Emergent phenomena in giant bulk Rashba semiconductors

Mohammad Saeed Bahramy

Center for Emergent Matter Science, RIKEN

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Collaborators

Experiment

- M. Sakano, K. Ishizaka (and her group members) (APRES)
- H. Murakawa. J. Checkelsky, Y. Kaneko (Sample growth, Transport)
- L. Demko, J. S. Lee, I. Kezsmarki, N. Ogawa (Optics)
- Y. Onose, Y. Tokura, ….

Theory

- B. J. Yang
- G. A. H. Schober
- R. Arita
- P. D. C. King, F. Baumberger
- N. Nagaosa

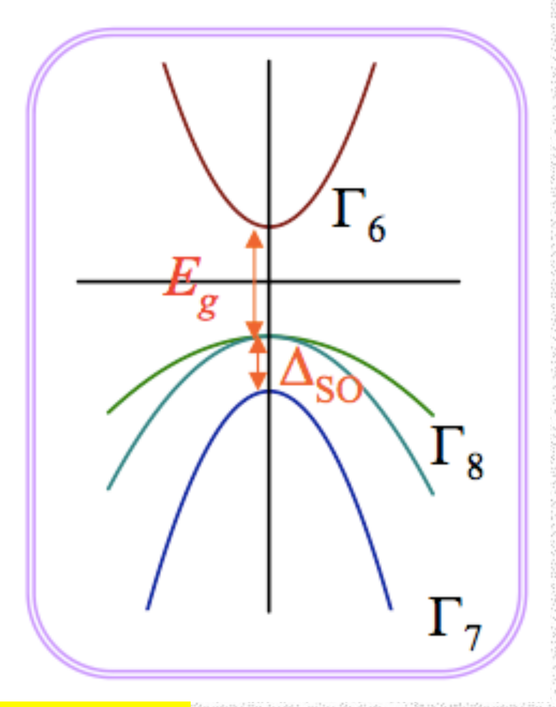
Spin-Orbit Coupling in semiconductors

Coupling of electron's spin with its momentum.

$$H = \frac{p^2}{2m} + V_{ext}(r)$$

$$\vec{B}_{eff} = \frac{1}{2m_0c^2}(\vec{p} \times \nabla V) \Rightarrow H_{so} = -\mu_B \vec{S} \cdot \vec{B}$$

$$\begin{cases} T-symmetry: \psi_{\mathbf{k},\uparrow} \leftrightarrow \psi_{-\mathbf{k},\downarrow} \\ I-symmetry: \psi_{\mathbf{k},\uparrow} \leftrightarrow \psi_{-\mathbf{k},\uparrow} \end{cases}$$

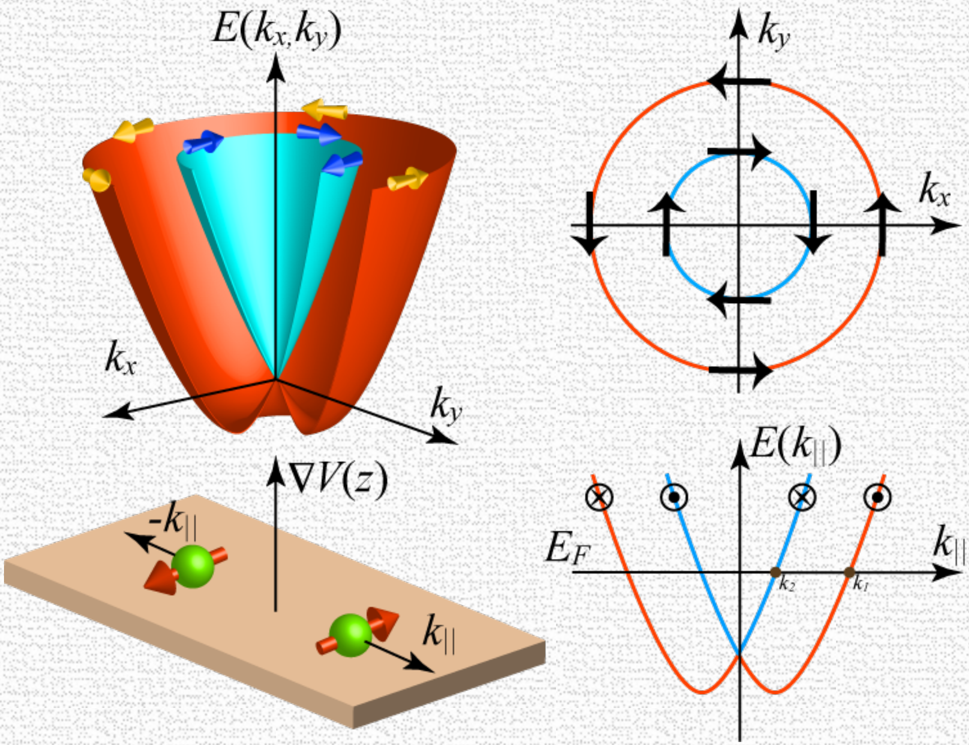


No spin splitting

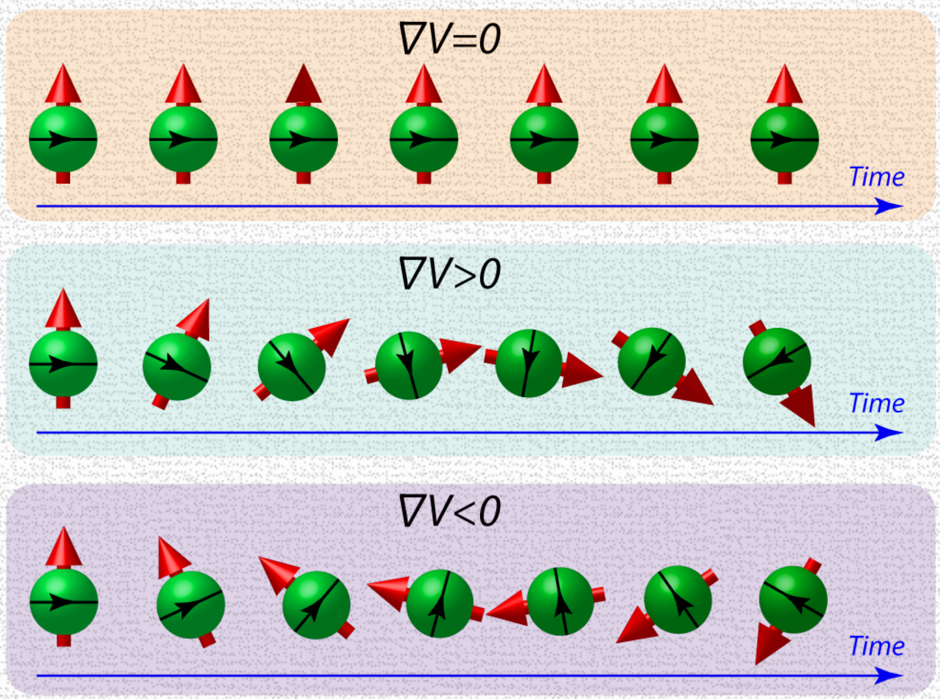
Rashba effect

Due to the **spin-orbit** interaction in inversion **asymmetric systems**.

Momentum space

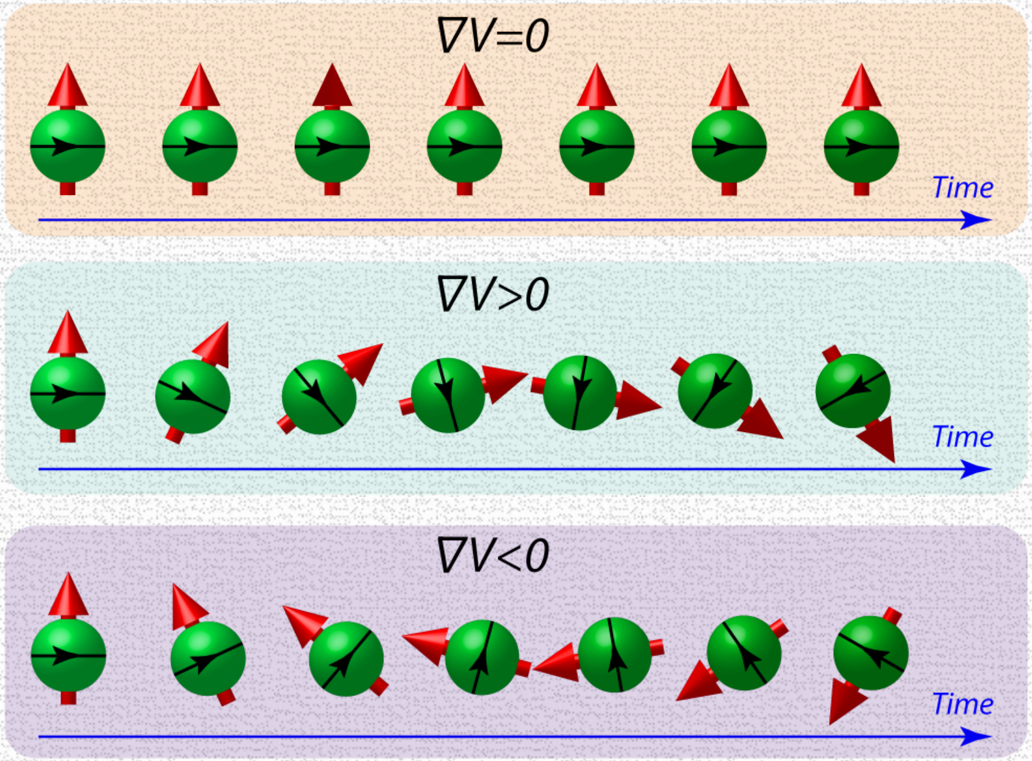


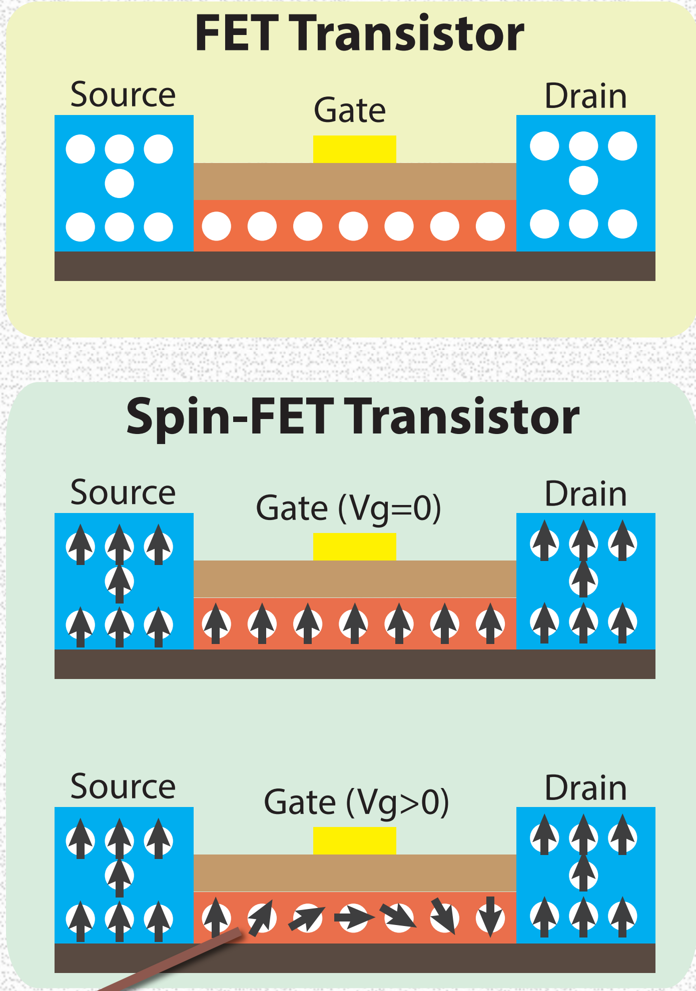
Real space



E. I. Rashba, Sov. Phys. Solid state (1960).

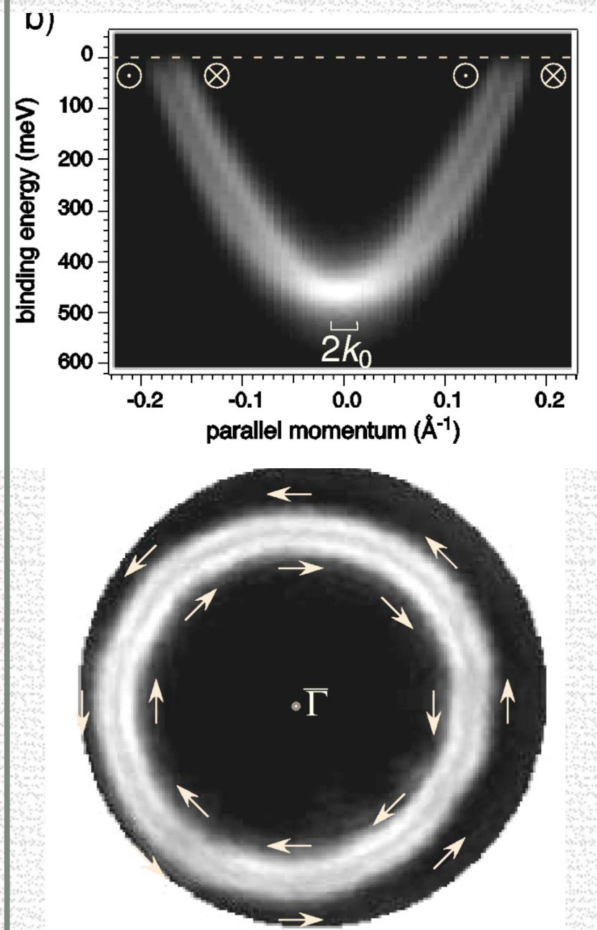
Possible application





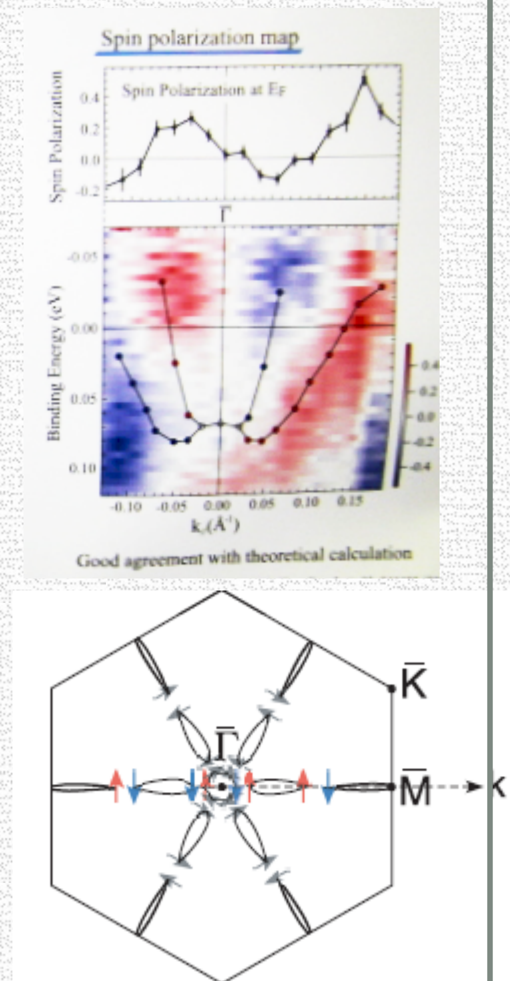
Non-magnetic semiconductor with large spin-orbit coupling
Rashba semiconductors ideal candidates!

Surface Rashba effect



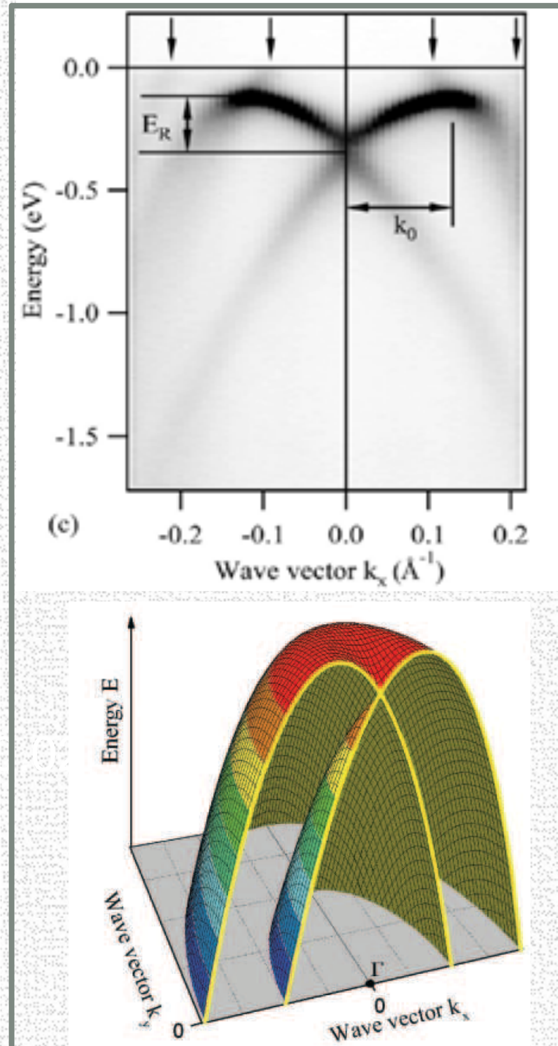
Au (111)

S. LaShell et al., PRL 77, 3419 (1996)



Bi(111
)

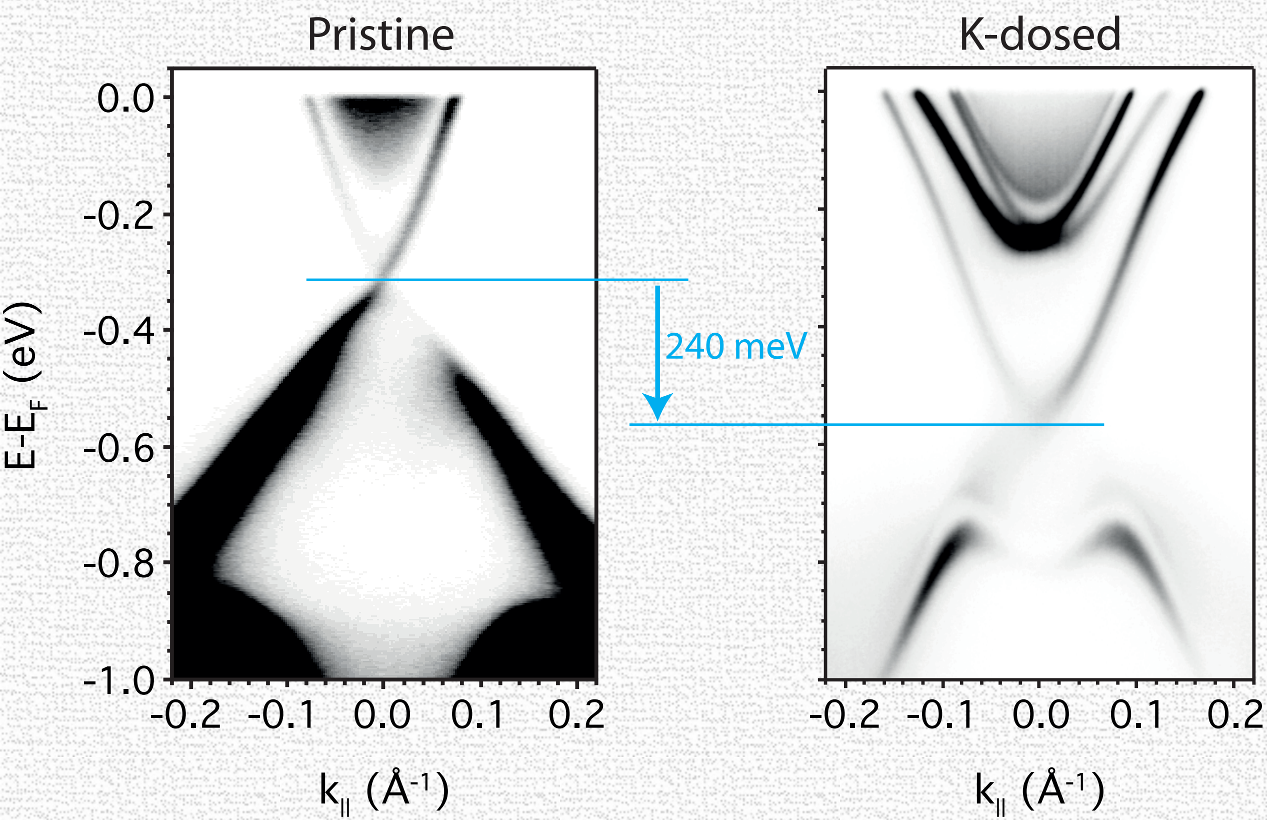
Y.M. Koroteev et al., PRL 93, 046403 (2004)



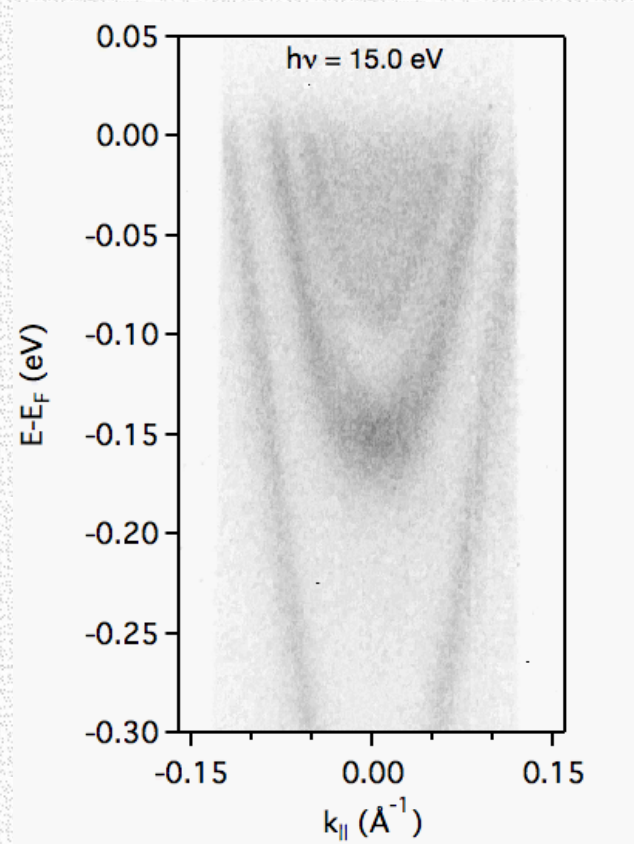
Bi/Ag(111)

C.R. Ast et al., PRL 98, 186807 (2007)

Relocation of the Dirac point and formation of 2D Rashba-split subbands at the surface of Bi2Se3

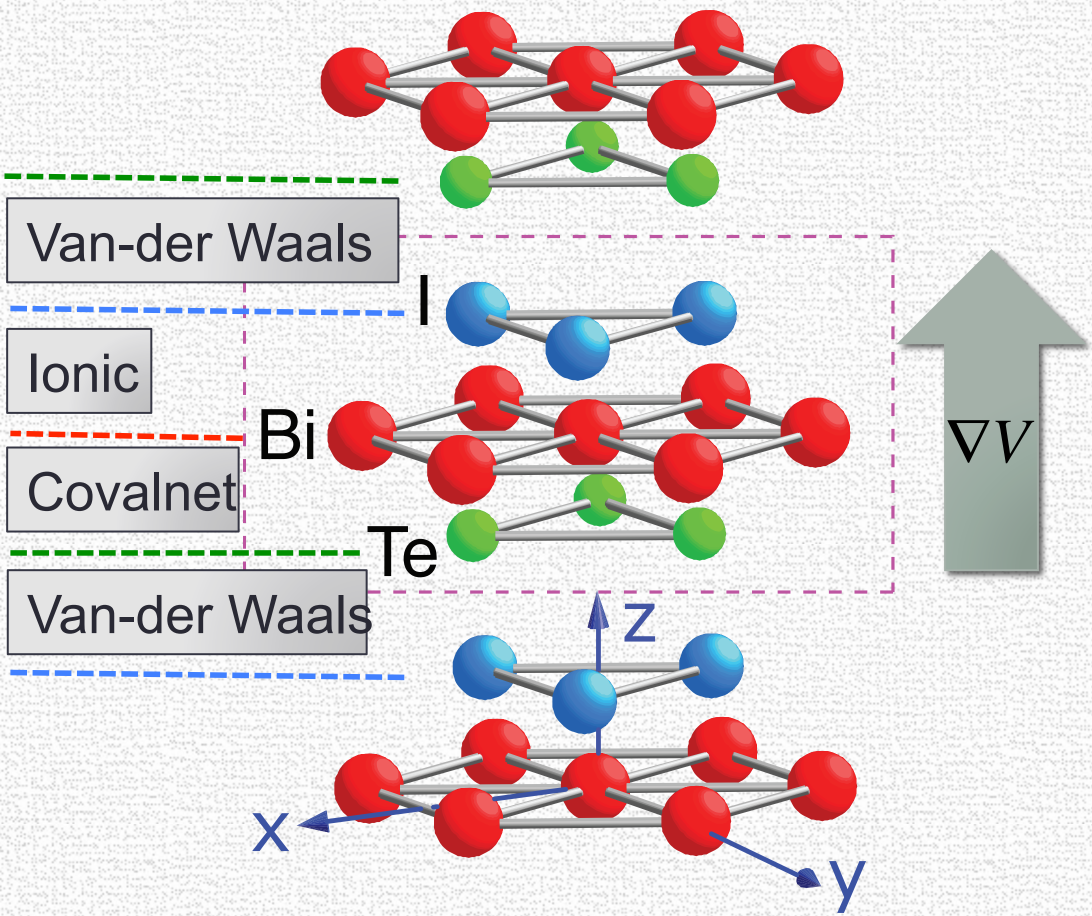


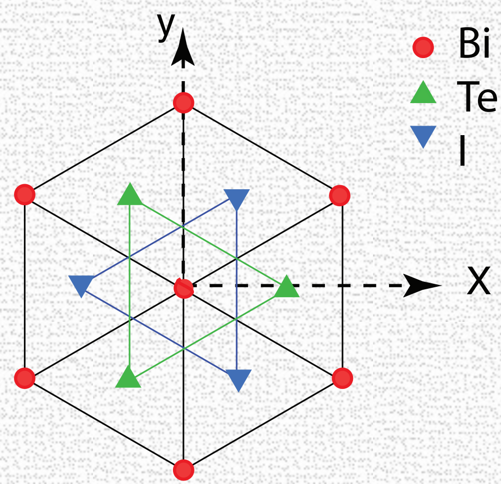
No kz-dependence

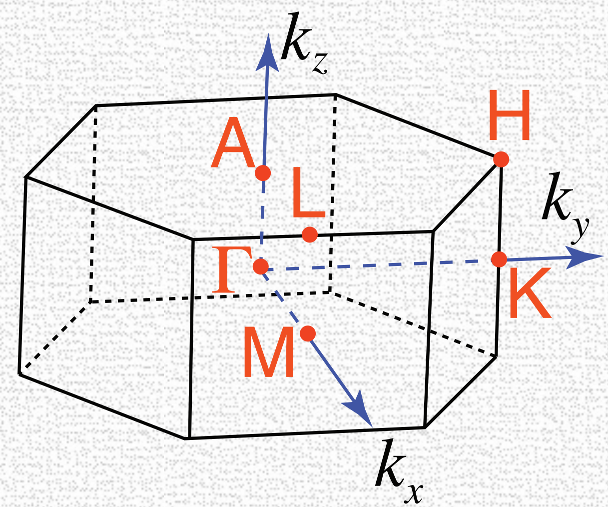


P.D.C. King et al., PRL 107, 096802 (2011).
M. S. Bahramy et al., Nature Communications 3, 1159 (2012).

BiTeI Crystal structure



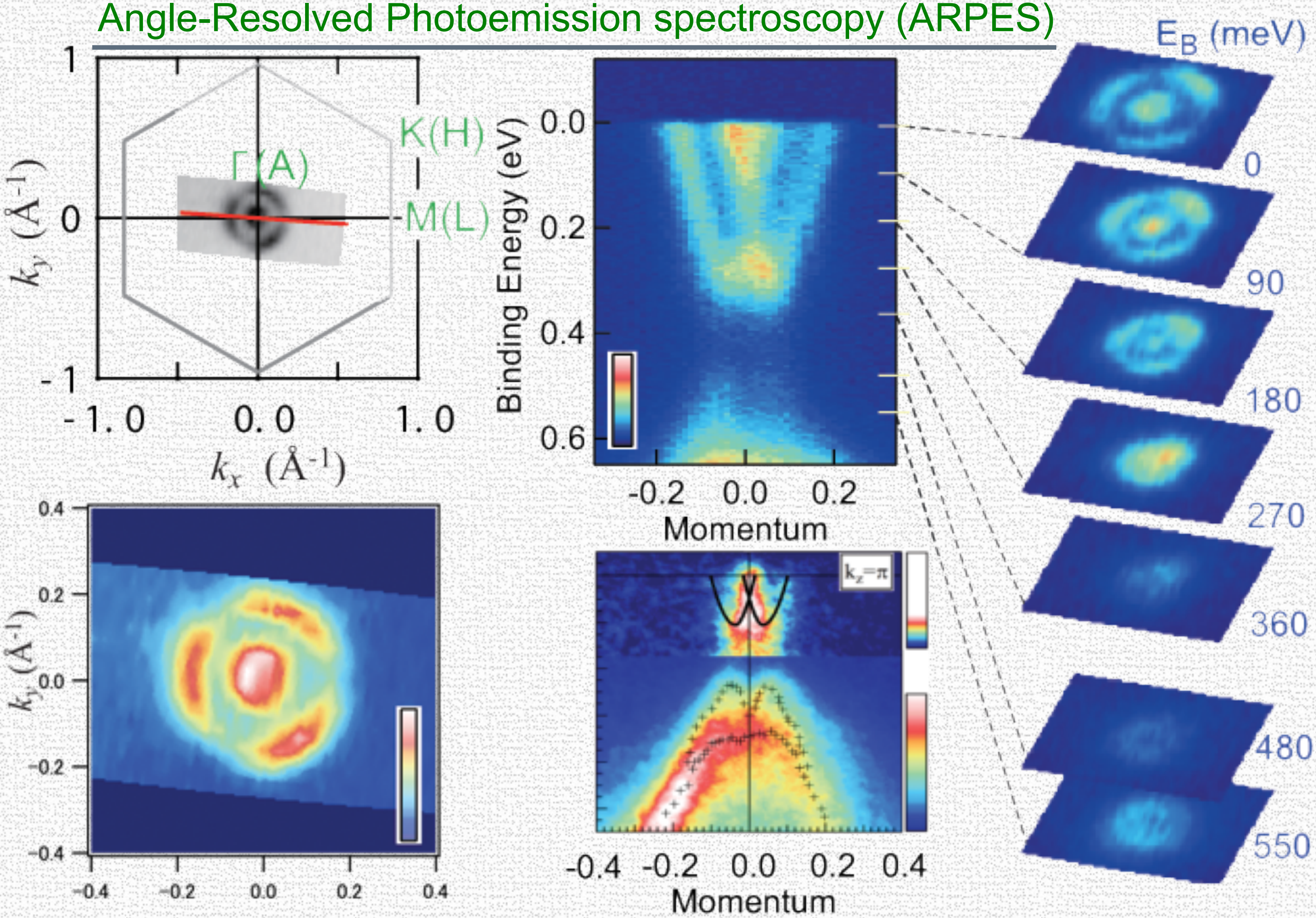




Broken I-symmetry + Strong atomic SOI of Bi

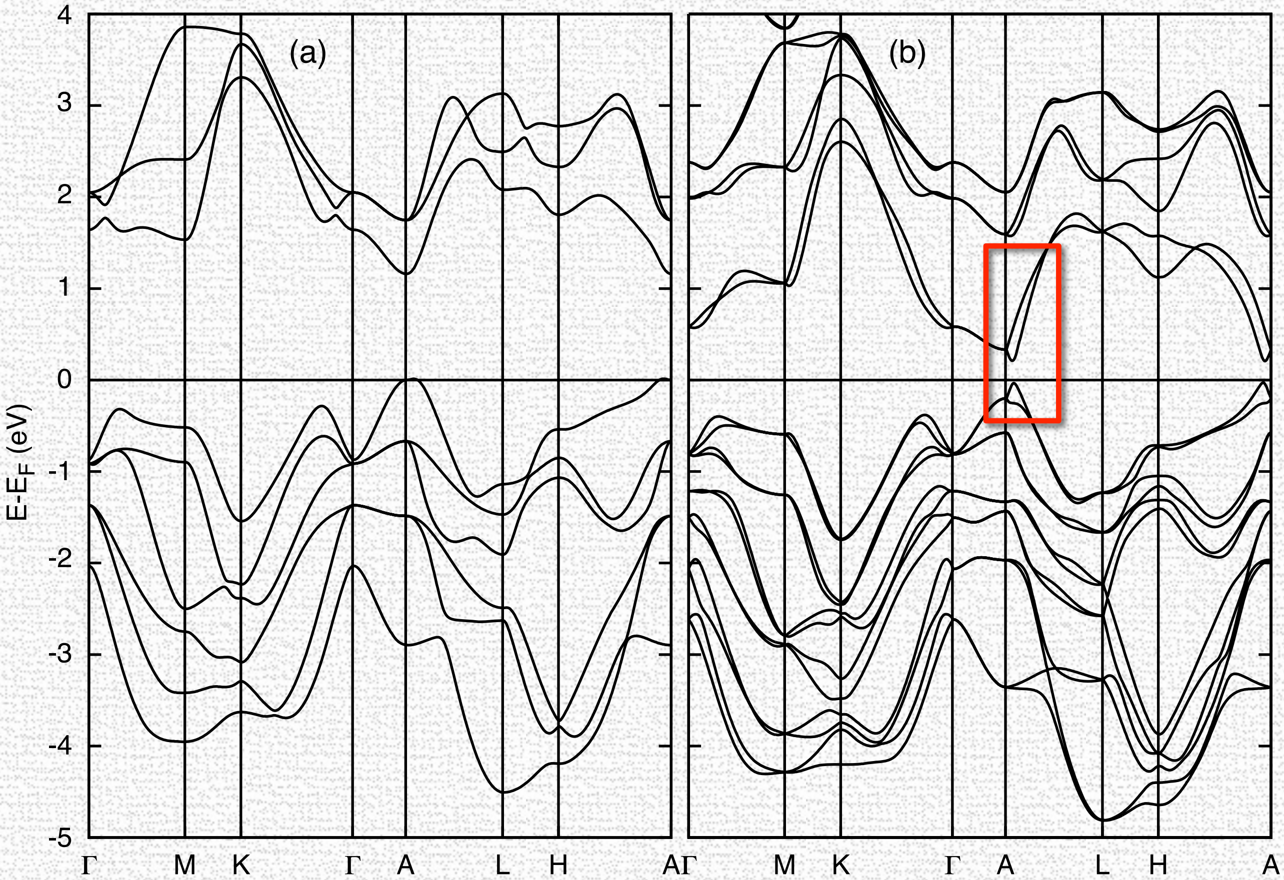
Giant ***bulk*** Rashba spin splitting in BiTeI

Angle-Resolved Photoemission spectroscopy (ARPES)



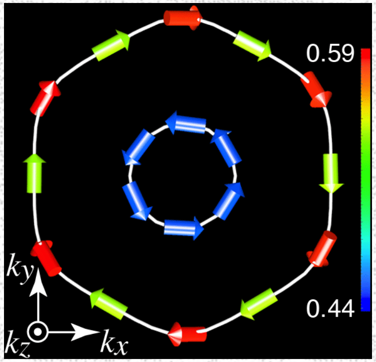
K. Ishizaka, MSB *et al.*, Nat. Mater. 10, 521 (2011).

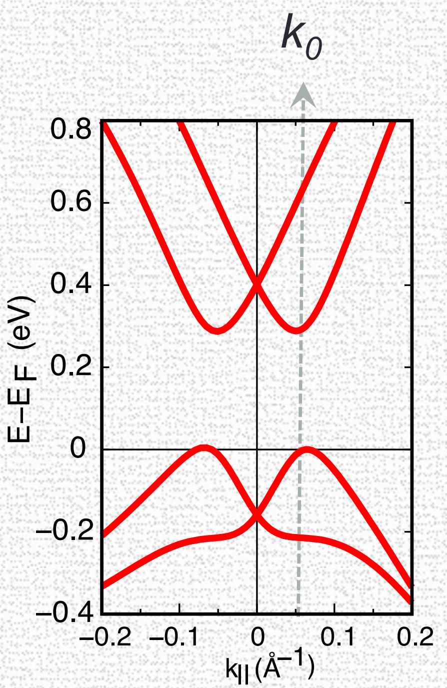
BiTeI band structure



Without SOC

With SOC

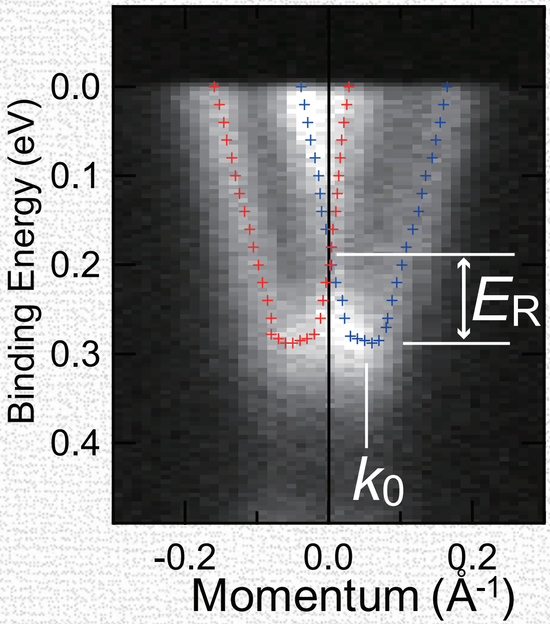




k_{CBM} and k_{VBM} ~k_0

K. Ishizaka, MSB *et al.*, Nat. Mater. 10, 521 (2011).

Comparison with 2D Rashba systems



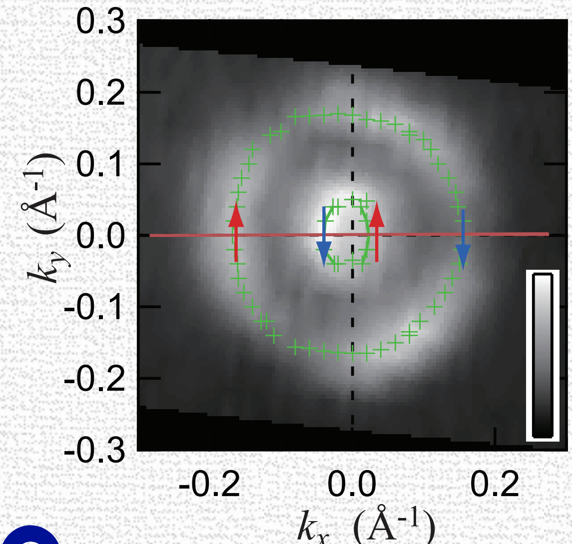


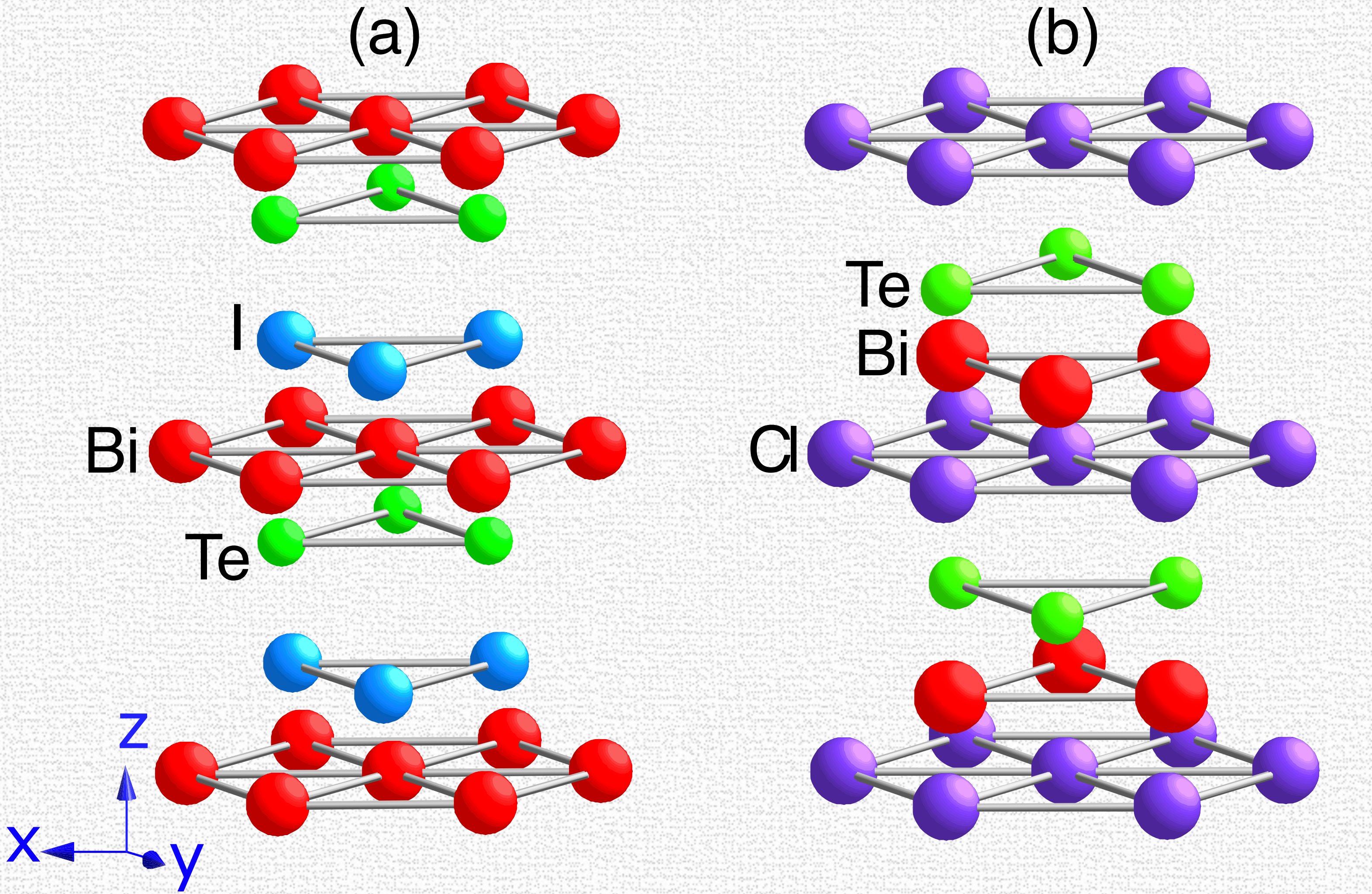
Table 1 | Selected materials and parameters characterizing spin band splitting: the momentum offset k_0 (Å^{-1}), Rashba energy E_R (meV) and Rashba parameter α_R (eV Å).

Sample	k_0	E_R	α_R	Reference
Surface state				
Au(111)	0.012	2.1	0.33	5
Bi(111)	0.05	14	0.55	16
1/3 ML Bi on Ag surface alloy	0.13	200	3.05	7
Interface				
InGaAs/InAlAs	0.028	<1	0.07	4
QW state				
Pb thin film (6–22 ML)	0.035	$\lesssim$10	0.04	36
Bi thin film (7–40 BL)	-	-	-	18,37
1 ML Bi on Cu	N/A	N/A	2.5	20
Bulk				
BiTeI	0.052	100	3.8	This work

For the Bi thin-film system in refs 18,37, the splitting was observed only for the surface states, not for the QW subband states. ML, monolayer.

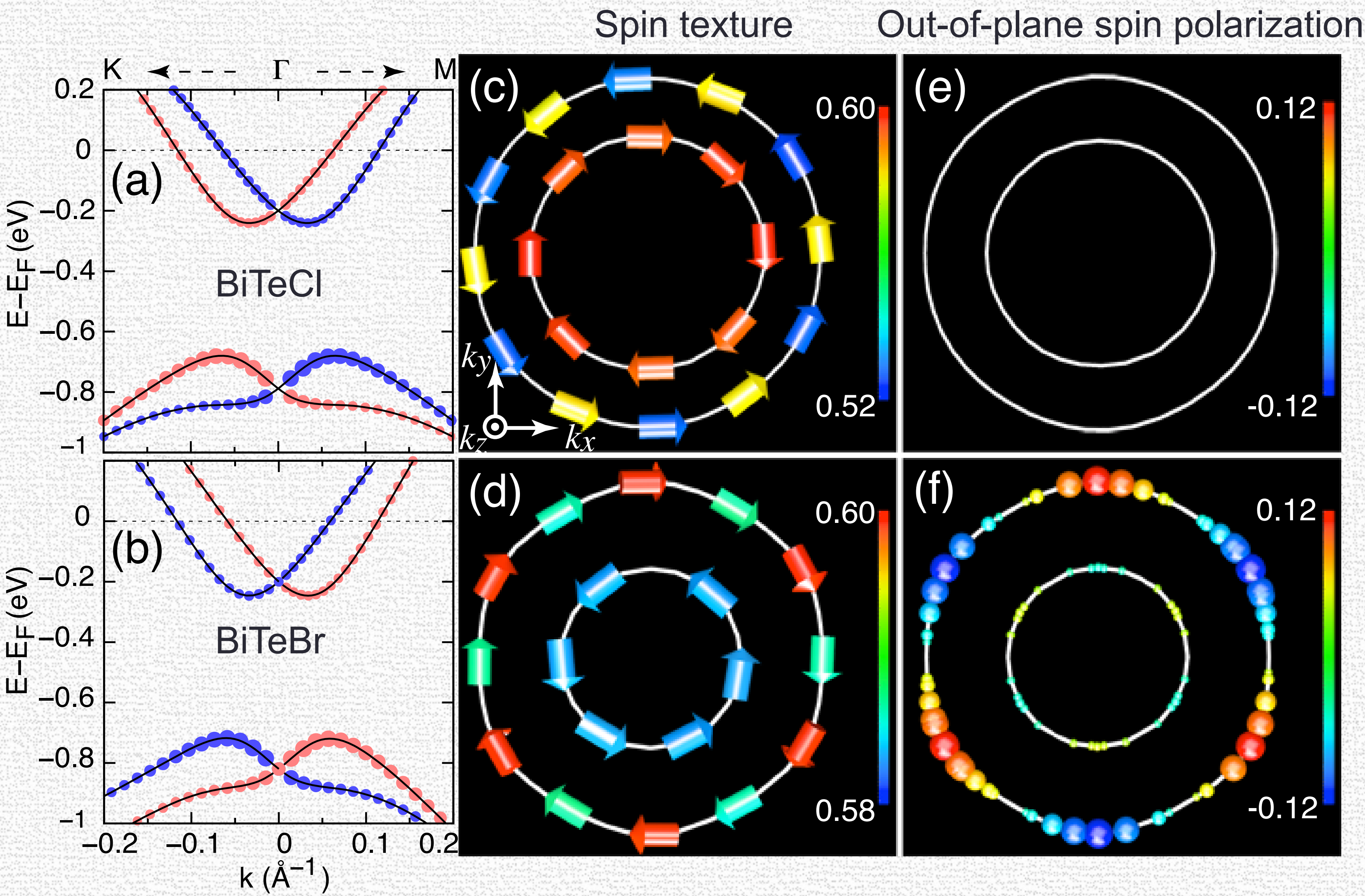
BiTeX Crystal structure

BiTeBr and BiTeI | BiTeCl



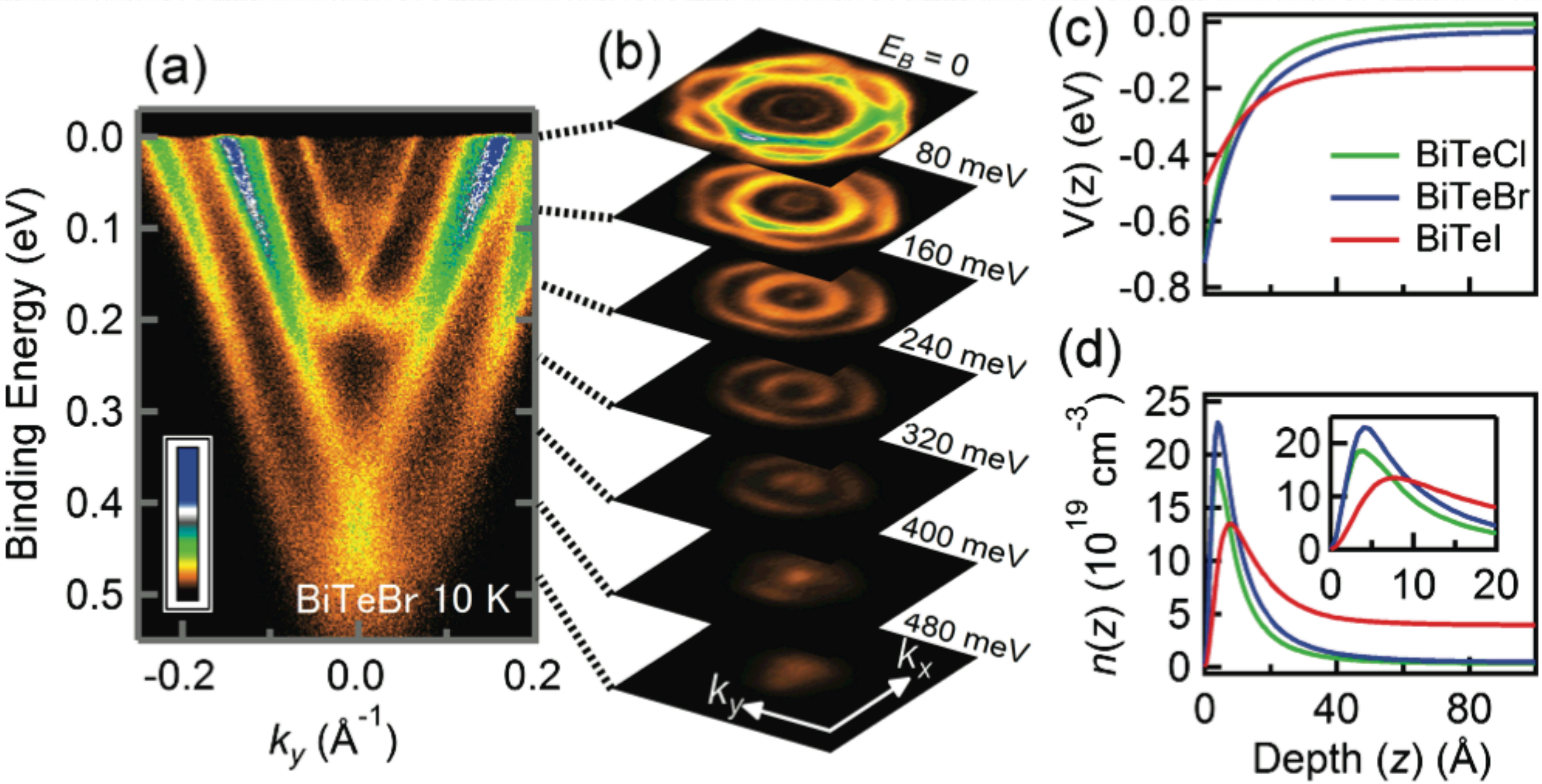
P3m1 | p63mc

Rashba effect in BiTeBr and BiTeCl



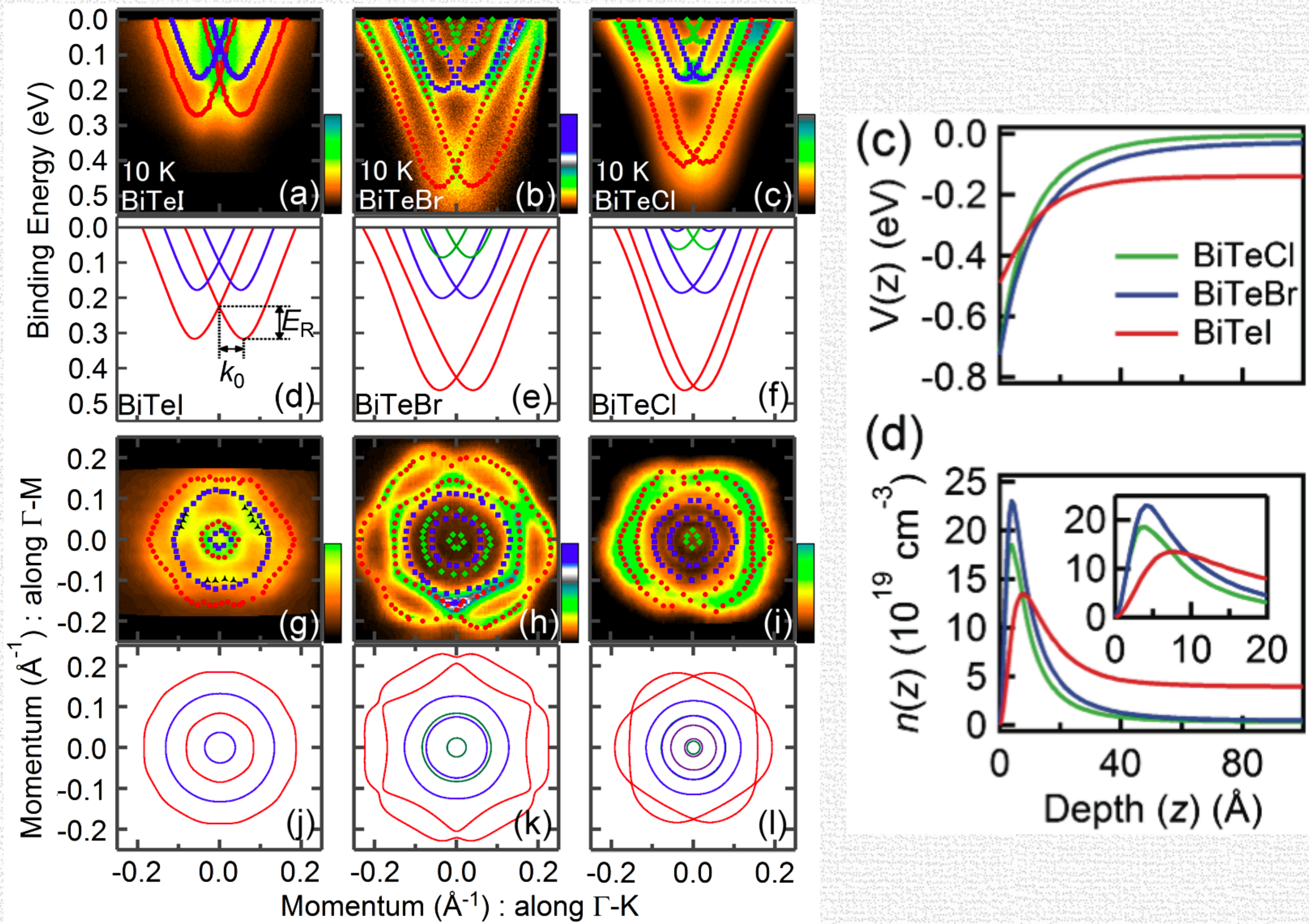
M. Sakano, MSB et al., PRL 110, 107204 (2013).

Band bending at the surface of BiTeX



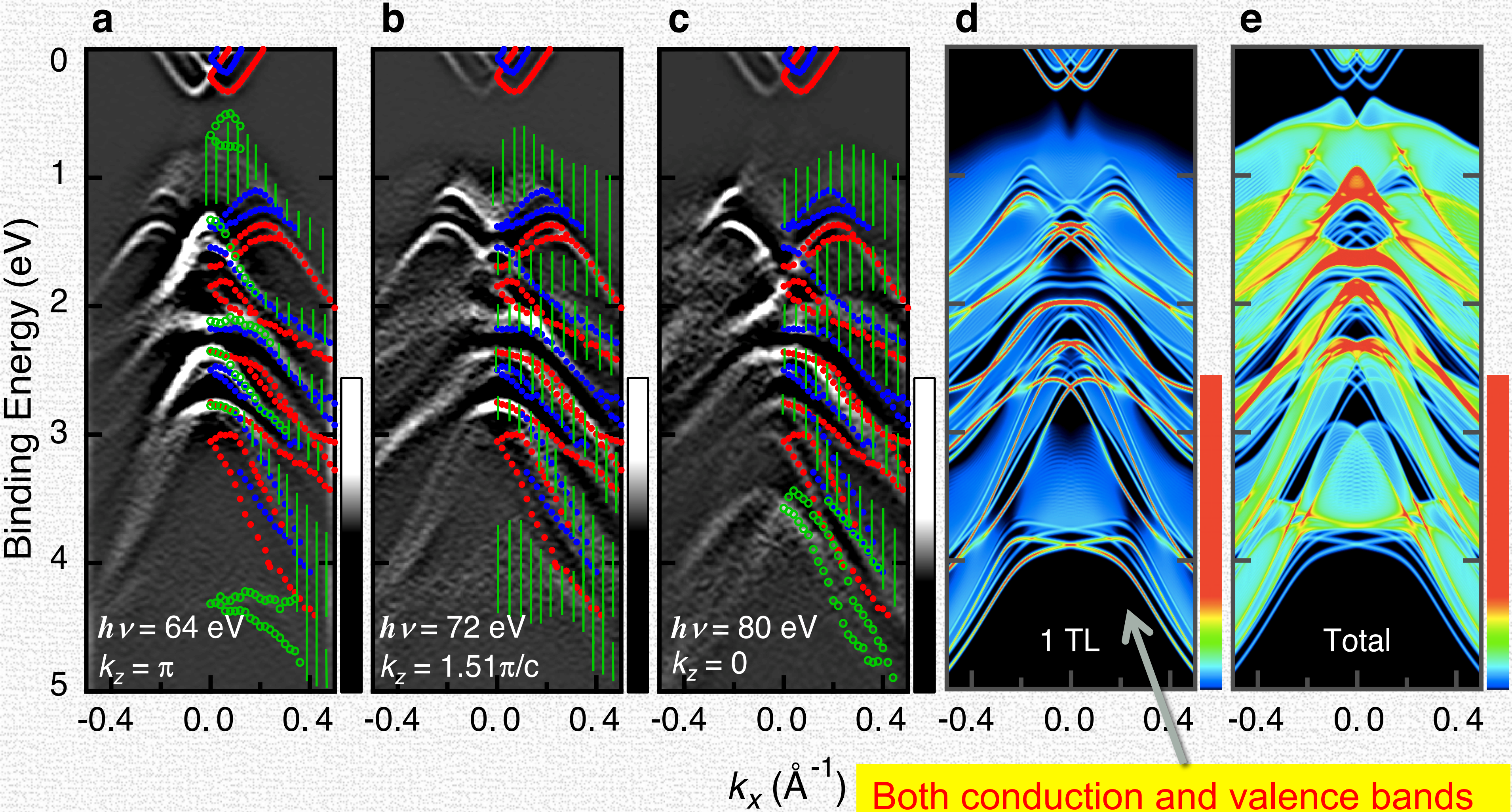
M. Sakano, MSB et al., PRL 110, 107204 (2013).

Band bending at the surface of BiTeX



M. Sakano, MSB et al., PRL 110, 107204 (2013).

Quantum confinement at BiTeI surface



Both conduction and valence bands are quantized at the surface.

K. Ishizaka, MSB et al., Nature Materials 10, 521 (2011).
M. Sakano, MSB et al., PRL 110, 107204 (2013).

Origin of bulk Rashba ffect

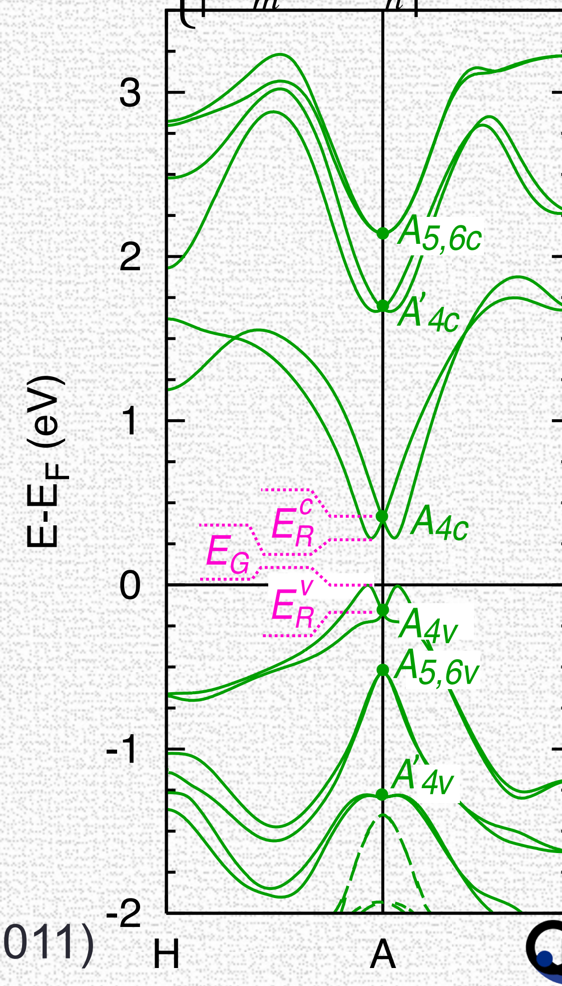
- $k.p$ Hamiltonian for spin splitting:

$$E_\sigma(k) = \frac{\hbar}{m_0}\sum_{n\neq m}\frac{\langle\psi_m|H^{(2)}|\psi_n\rangle\langle\psi_n|\vec{k}\cdot\vec{p}|\psi_m\rangle + c.c.}{E_m - E_n} \rightarrow \begin{cases}\langle\psi_m|H^{(2)}|\psi_n\rangle \Uparrow \\ |E_m - E_n| \Downarrow\end{cases}$$

$$H^{(2)} = (\nabla V\cdot\vec{p})\cdot\sigma = (k_x\sigma_y - k_y\sigma_x)$$

Necessary conditions:

1. Strong spin-orbit coupling without inversion symmetry
2. Narrow band gap
3. Symmetrically same Valence and conduction bands.



MSB, R. Arita and N. Nagaosa PRB 84, 041202(R) (2011)

Novel features of bulk Rashba effect

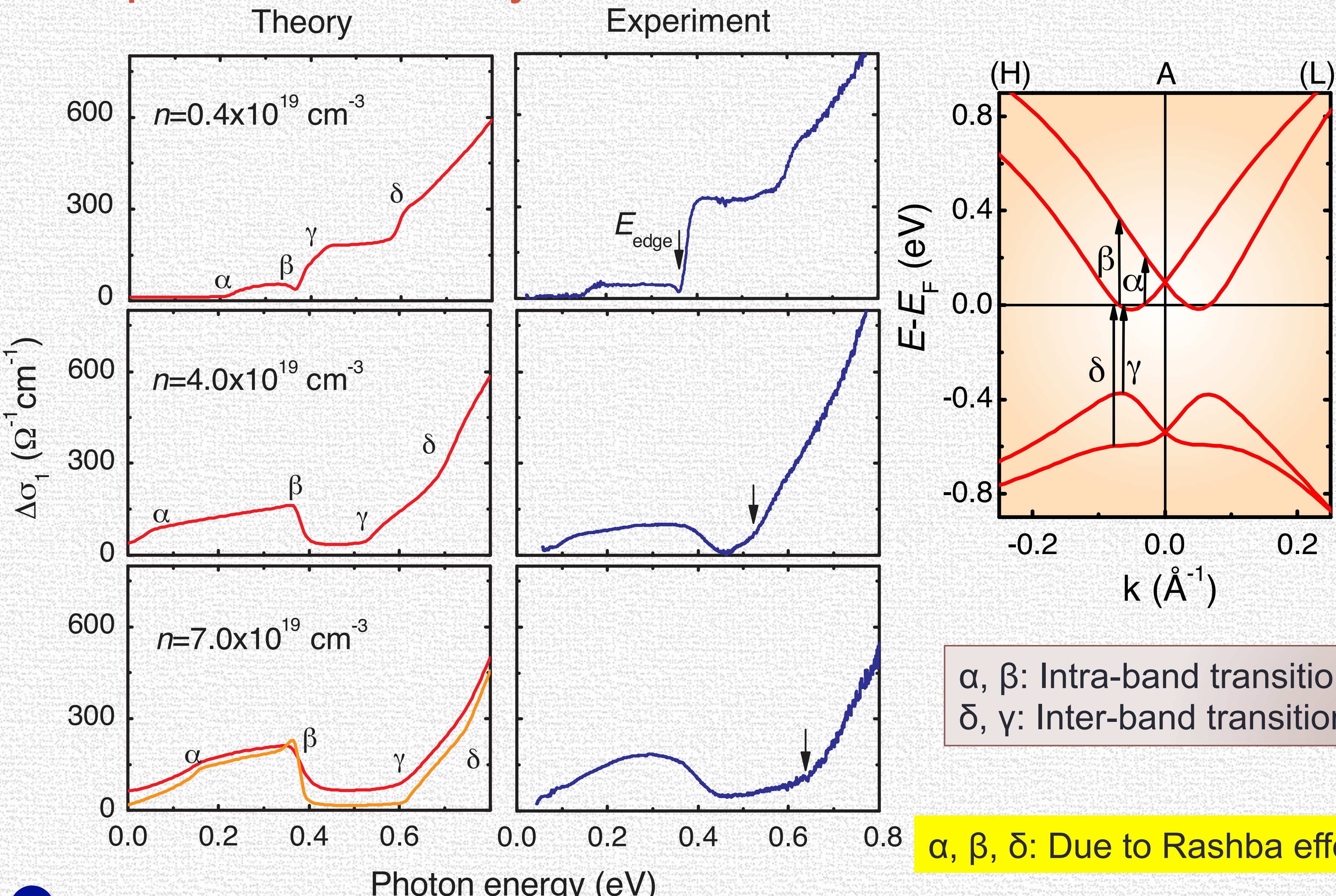
① Unique features in optical spectra

② Enhanced magneto-optical response

③ Enhanced orbital dia- and paramagnetism

④ Spin polarized photocurrent

Optical conductivity in Rashba semiconductor BiTeI



α, β: Intra-band transition
δ, γ: Inter-band transition

α, β, δ: Due to Rashba effect

J. S. Lee et al., PRL 107, 117401 (2012).

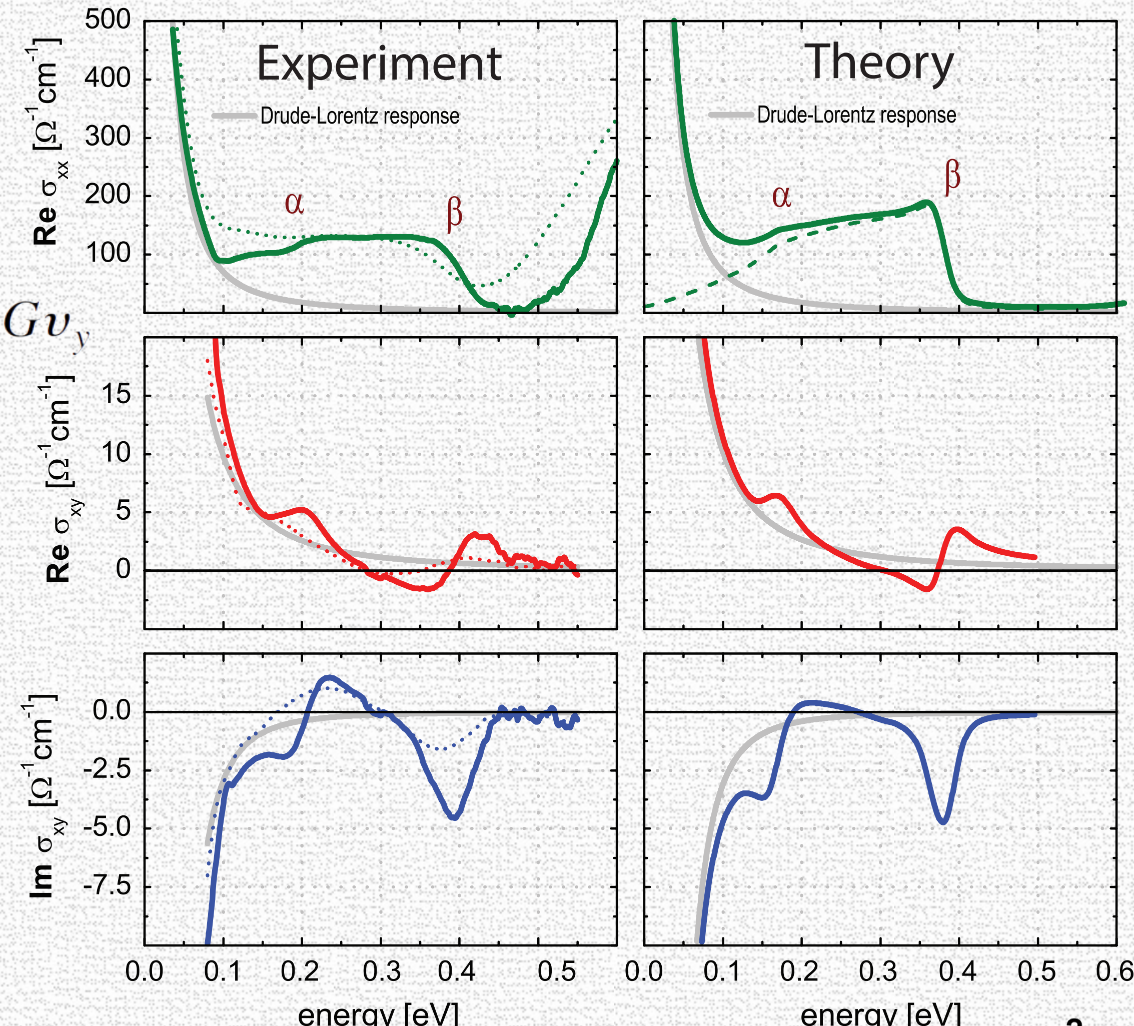
Enhanced Infrared magneto optical response

MO Kerr angle spectra $\Phi_K = \theta_K + i\eta_K = -\dfrac{\sigma_{xy}}{\sigma_{xx}\sqrt{1+(4\pi i/\omega)\sigma_{xx}}}$

Fukuyama formula (H. Fukuyama 1969)

$$\sigma_{xy}(i\omega_\ell) = B\frac{e^3\hbar}{2\omega}k_B T\sum_n \frac{1}{V}\sum_{\mathbf{k}} \{m\mathrm{Tr}[G_- v_x G v_x G - G_- v_x G_- v_x G] + m^4\mathrm{Tr}[G_- v_y G_- v_x G v_x G v_y - G_- v_x G_- v_x G v_y G v_y + v_x G v_y G_- v_x G_- v_y G_- - v_x G v_y G_- v_y G_- v_x G_- + G_- v_x G v_x G v_y G v_y - G_- v_x G v_y G v_x G v_y]\},$$

$$G = [i\tilde{\epsilon}_n + E_F - H]^{-1}$$



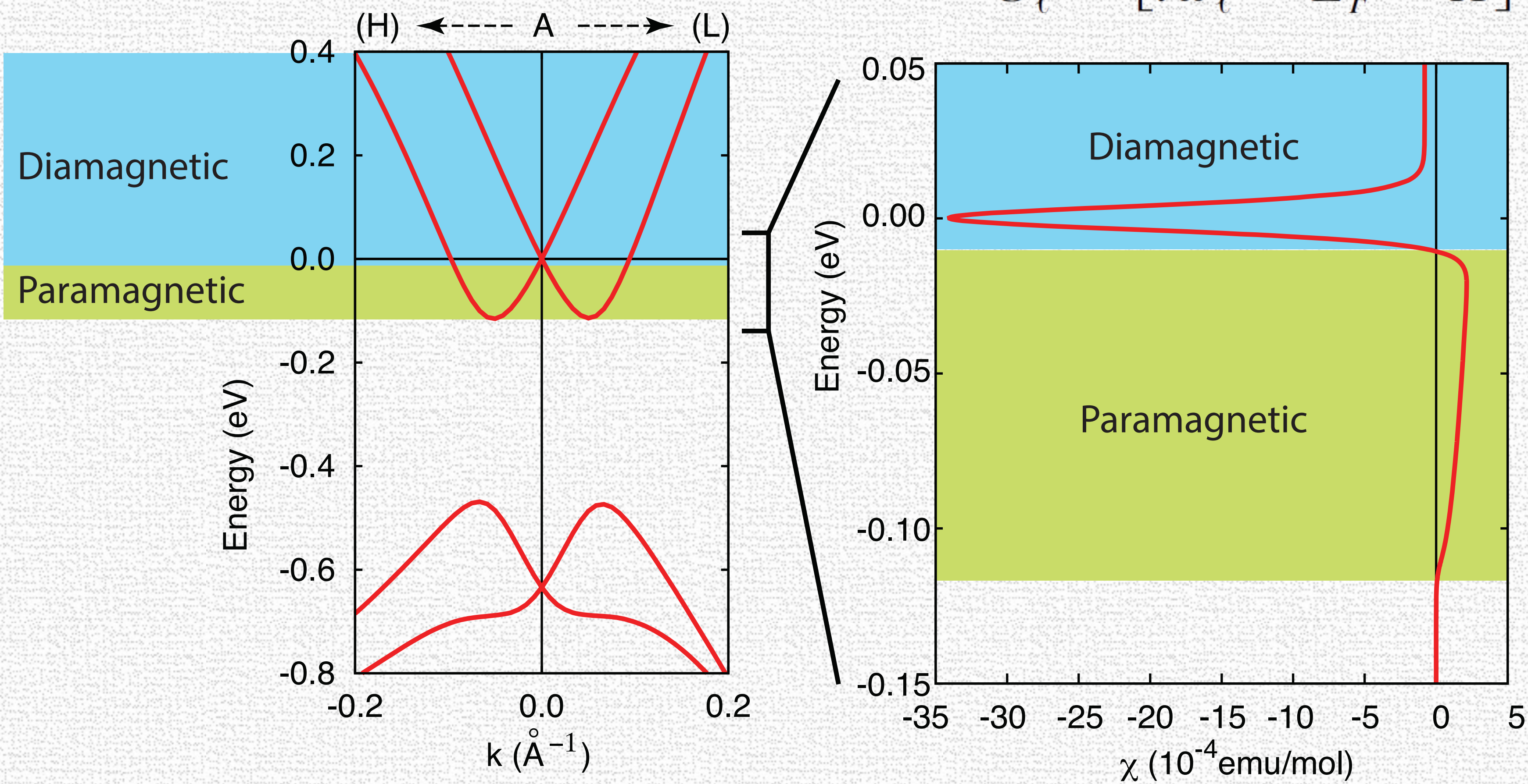
L. Demko et al., PRL 109, 167401 (2012).

Enhanced orbital dia/para-magnetism

Fukuyama formula (H. Fukuyama 1971)

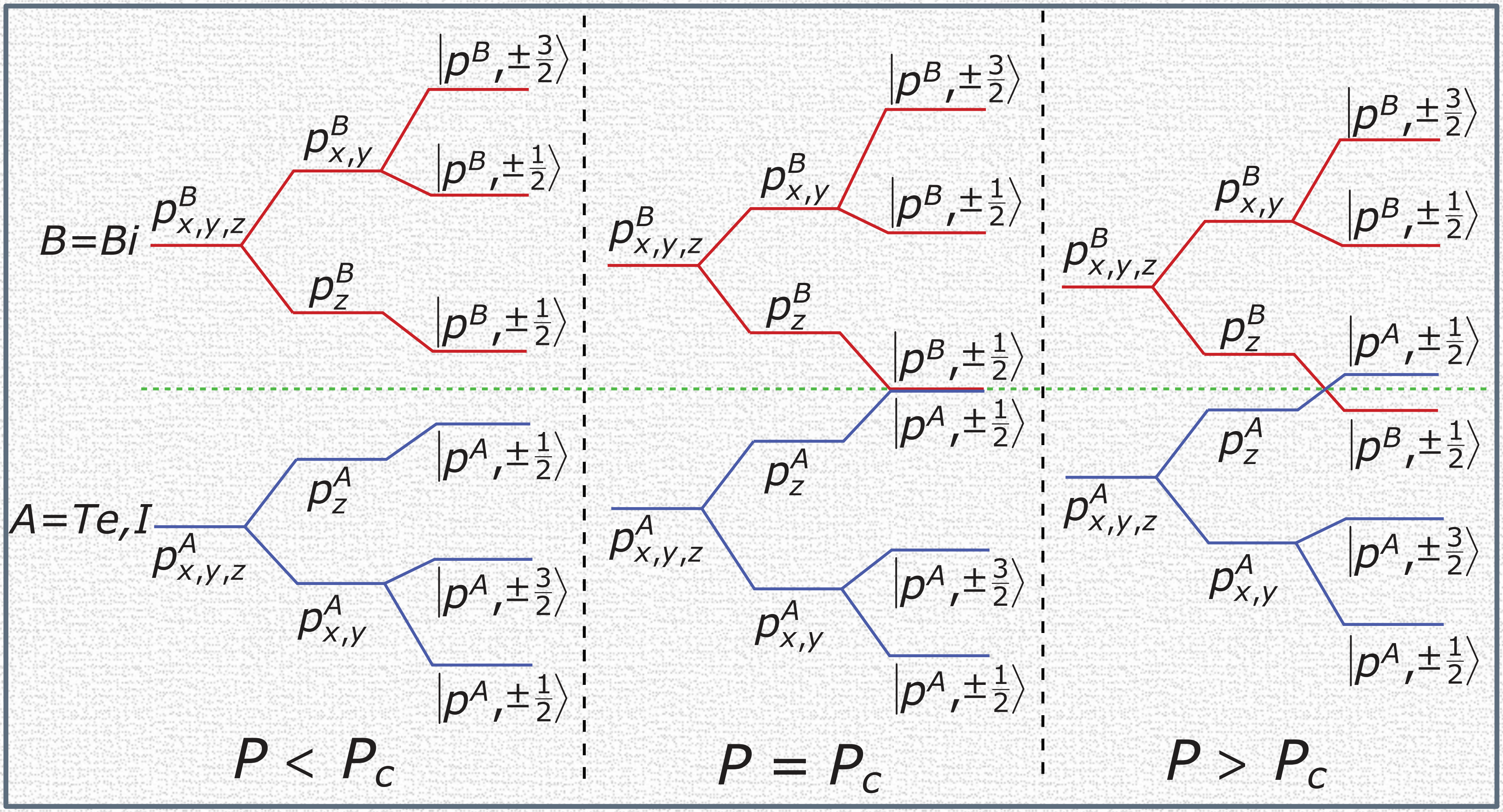
$$\chi(T) = \mu_0 \frac{N_A}{N} \frac{e^2\hbar^2}{2} k_B T \sum_\ell \sum_\mathbf{k} \mathrm{Tr}[G_\ell v_x G_\ell v_y G_\ell v_x G_\ell v_y],$$

$$G_\ell = [i\omega_\ell + E_F - H]^{-1}$$

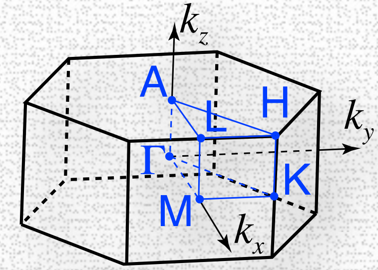


G. Schober, H. Murakawa, MSB, R. Arita, Y. Kaneko , Y. Tokura, N. Nagaosa
PRL 108, 247208 (2012)

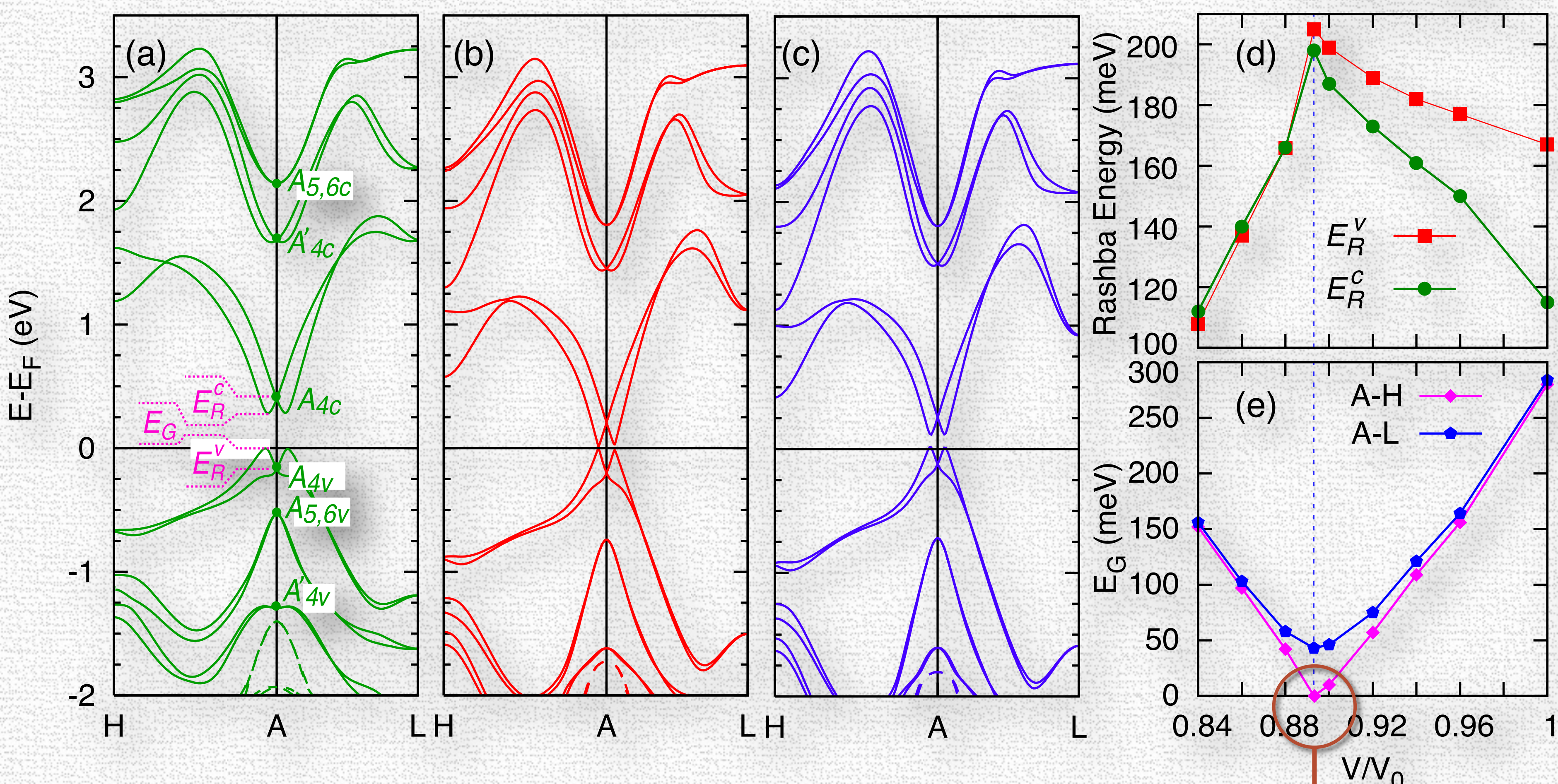
Topological phase transition by pressure



Effect of pressure on Rashba splitting



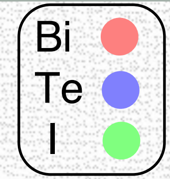
Enhancement of Rashba spin splitting for $P<P_c$

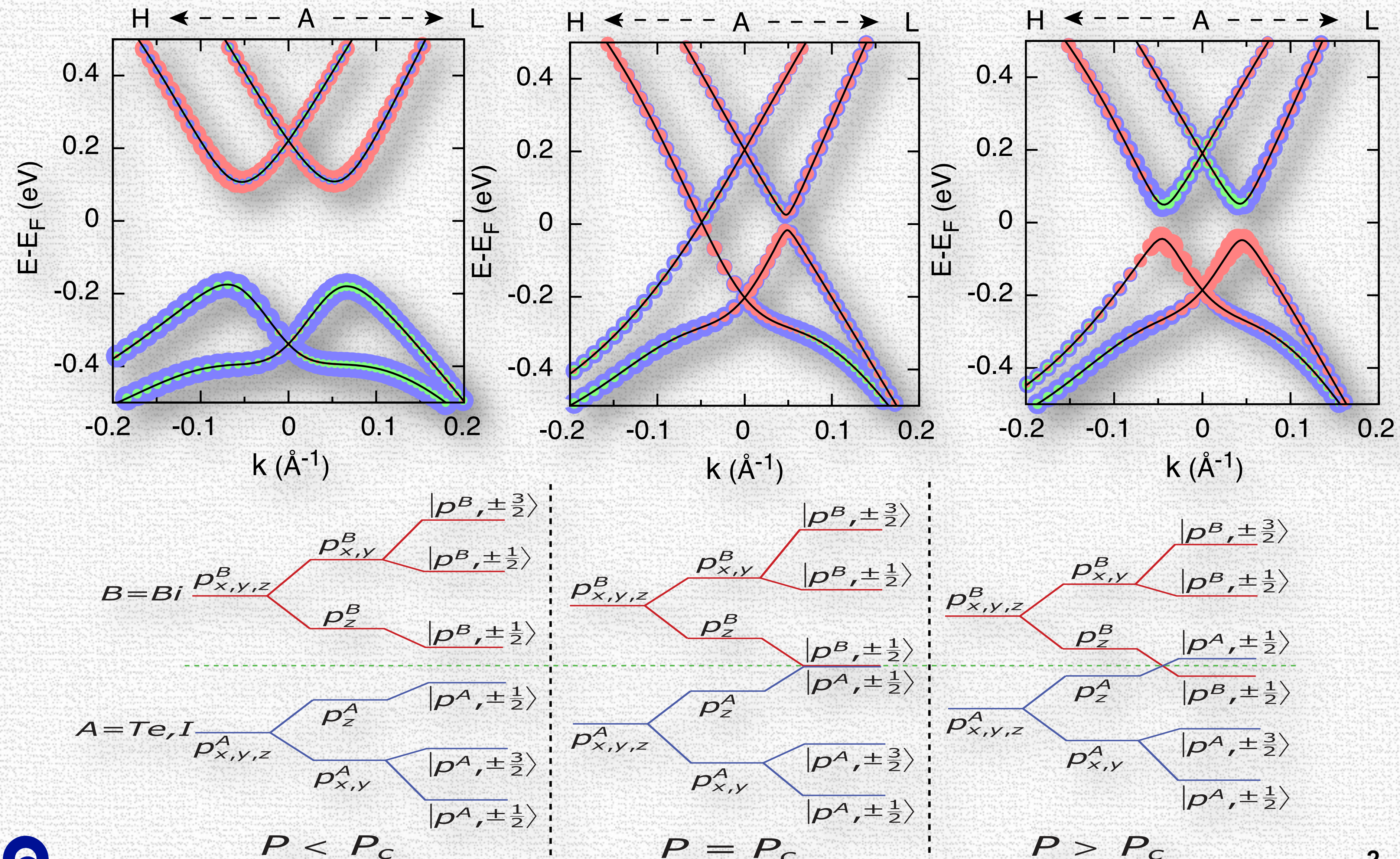


$P<P_c$ | $P=P_c$ | $P>P_c$

Gapless along A-H at P_c

Pressure-induced band inversion



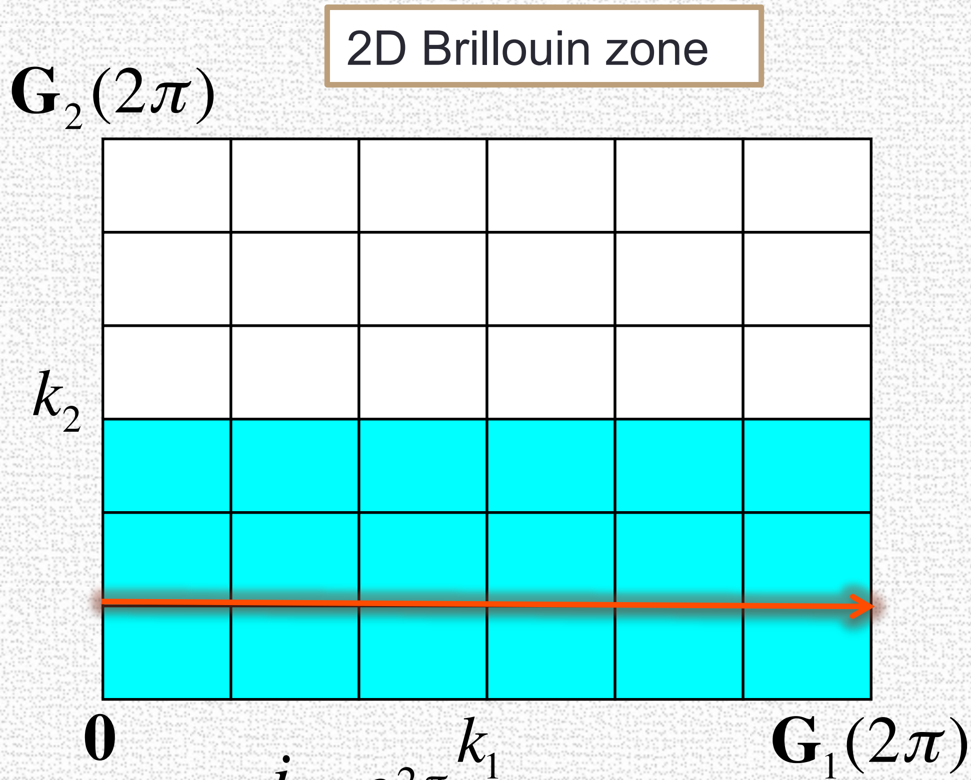


M. S. Bahramy, B. –J. Yang, R. Arita, N. Nagaosa, Nat. Commun. 3, 679 (2012).

Z_2 topological invariant of BiTeI

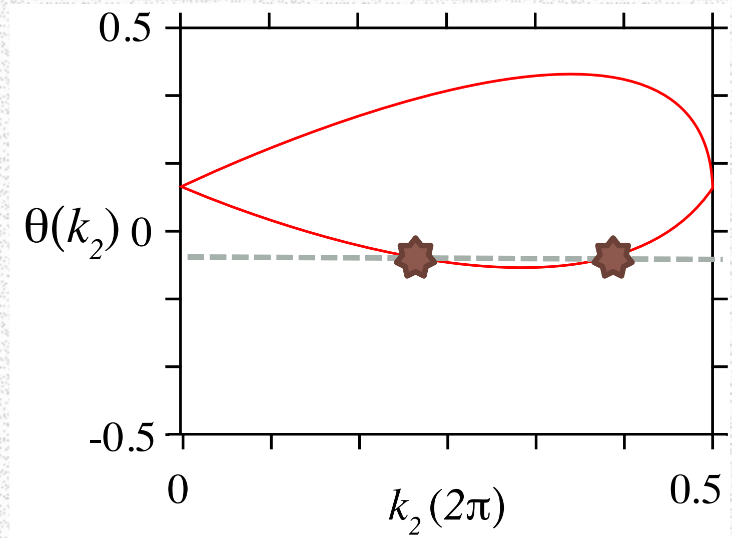
$$
\begin{cases}
Z_2 = \nu_0;(\nu_1\nu_2\nu_3) \\
\nu_0 = 1: \quad \text{Strong topological insulator} \\
\nu_0 = 0: \begin{cases} \nu_{1-3} = 1: \quad \text{Weak topological insulator} \\ \nu_{1-3} = 0: \quad \text{Normal insulator} \end{cases}
\end{cases}
$$

Computation of Z_2 topological invariants

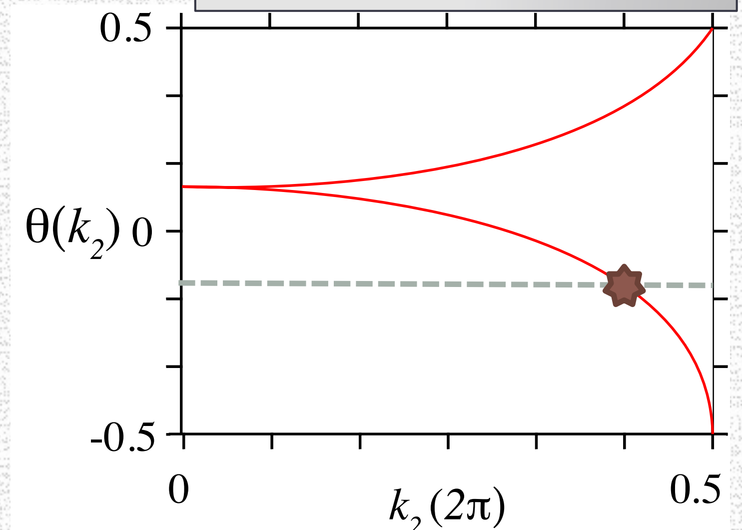


$$\theta_n(k_2) = \frac{i}{2\pi}\int_0^{2\pi} dk_1 \langle u_{n,\mathbf{k}} | \nabla_{k_1} | u_{n,\mathbf{k}} \rangle$$

1D-Wannier charge center



Normal insulator; $\nu=0$



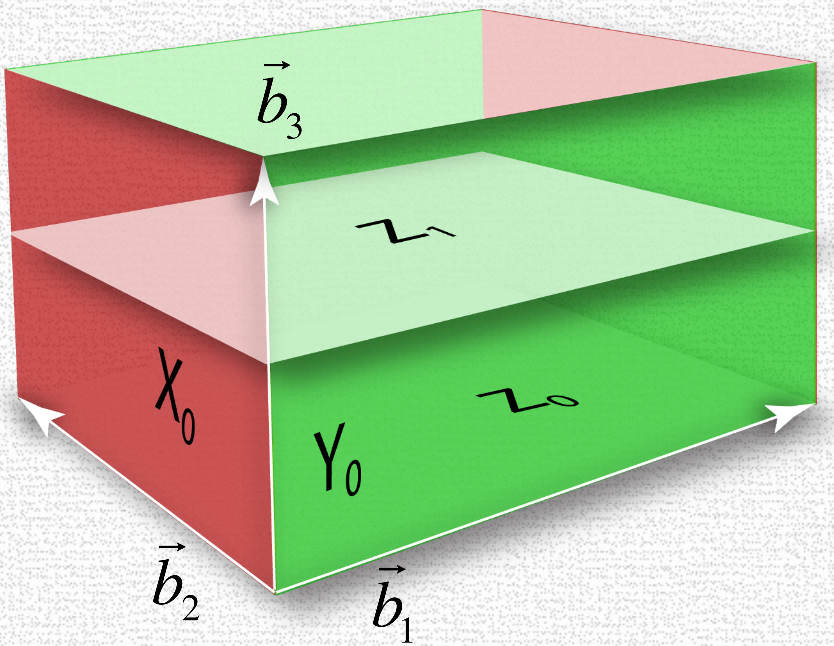
Topological insulator; $\nu=1$

A.A. Soluyanov and D. Vanderbilt, PRB 83, 235401 (2011).
R. Yu, X. L. Qi, A. Bernevig, Z. Fang, and X. Dai, PRB 84, 075119 (2011)

Z_2 topological invariants in 3D

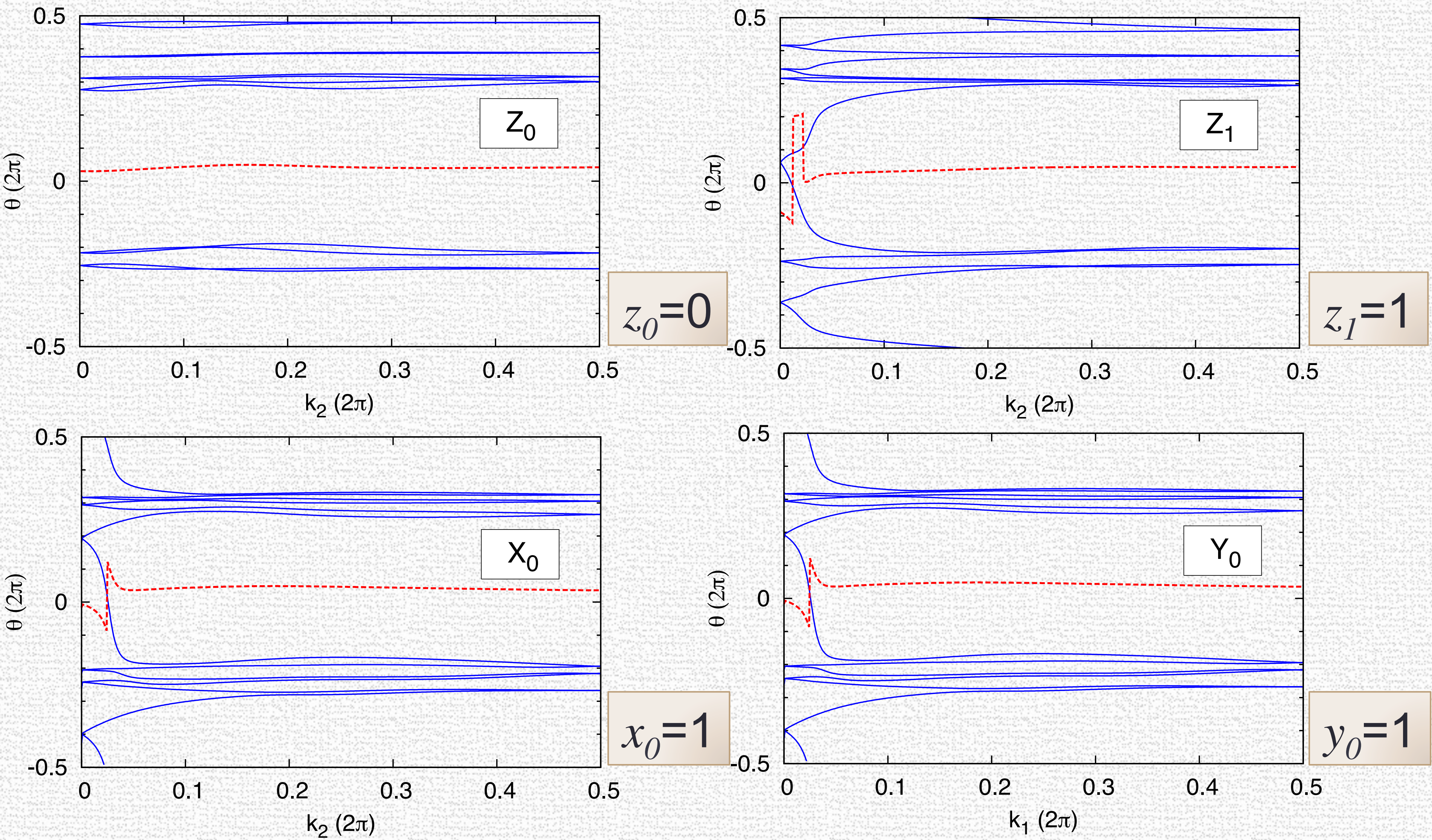
$$Z_2 = \nu_0;(\nu_1\nu_2\nu_3)$$

Strong TI index: $\nu_0 = \left[\left(z_0 + z_1\right)\bmod 2\right] = \left[\left(x_0 + x_1\right)\bmod 2\right] = \left[\left(y_0 + y_1\right)\bmod 2\right]$



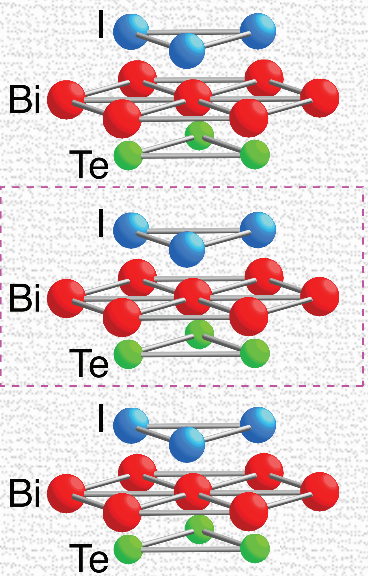
Weak TI index: $\begin{cases} \nu_1 = x_1 \\ \nu_2 = y_1 \\ \nu_3 = z_1 \end{cases}$

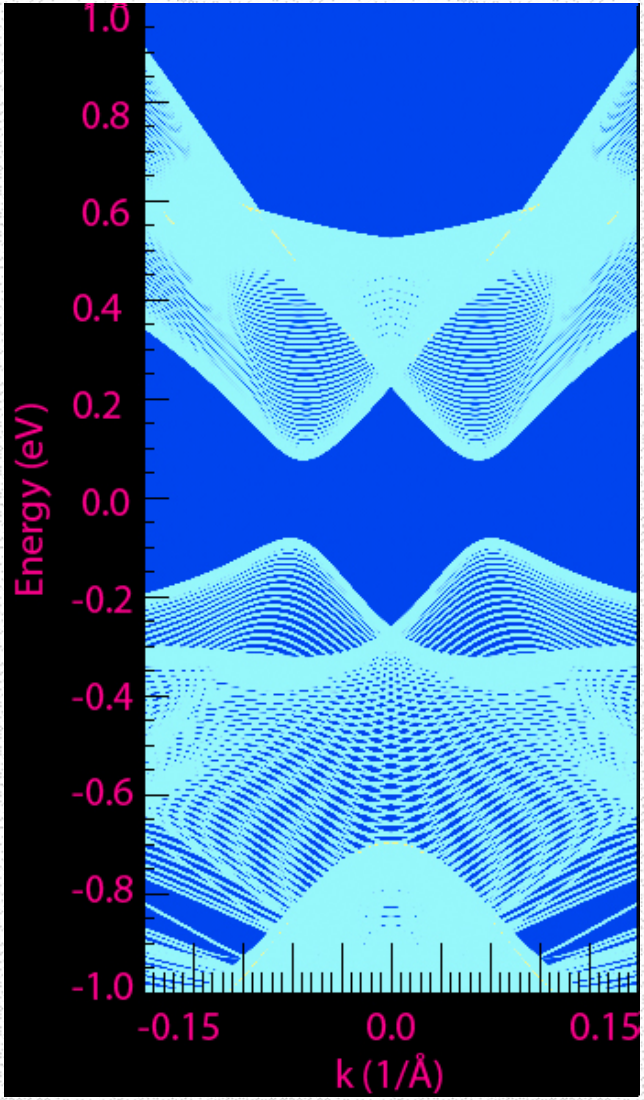
Z_2 topological invariants



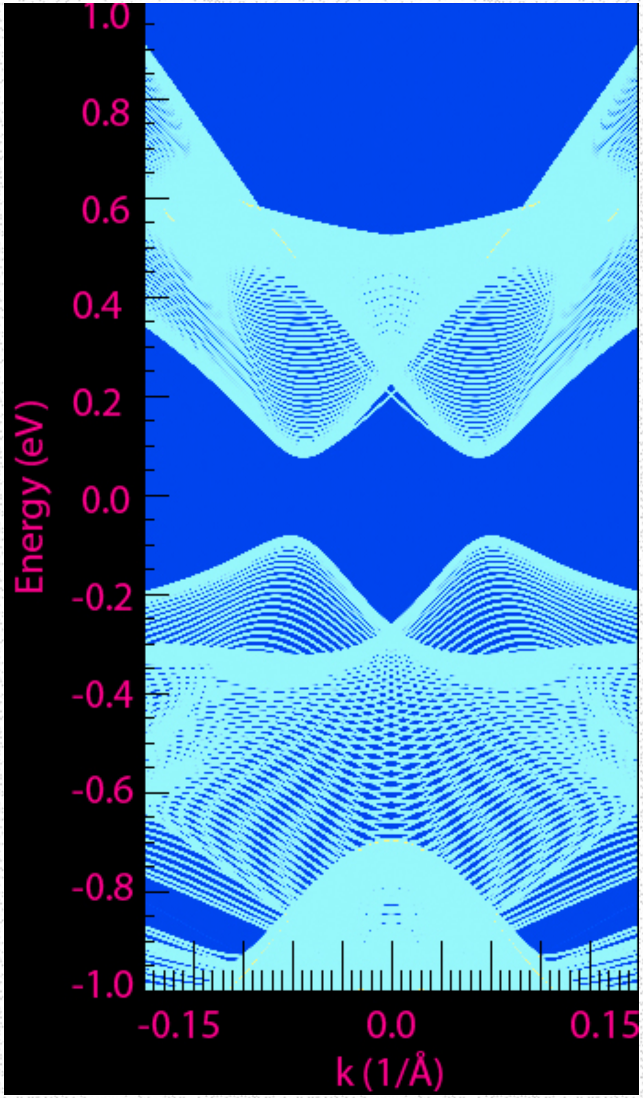
$$Z_2 = \nu_0; (\nu_1 \nu_2 \nu_3) = 1; (001)$$

Pressure-induced topological phase transition in BiTeI





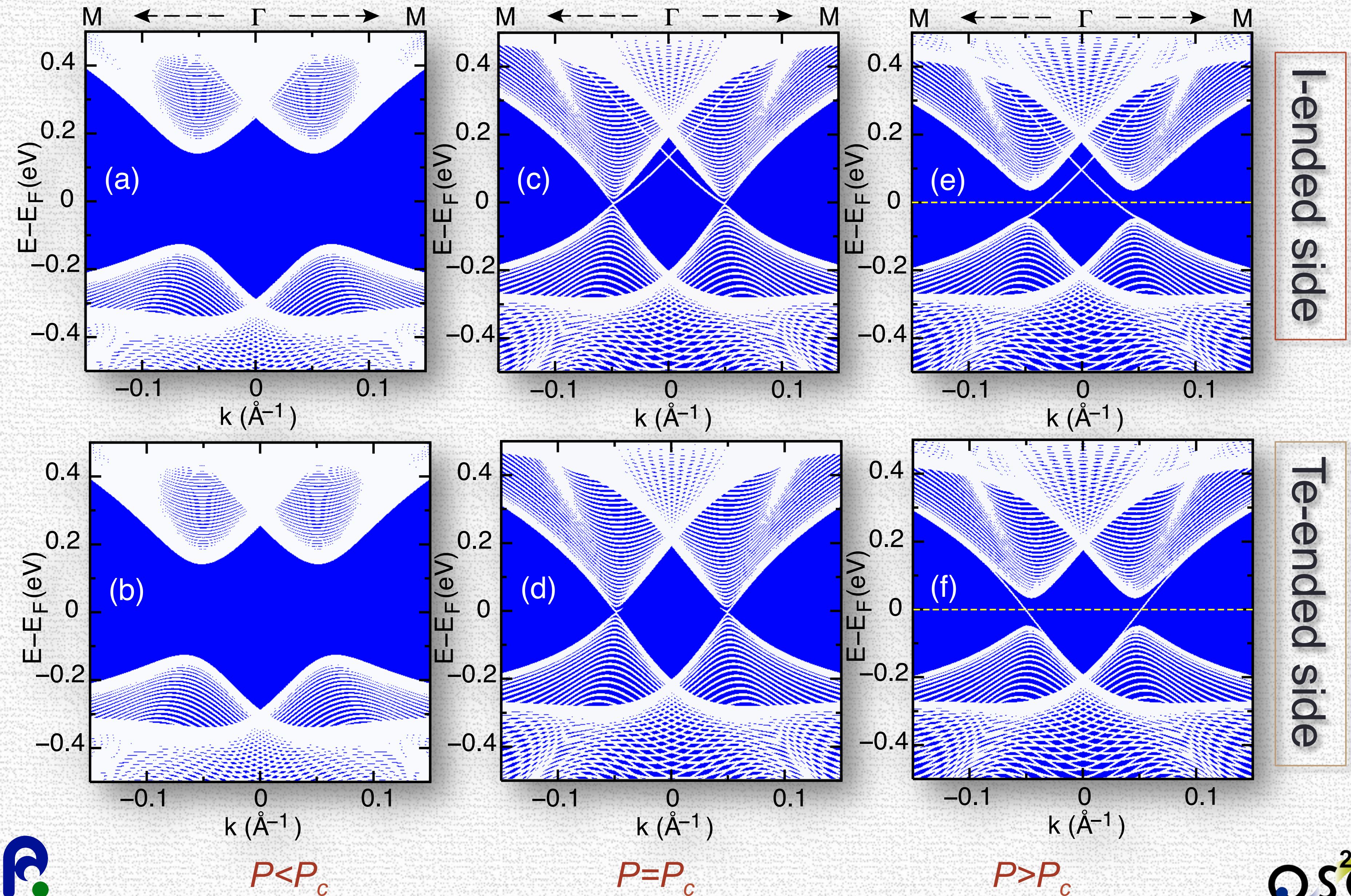
Te-terminated side



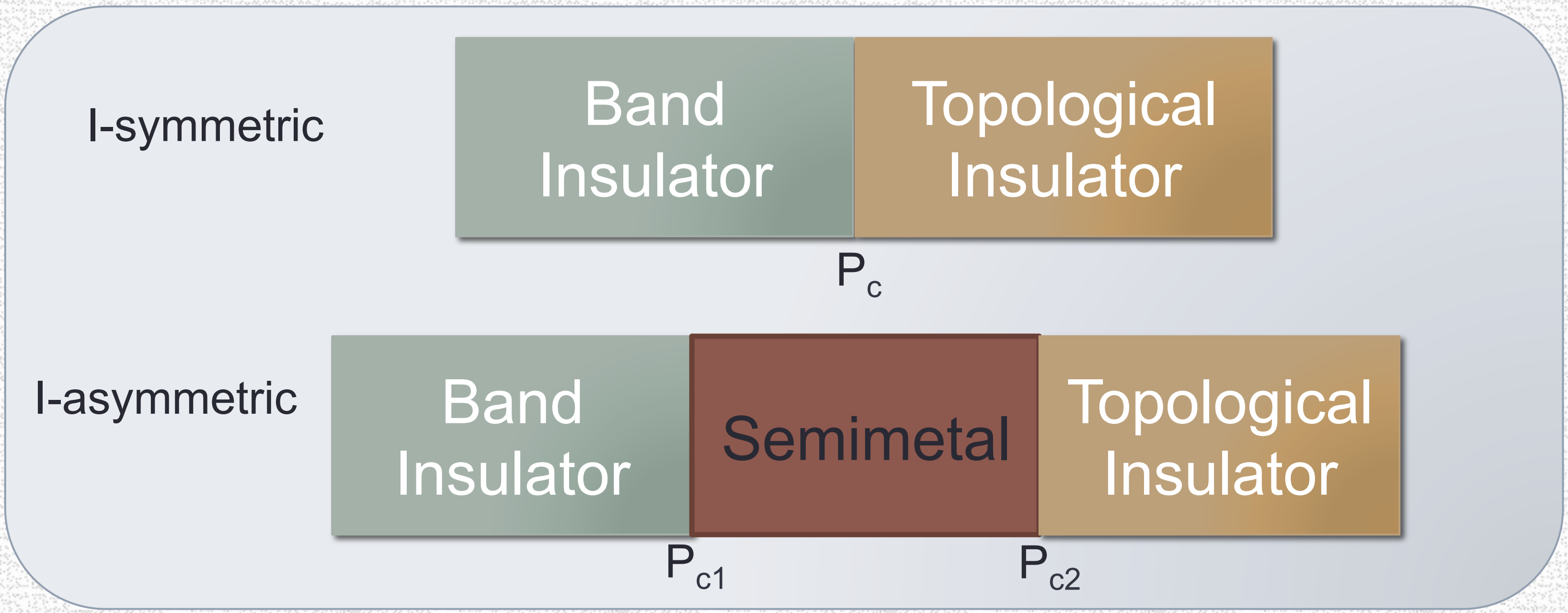
I-terminated side

Nature Communications (2012).

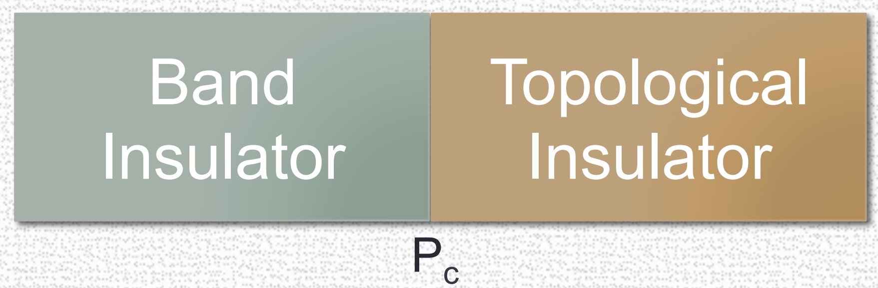
Inequivalence of Dirac surface states



Unconventional quantum phase transition



S. Murakami, and S. Kuga PRB 78, 165313 (2008).



BiTeI

Theory of topological phase transition

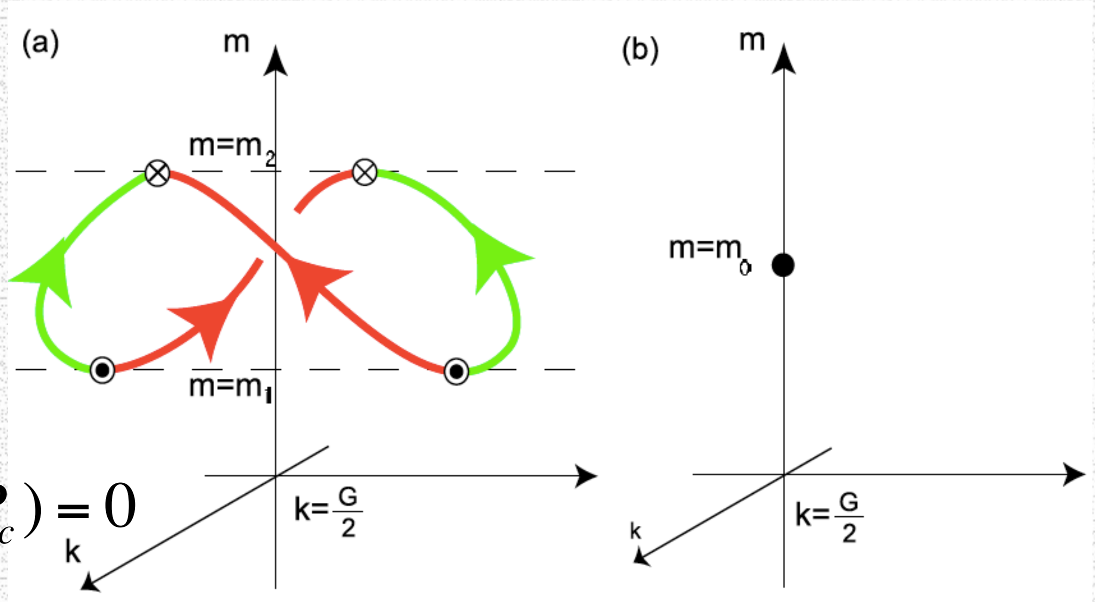
$$H_{2\times 2}(\mathbf{k},P) = \sum_{i=1}^{3} f_i(\mathbf{k},P)\ \tau_i$$

$$= f_0(\mathbf{k},P)\tau_0 + f_1(\mathbf{k},P)\tau_1 + f_2(\mathbf{k},P)\tau_2 + f_3(\mathbf{k},P)\tau_3$$

$f_i(\mathbf{k},P): real\ \ functions$

$\tau_0\ :\ unit\ \ matrix$

$\tau_{1-3}\ :\ Pauli\ matrices$



At band touching point:

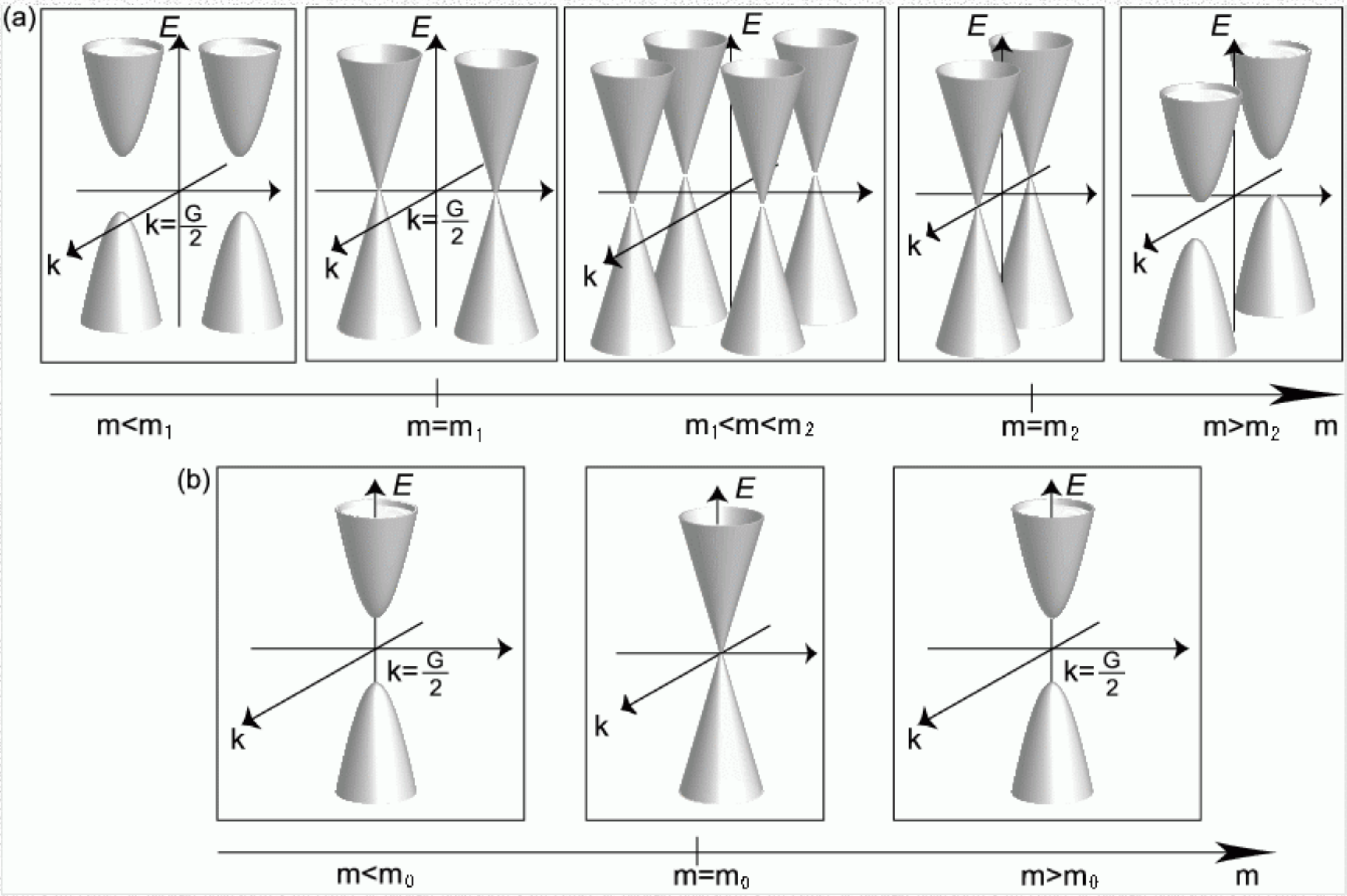
$$f_1(\mathbf{k}_c,P_c) = f_2(\mathbf{k}_c,P_c) = f_3(\mathbf{k}_c,P_c) = 0$$

$$(\mathbf{k}_c,P_c) : (k_{xc},\ k_{yc},\ k_{zc},P)$$

3 conditions can not be uniquely satisfied by 4 parameters.

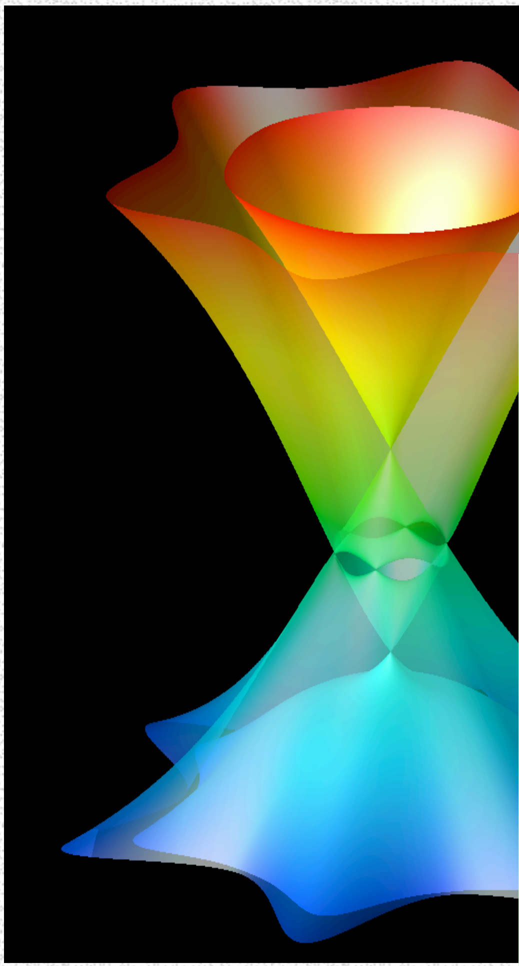
S. Murakami, New J. Phys. 9, 356 (2007).
S. Murakami, and S. Kuga PRB 78, 165313 (2008).

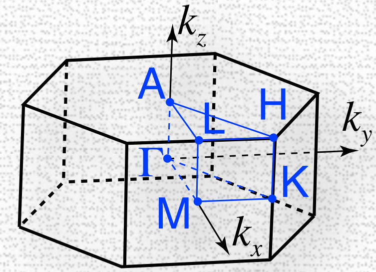
Monopole-Antimonopole creation/annihilation

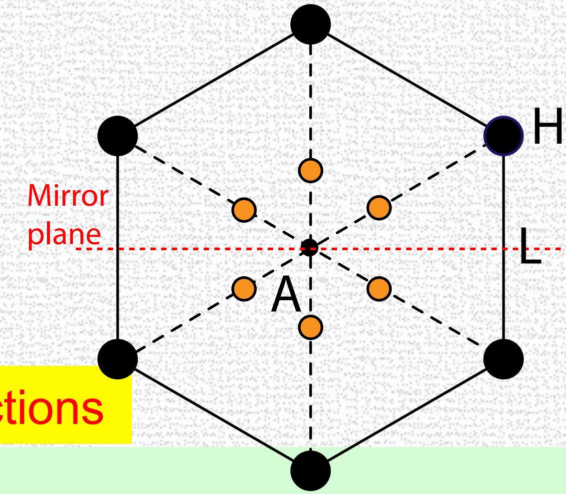


S. Murakami, New J. Phys. 9, 356 (2007).

Topological phase transition in BiTeI







Band touching along A-H directions

$$(k_x, k_z) = (0, \pi / c)$$

M: Mirror symmetry, *T*: Time reversal symmetry

$$M = i\sigma_y; \quad T = i\sigma_y K \Rightarrow \Omega = MT = K$$

$$\Omega H_{2\times2}(k_{yc}, P_c)\Omega^{-1} = H^{*}_{2\times2}(k_{yc}, P_c) = H_{2\times2}(k_{yc}, P_c)$$

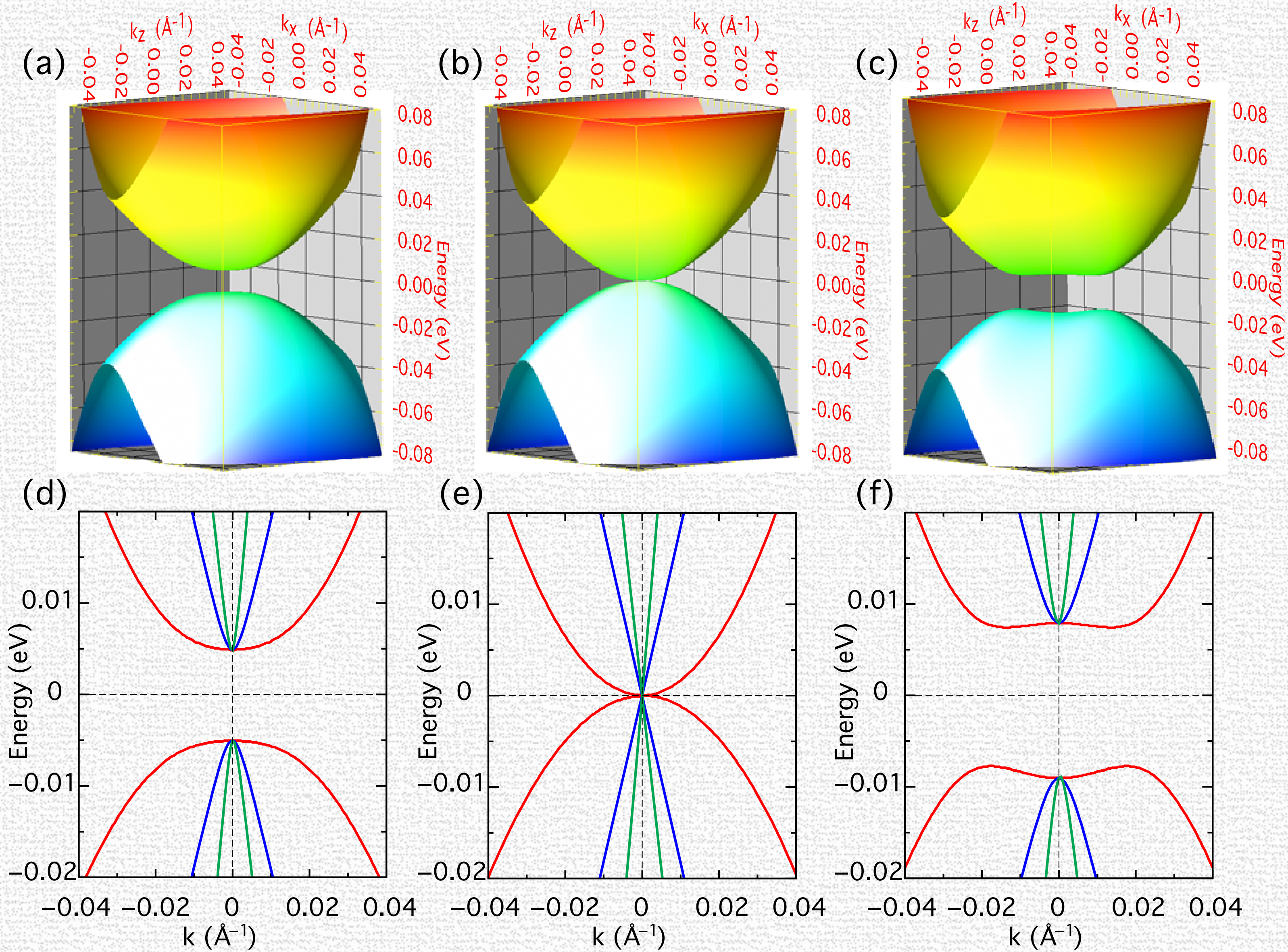
$$\Rightarrow f_2(k_{yc}, P_c) = 0$$

Remaining 2 conditions can be uniquely satisfied by k_{yc} and P_c

$$f_1(k_{yc}, P_c) = f_3(k_{yc}, P_c) = 0$$

MSB, B. –J. Yang, R. Arita, N. Nagaosa, Nature Commun. 3, 679 (2012).
B. –J. Yang, MSB, R. Arita, H. Isobe, E. Moon, N. Nagaosa, PRL 110, 086402 (2013).

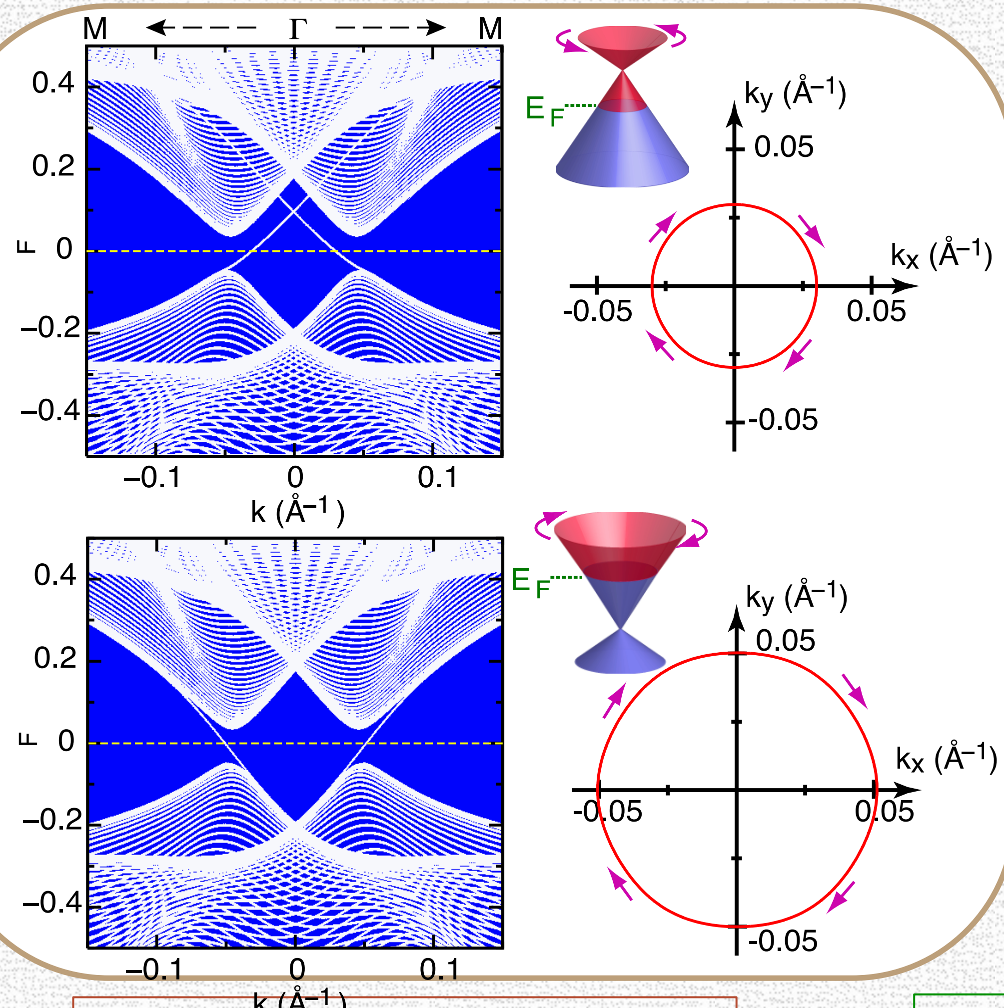
Evolution of band dispersions at band touching point



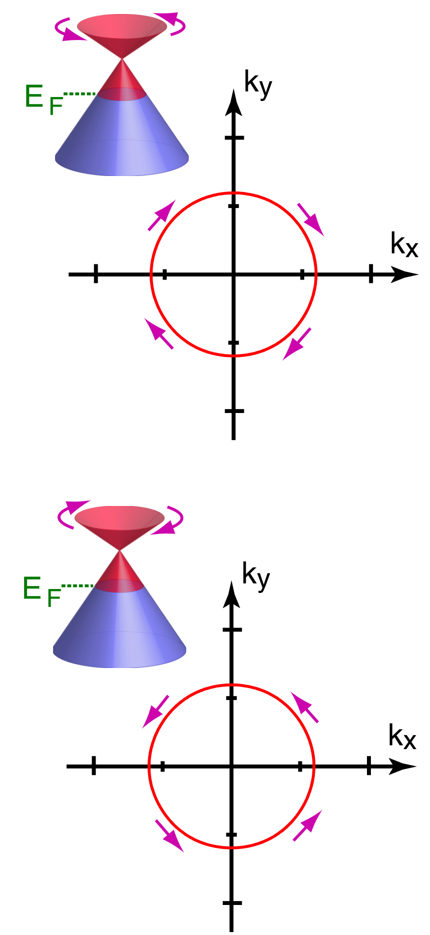
B. –J. Yang, MSB, R. Arita, H. Isobe, E. Moon, N. Nagaosa, PRL 110, 086402 (2013).

Comparison with centrosymmetric TI's

BiTeI



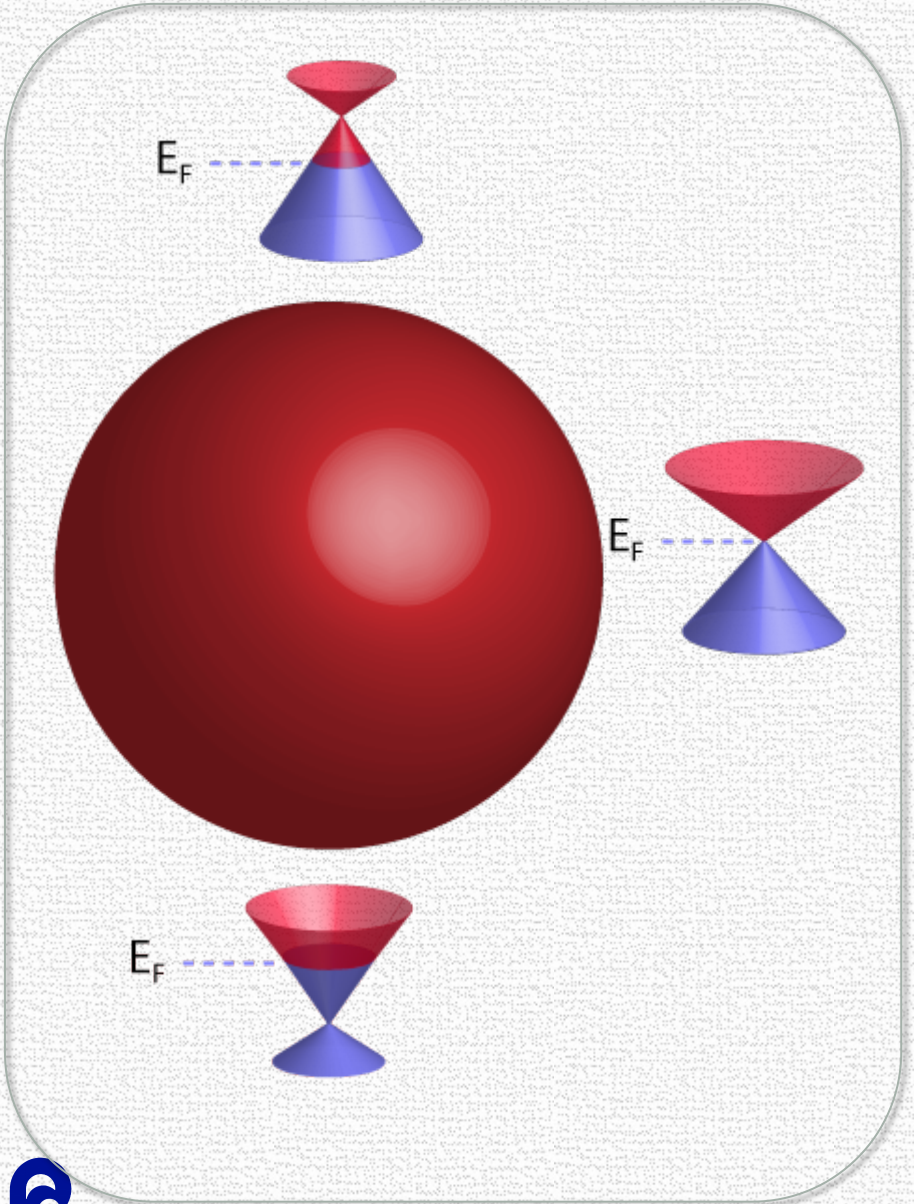
Centrosymmetric TI's

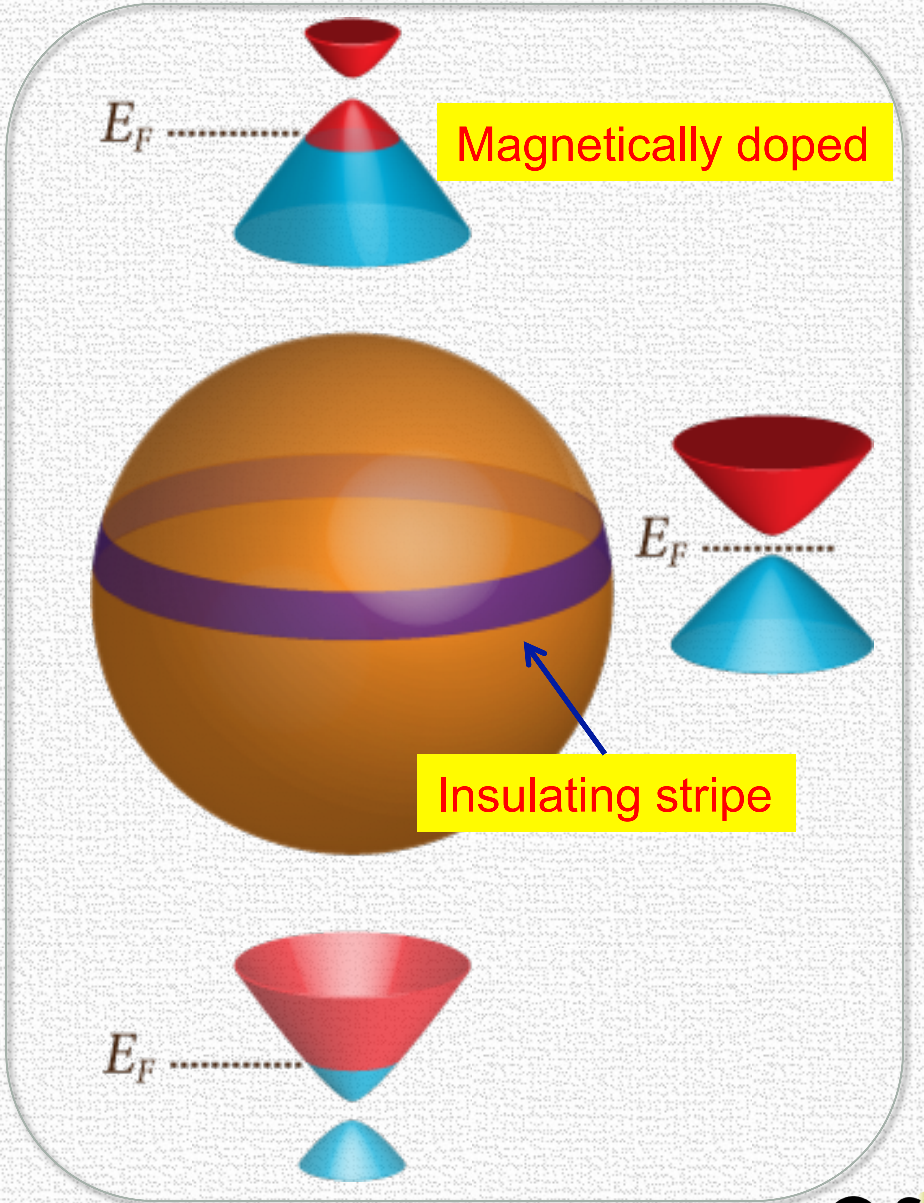


Different shapes
Similar spin helicities

Similar shapes
Different spin helicities

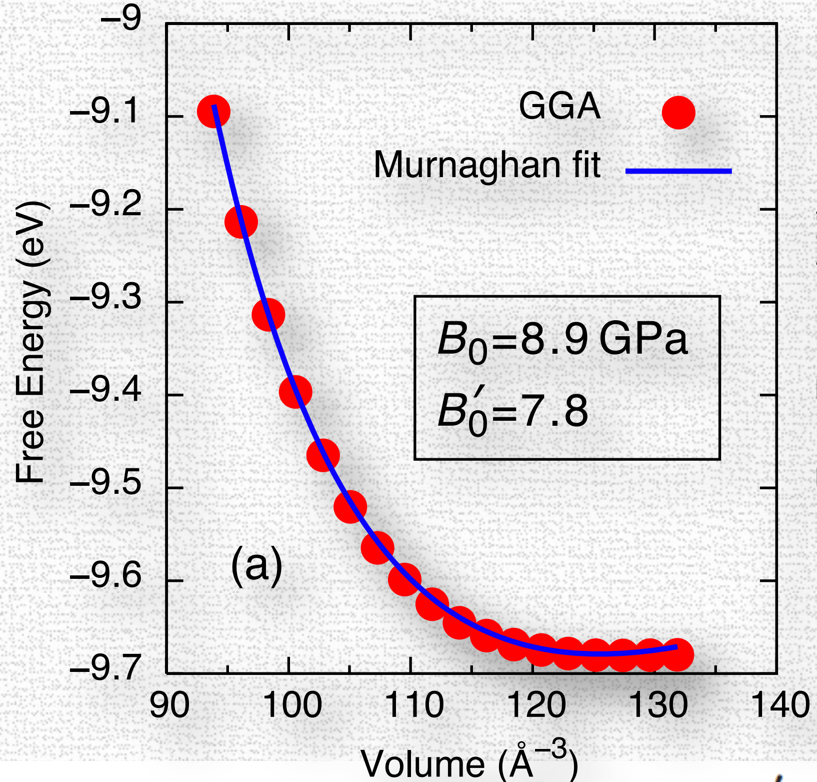
Evolution of Dirac cone on side surface

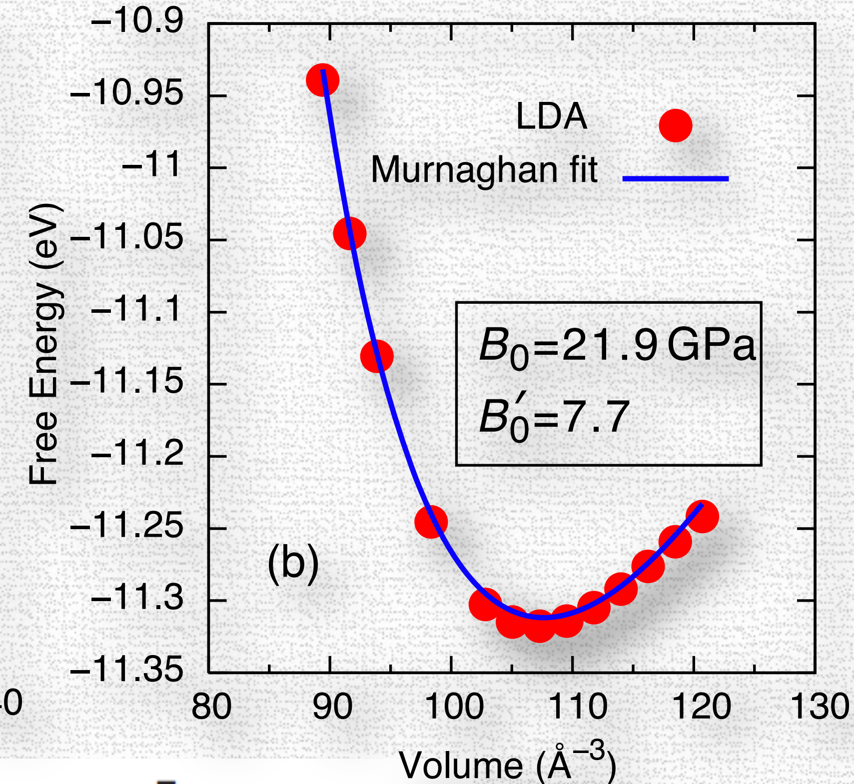




Assuming E_F is within the bulk band gap

Estimation of critical pressure





$$E(V) = E_0 + \frac{B_0 V}{B'_0}\left[\frac{(V_0/V)^{B'_0}}{B'_0 - 1} + 1\right] - \frac{B_0 V_0}{B_0\prime - 1}$$

$$P(V) = \frac{B_0}{B'_0}\left[\left(\frac{V_0}{V}\right)^{B'_0} - 1\right]$$

$$1.7\ GPa \leq P_c \leq 4.5\ GPa$$

Experimental demonstration

Observation of a Pressure-Induced Topological Quantum Phase Transition in BiTeI

Xiaoxiang Xi,[1] Chunli Ma,[2,3] Zhenxian Liu,[2] Zhiqiang Chen,[4]
Wei Ku,[5] H. Berger,[6] C. Martin,[7] D. B. Tanner,[7] and G. L. Carr[1]

[1]*Photon Sciences, Brookhaven National Laboratory, Upton, New York 11973, USA*
[2]*Geophysical Laboratory, Carnegie Institution of Washington, Washington D.C. 20015, USA*
[3]*State Key Laboratory of Superhard Materials, Jilin University, Changchun 130012, China*
[4]*Department of Geosciences, Stony Brook University, Stony Brook, New York, USA*
[5]*Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, New York 11973, USA*
[6]*Institute of Condensed Matter Physics, École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland*
[7]*Department of Physics, University of Florida, Gainesville, Florida 32611, USA*

(Dated: May 7, 2013)

We report the observation of a pressure-induced topological quantum phase transition in the polar semiconductor BiTeI using X-ray powder diffraction and infrared spectroscopy. The X-ray data confirm that BiTeI remains in its ambient-pressure structure up to 8 GPa. The lattice parameter ratio c/a shows a minimum between 2.0–2.9 GPa, indicating an enhanced c-axis bonding through p_z band crossing as expected during the transition. Over the same pressure range, the infrared spectra reveal a maximum Drude spectral weight, reflecting the closing and reopening of the semiconducting gap through band inversion. Both of these features are characteristics of a topological quantum phase transition, and are consistent with a recent theoretical proposal.

arXiv: 1305.0959v1

Conclusions

- BiTeX exhibit giant bulk Rashba spin splitting
- This effect leads to many novel phenomena (enhanced magneto-optical response, divergent dia/para-magnetism, spin-polarized photcurrent ….)
- BiTeI is expected to become a strong TI under pressure
- The material is expected to undergo an unusual topological phase transition