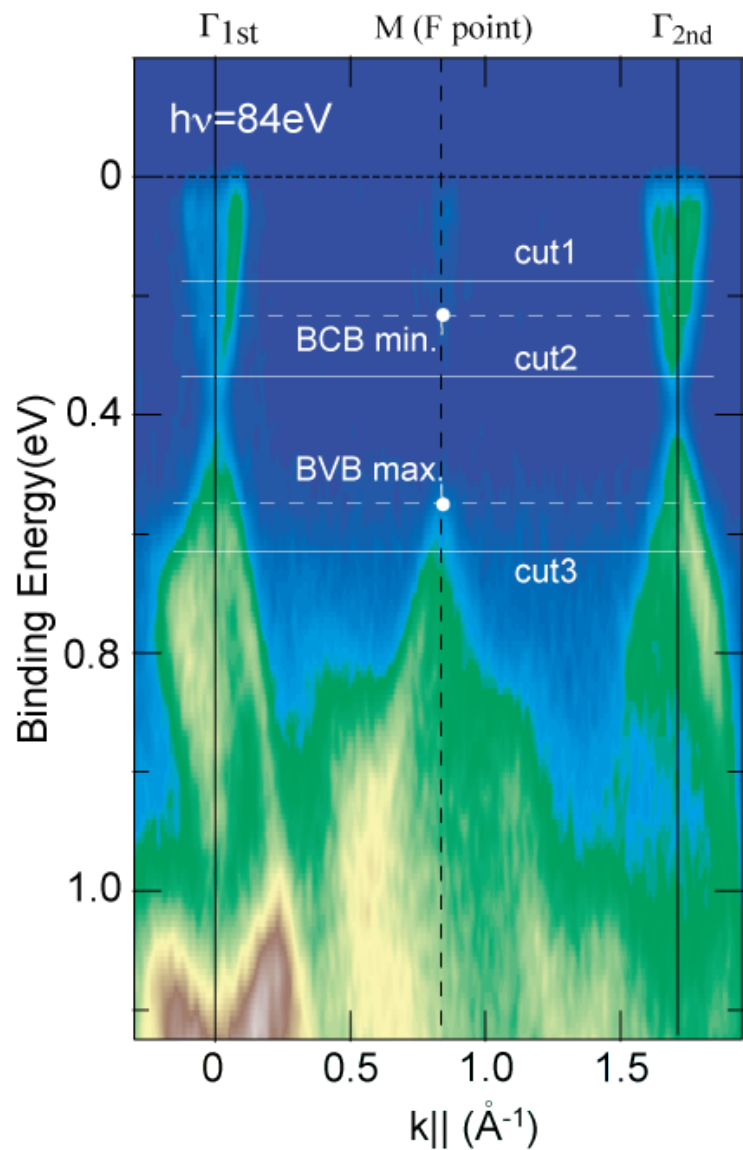
BL-1



Bi ₂ Se ₃	TIBiSe ₂
2.9x10 ⁵ m/s	3.9x10 ⁵ m/s

Photon energy dependence

BL-1



No overlap with bulk continuum states.

トポロジカル物質のspin分解ARPES

- **3D spin解析**: 複雑なspinテクスチャーを可視化
- **放射光の利用**: 表面Dirac coneの抽出、バルクバンドの決定
- **高い運動量分解能**: $\delta k < 0.5\% \cdot BZ$

- **トポロジカル絶縁体の新物質探索**
 - a single, ideal, faster and well-isolated Dirac cone.

例: **TlBiSe₂**  K. Kuroda et al., Phys. Rev. Lett. 105, 146801 (2010).



量子トポロジー物性、物質中の宇宙への深い理解