A New Look at Rashba-related Phenomena from Multi-orbital Perspective

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Collaboration

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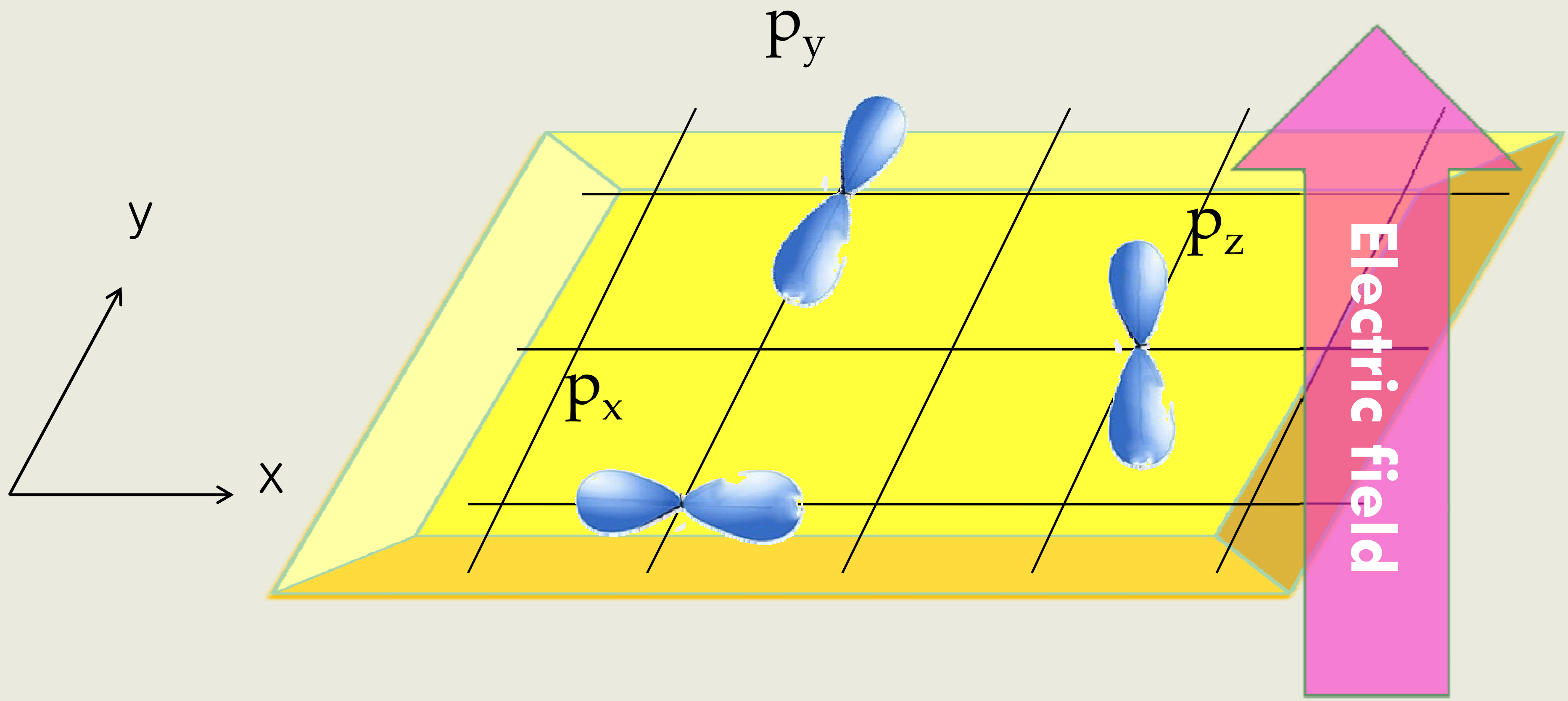
Ref: SR Park et al. PRL 107, 156803 (2011)
SR Park et al. PRL 108, 046805 (2012)
JH Park et al. PRB 85, 195401 (2012)
JH Park et al. PRB 87, 041301 (2013)
PJ Kim & JHH, PRB 87, 205119 (2013)

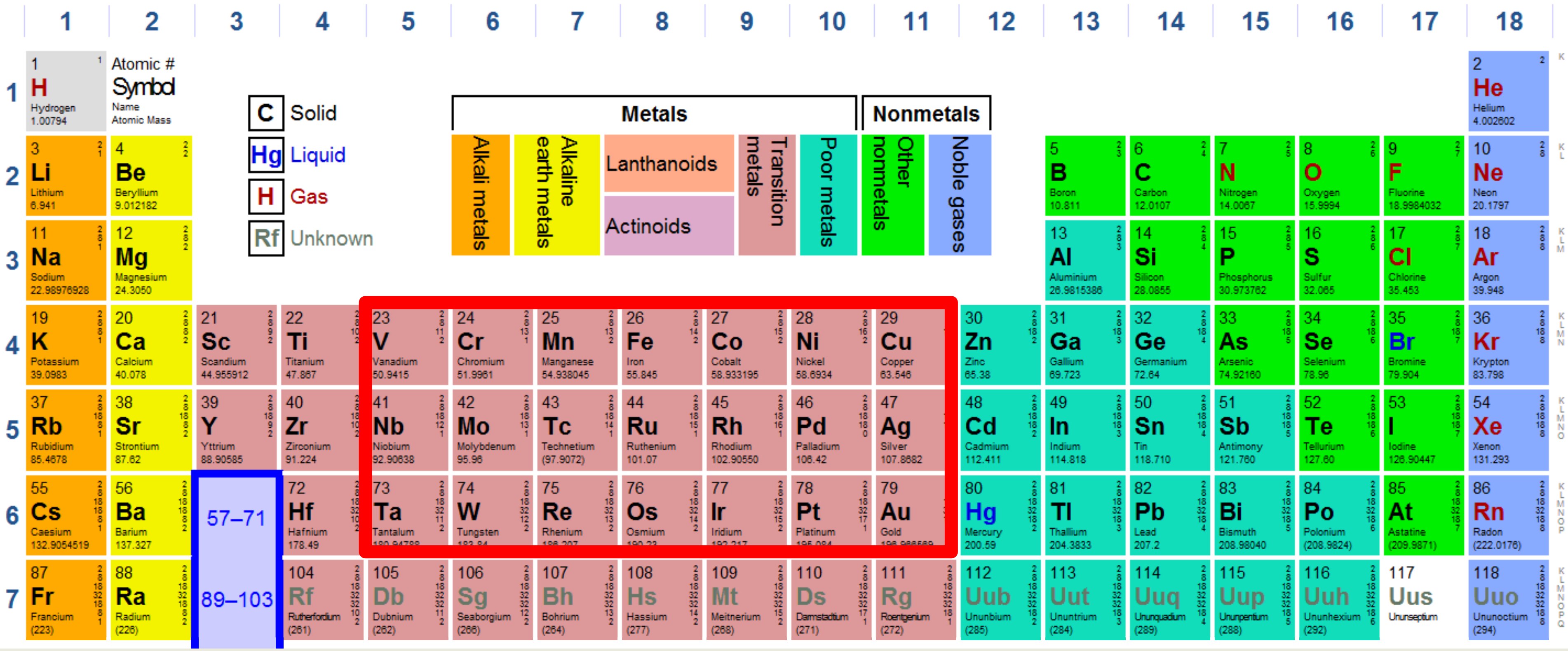
Ingredients



I. Multi-orbital electronic bands

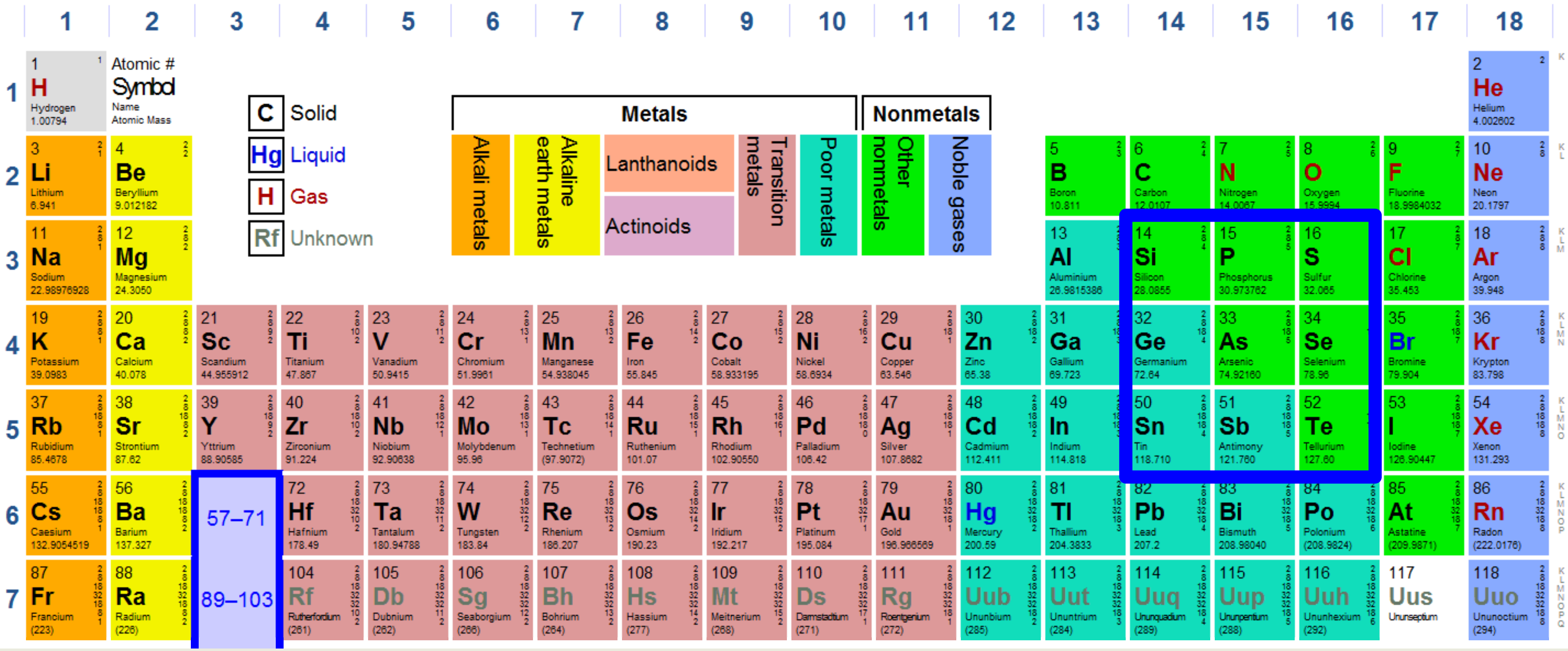
II. Surface (inversion symmetry breaking, E-field perpendicular to surface)

Examples I



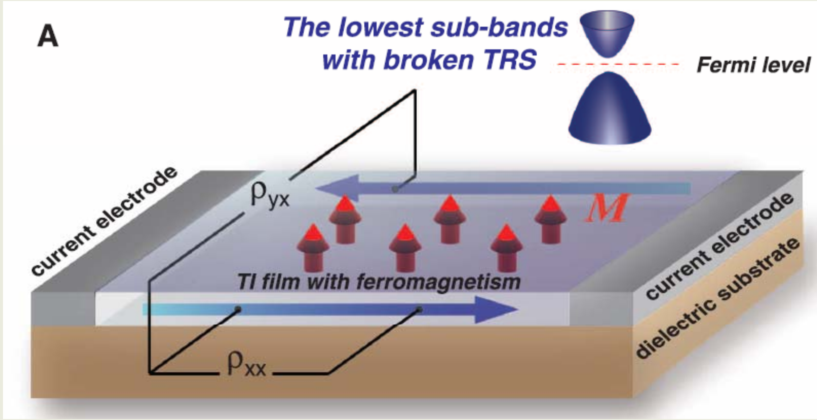
Transition metal surface (incomplete d-shells form multi-d-orbital bands)

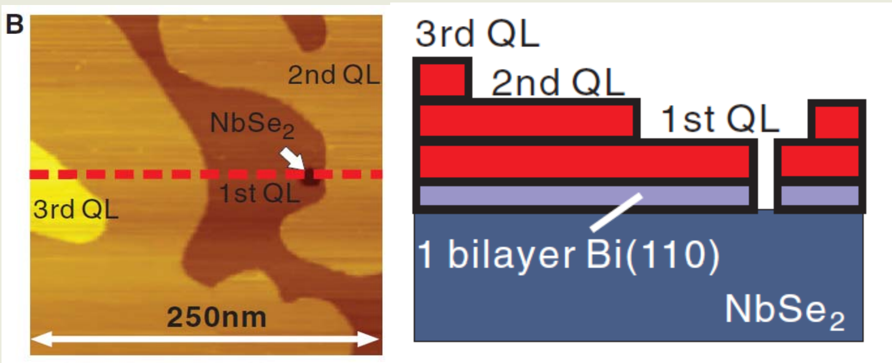
Examples II

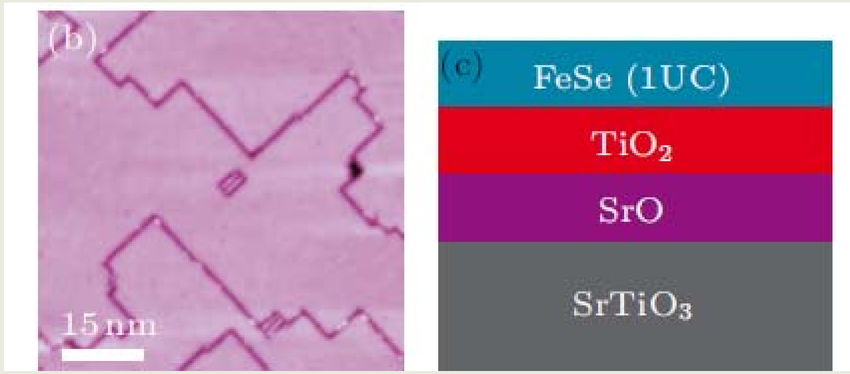


(metallic) surface of semiconductors

Recent examples (from Tsinghua)







Atomically thin layers of topological insulators (heavy p-orbitals) or iron pnictides (3d-orbitals)

Multi-orbital bands are quite ubiquitous; yet we hardly teach them in solid state classes.

The other overlooked subject, i.e. spin-orbit interaction, has been remedied of its neglect due to discovery of topological insulators

Multi-orbital bands are at least as ubiquitous as SOI

Multi-orbitality & SOI

$$H_{so} = L*S = L^z S^z + (L^+S^- + L^-S^+)/2$$

Orbital state: (L_z -> L_z+1 or L_z-1)
Spin state: (S_z -> S_z-1 or S_z+1)

Exchange of angular momentum between orbital and spin; in a single-orbital (L=0) situation this exchange cannot occur

Multi-orbitality is the pre-requiste for SOI. It is possible to consider multi-orbitality without SOI; the converse cannot be true

In the first part, SOI will be neglected (thus, Rashba effect will be neglected).

Later, we will re-visit Rashba effect from multi-orbital perspective

Symmetry & Band Structure

A. TR symmetry: $E_{\uparrow}(\mathbf{k}) = E_{\downarrow}(-\mathbf{k})$

B. Inversion symmetry: $E_{\uparrow}(\mathbf{k}) = E_{\uparrow}(-\mathbf{k})$

C. TR+I: $E_{\uparrow}(\mathbf{k}) = E_{\downarrow}(\mathbf{k})$

D. Crystal symmetry dictates symmetry of energy dispersion

$$E(k_x, k_y) = E(k_y, -k_x)$$

Symmetry & Band Structure

If certain symmetry is lost, a corresponding change in the Hamiltonian, hence the band dispersion, takes place

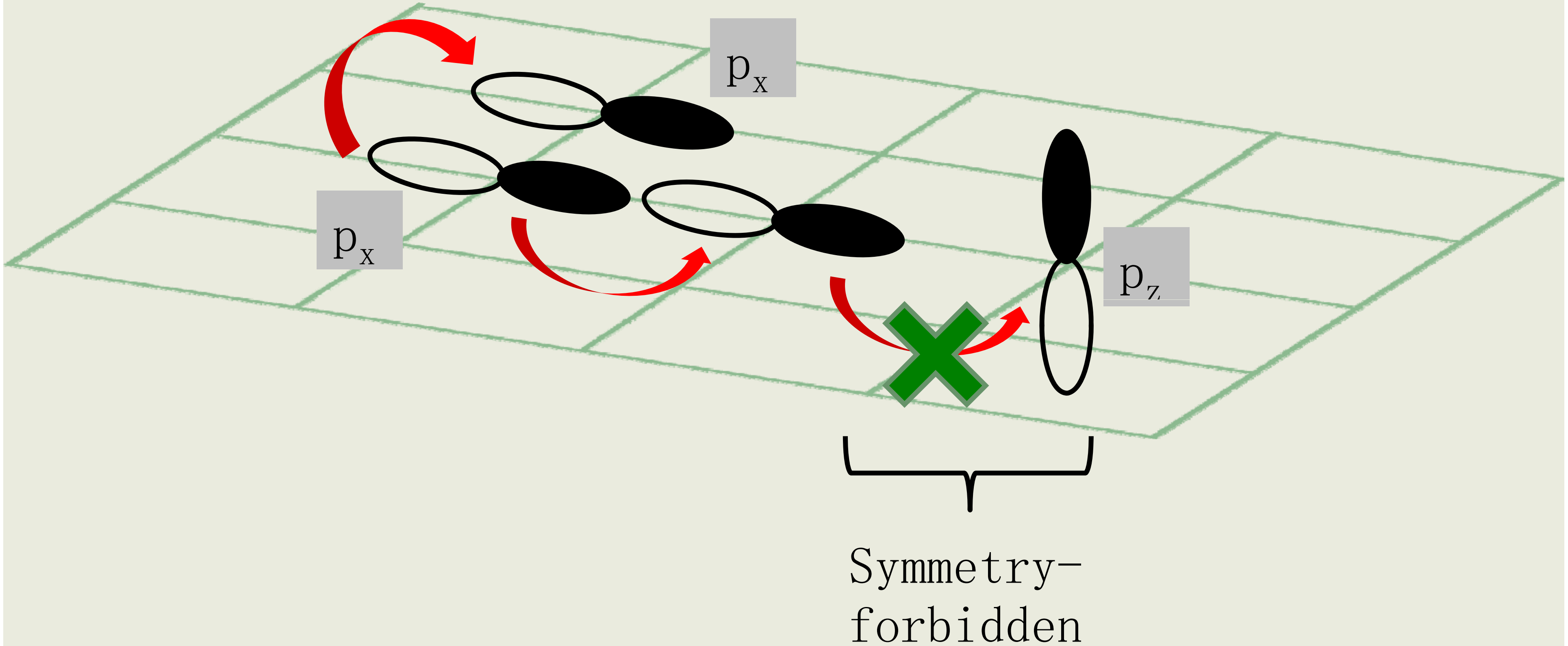
When inversion symmetry is lost (ISB), what happens to band structure?

Answer: Orbital Rashba effect

Conventional Rashba effect won't do because we neglected SOI (spinless fermions, basically)

Tight-binding (Microscopic) View of ISB

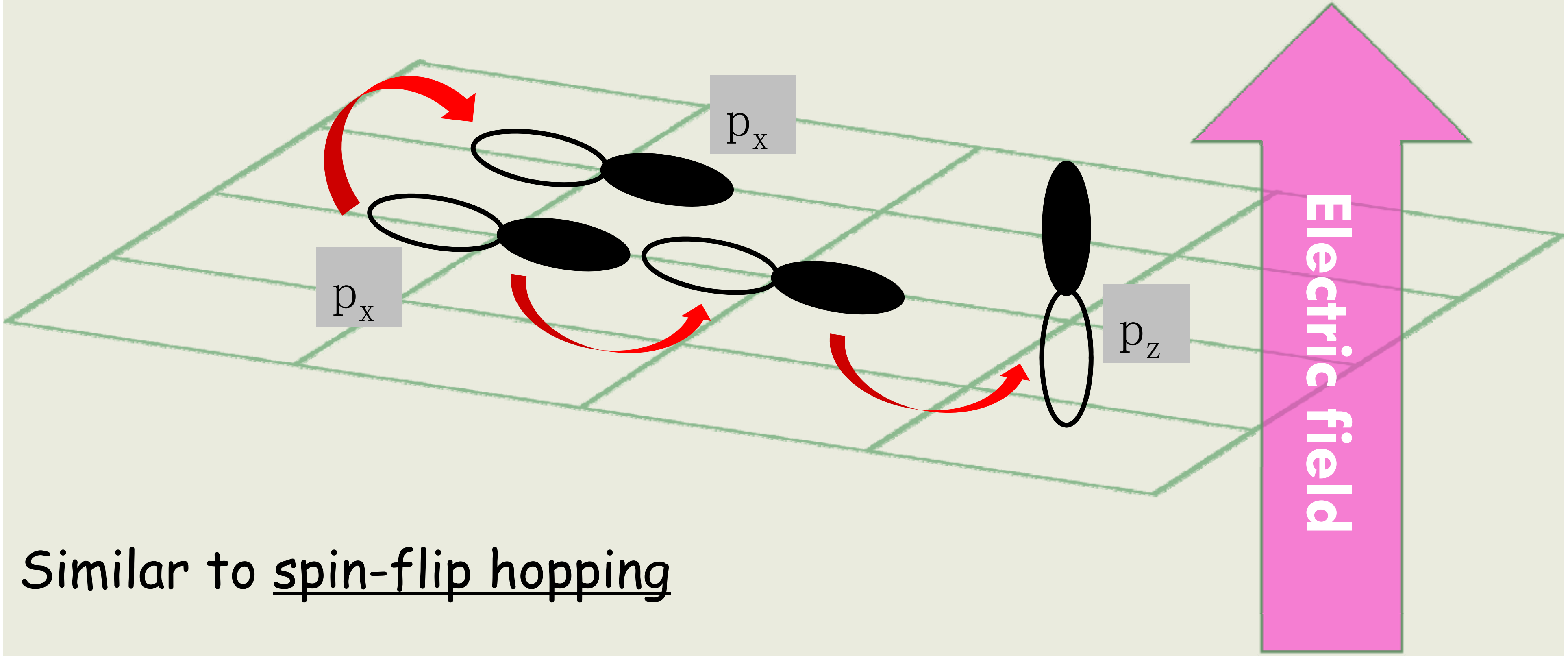
In a p-orbital system without ISB, p_x-, p_y-, p_z-orbital bands are all separate because one orbital state cannot hop onto (hybridize with) any other orbitals



Petersen&Hedegard, Surf. Sci. (2000); JH Park et al. PRB (2012)

Tight-binding (Microscopic) View of ISB

Once inversion symmetry breaking (ISB) occurs by electric field, p_z hybridizes with p_x, p_y



Similar to spin-flip hopping

(p_z has L_z=0, p_x p_y has L_z=+1 and L_z=-1)

Petersen&Hedegard, Surf. Sci. (2000); JH Park et al. PRB (2012)

Some new terms appear due to allowed mixing

$$\begin{pmatrix} 2(V_2c_y - V_1c_x) & 0 & -3\gamma i s_x \\ 0 & 2(V_2c_x - V_1c_y) & -3\gamma i s_y \\ 3\gamma i s_x & 3\gamma i s_y & 2V_2(c_x + c_y) \end{pmatrix}$$

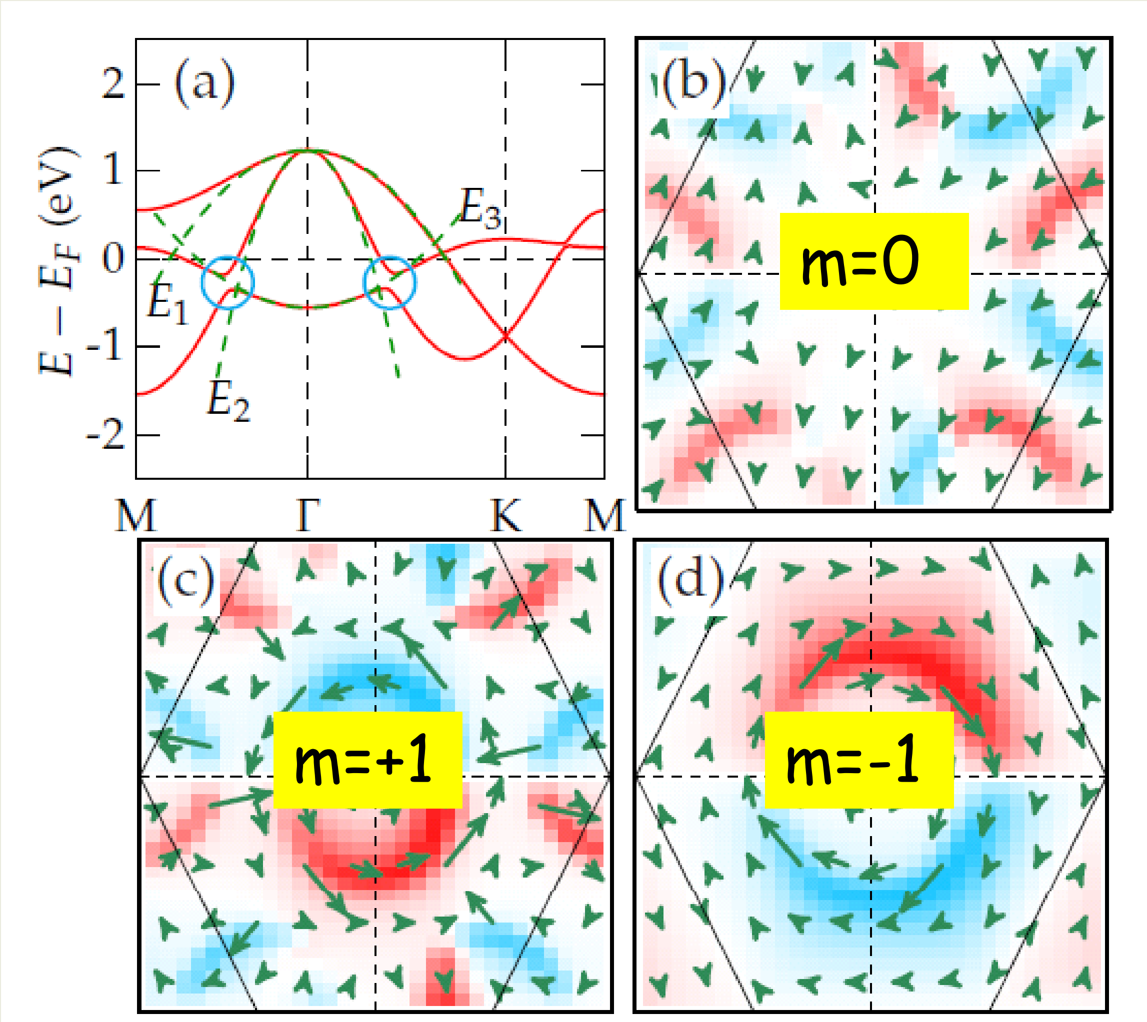
$$H_{\text{ISB}} \sim \gamma(\sin k_x L_y - \sin k_y L_x)$$

$$\sim \gamma(\hat{z} \times \mathbf{k}) \cdot \mathbf{L}$$

L=orbital angular momentum operator (OAM) in p-orbital basis
γ = a measure of ISB

Note the COMPLETE ANALOGY to spin Rashba term!

Hence, we call it orbital Rashba effect

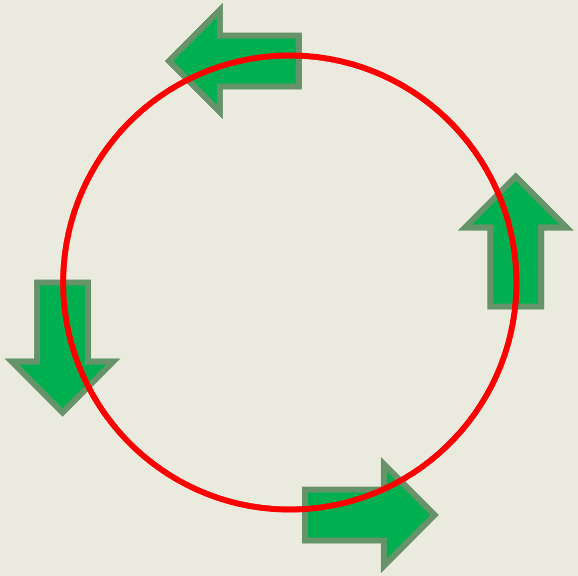


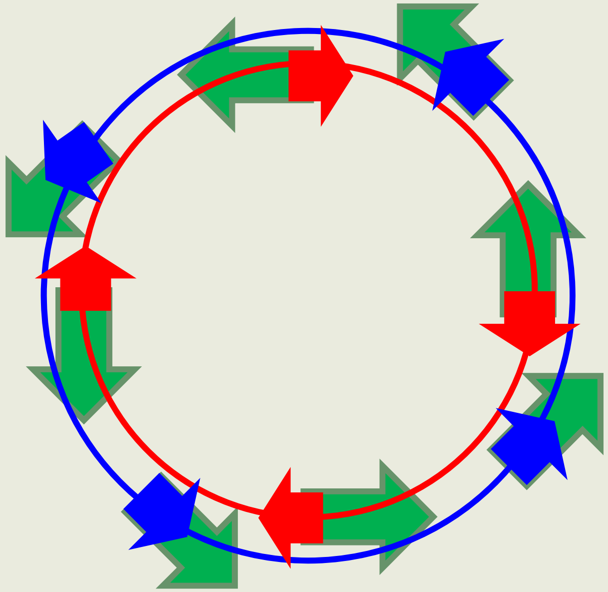
$$H_{\mathrm{ISB}} \sim \gamma(\hat{z} \times \mathbf{k}) \cdot \mathbf{L}$$

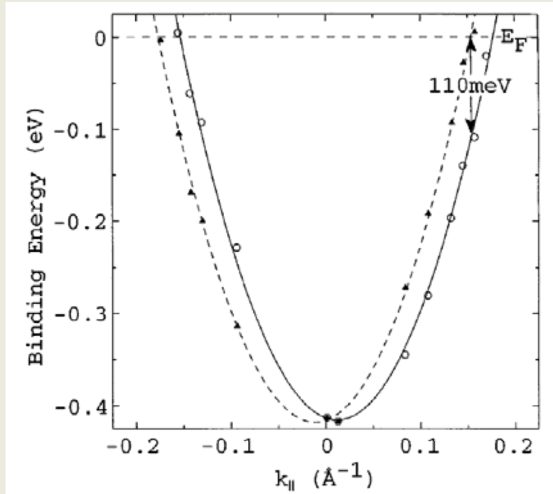
One band with CCW OAM (m=+1),
One band with CW OAM (m=-1),
One band with zero OAM (m=0).

Where is Rashba (as we know it)?

Restore spin, each band is doubly degenerate







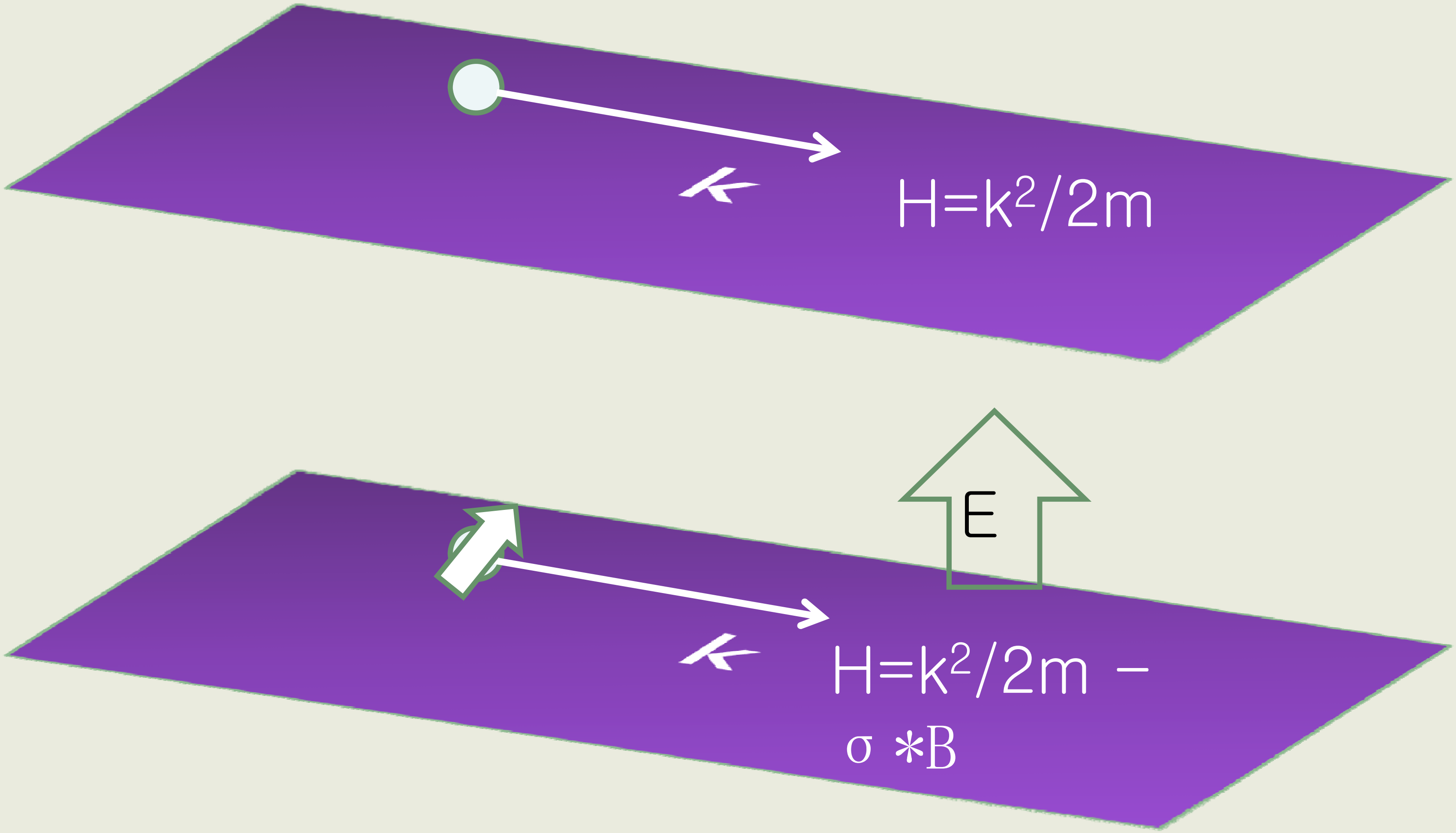
Introduce $H_{SOI} \sim L^*\sigma$, project onto the degenerate state

$$P(k)\, H_{SOI}\, P(k) \sim (k x z)^* \, \sigma$$

This is Rashba !

Orbital Rashba is the PRE-REQUISITE for spin Rashba!

Where it went wrong with free-electron explanation of spin
Rashba effect



$B = v \times E = k \times E/m$

Relativistic effect forces electrons to see E-field as B-field and experience Zeeman splitting

$$H = \frac{\mathbf{k}^2}{2m} + \lambda_{\mathsf{R}}(\boldsymbol{\sigma} \times \hat{z}) \cdot \mathbf{k}$$

Rashba scale is very small:

$$\lambda_{\mathsf{R}} \sim (\alpha_B \alpha_f)^2 e$$

$$H_{\mathsf{R}} \sim (\alpha_f)^2 \times W$$

Relativstic free-electron argument is irrelevant

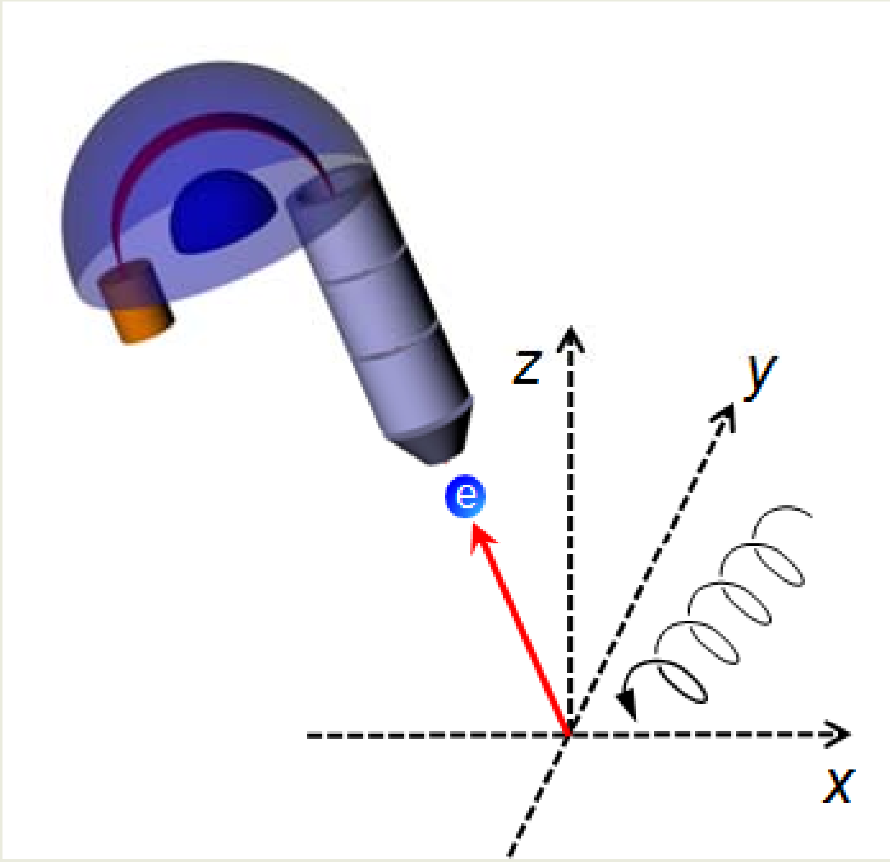
How to detect chiral OAM

Circular Dichroism ARPES

- Polarized source light (RCP/LCP) in ARPES

- RCP/LCP lights give different intensities

- Map of D(k) = (RCP-LCP)/(RCP+LCP)



Theory of Circular Dichroism

- Matrix element ~ <F|p*A|I> ~ <F|r*A|I>
- LCP/RCP lights are given by A and A*

- $D(k)=(I_{RCP}(k)-I_{LCP}(k))/(I_{RCP}(k)+I_{LCP}(k))$

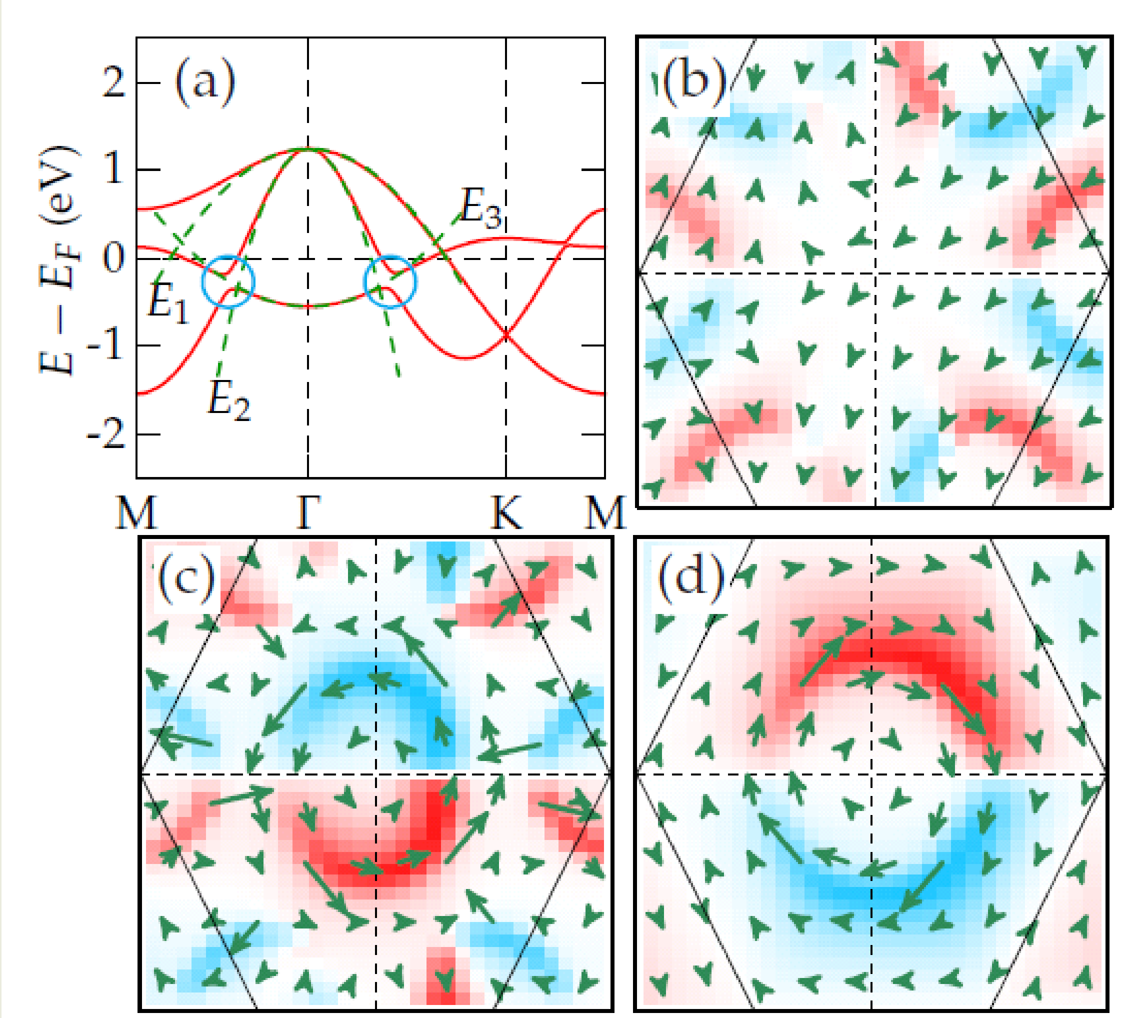
- D(k) is proportional to OAM average of the initial state

$$D(k) \sim F_{ij}(E_f)\,(k_{ph})_i \langle k|\, L_j \,|k\rangle$$

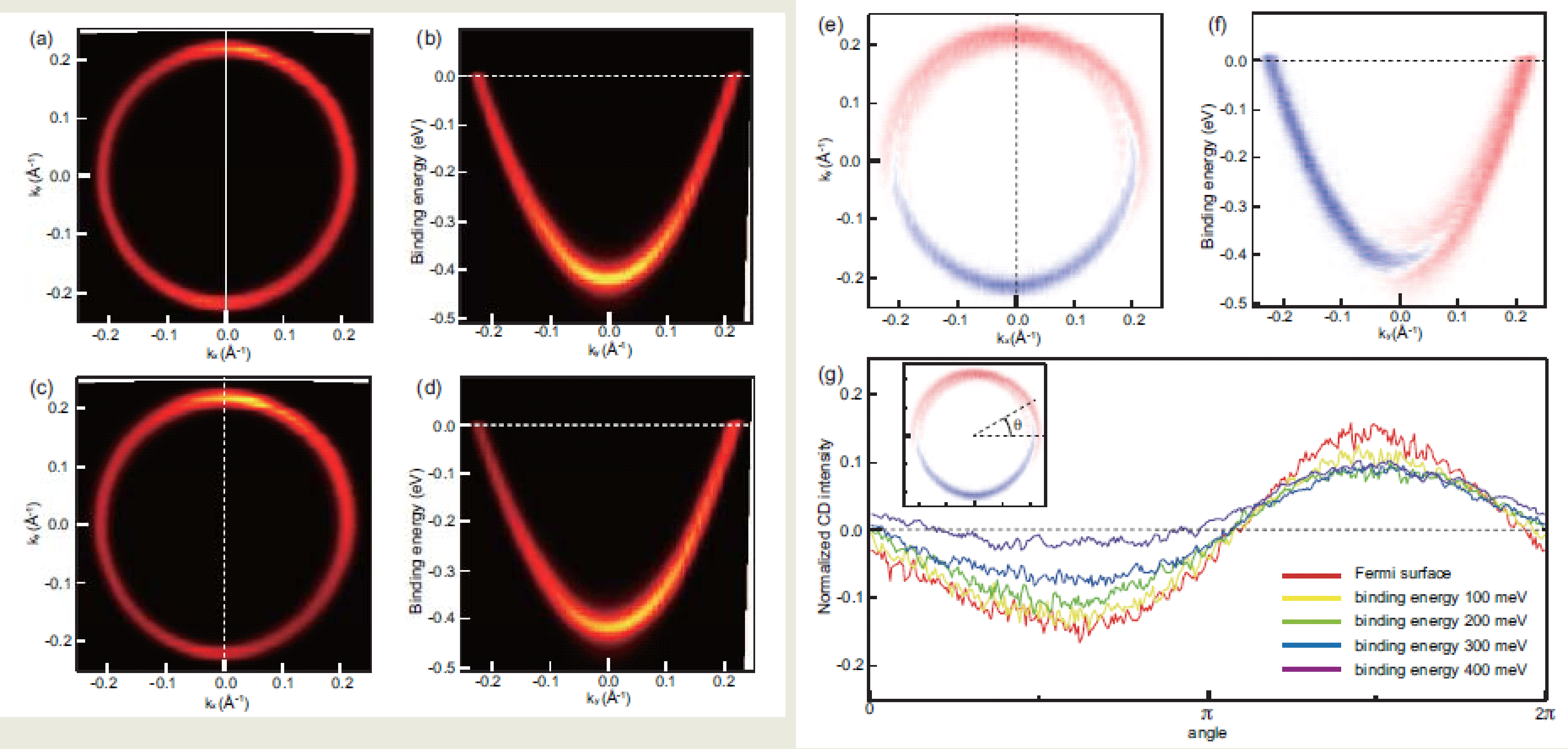
- True for p- and d-orbitals (presumably for any multi-orbital band structure)

SR Park et al PRL (2012); JH Park et al. PRB (2012)

Circular Dichroism Map

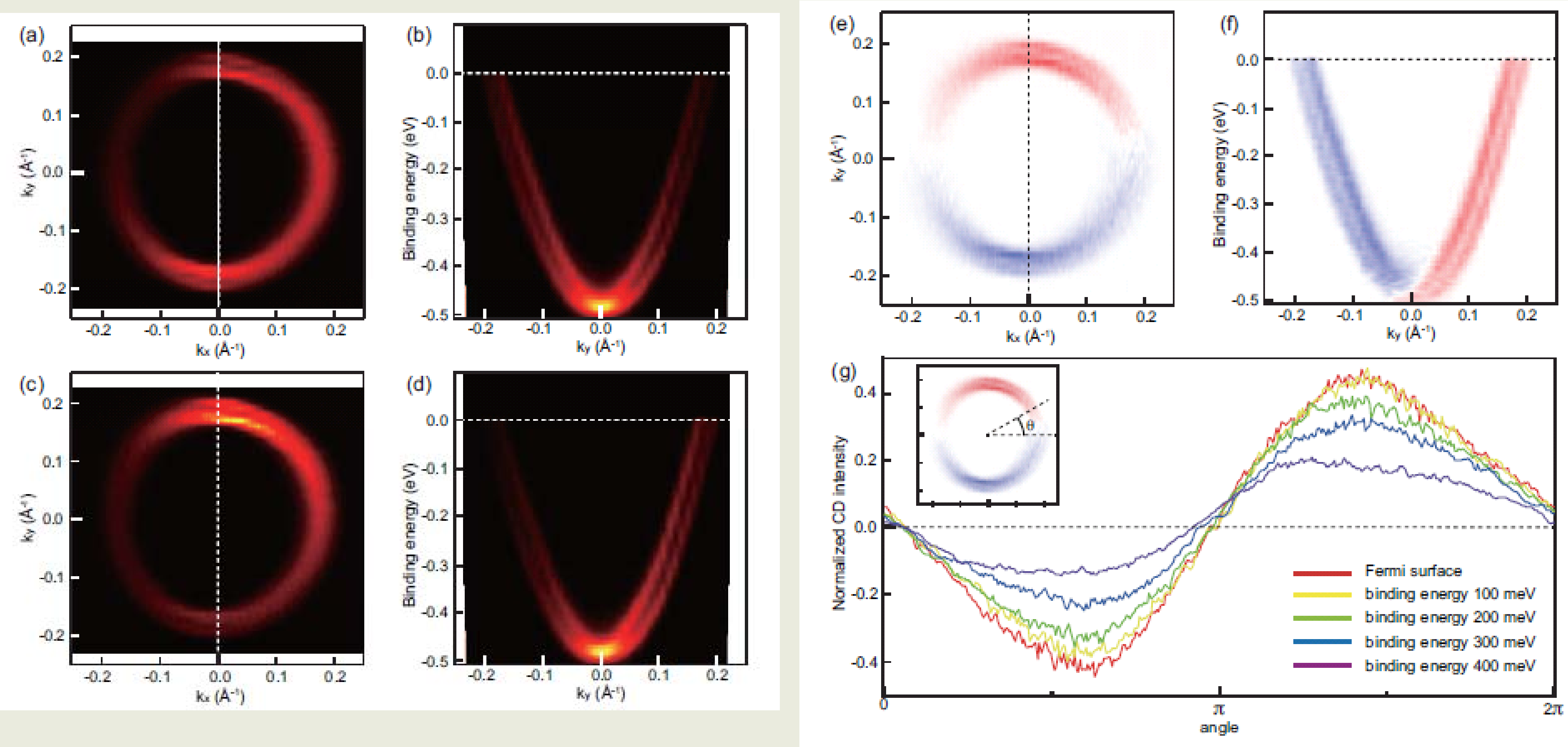


Testing it Out on Cu (weak SOI)



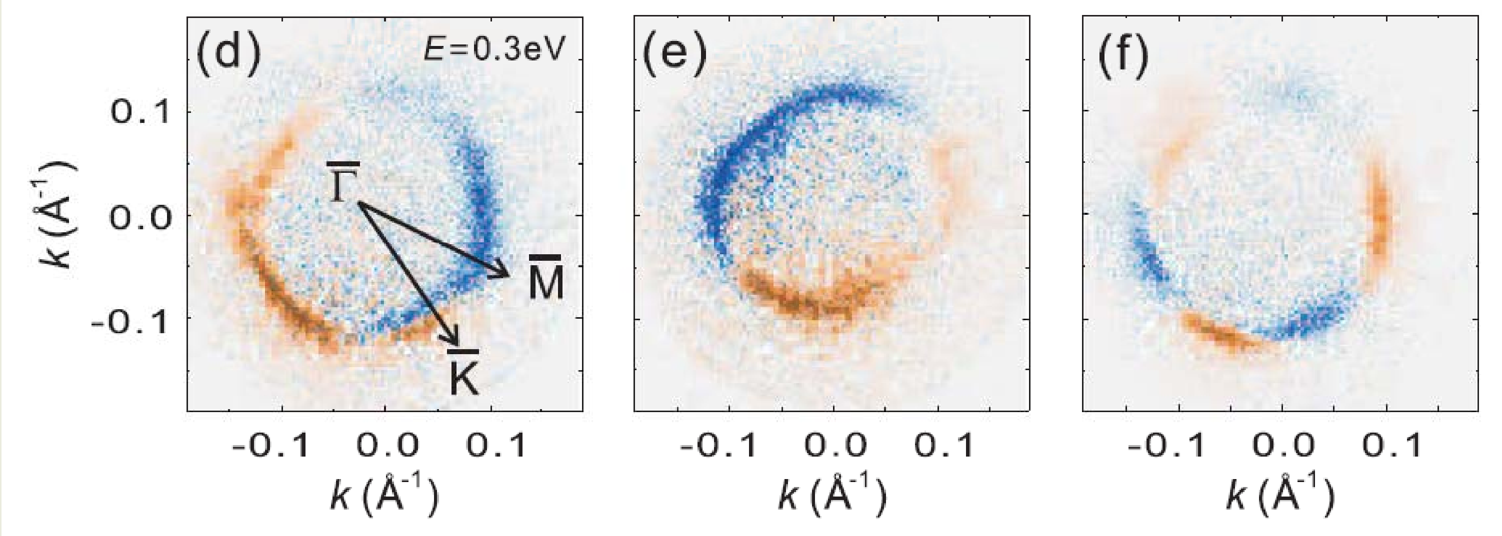
- PRB (2012) Yonsei group

Testing it Out on Au (medium SOI)

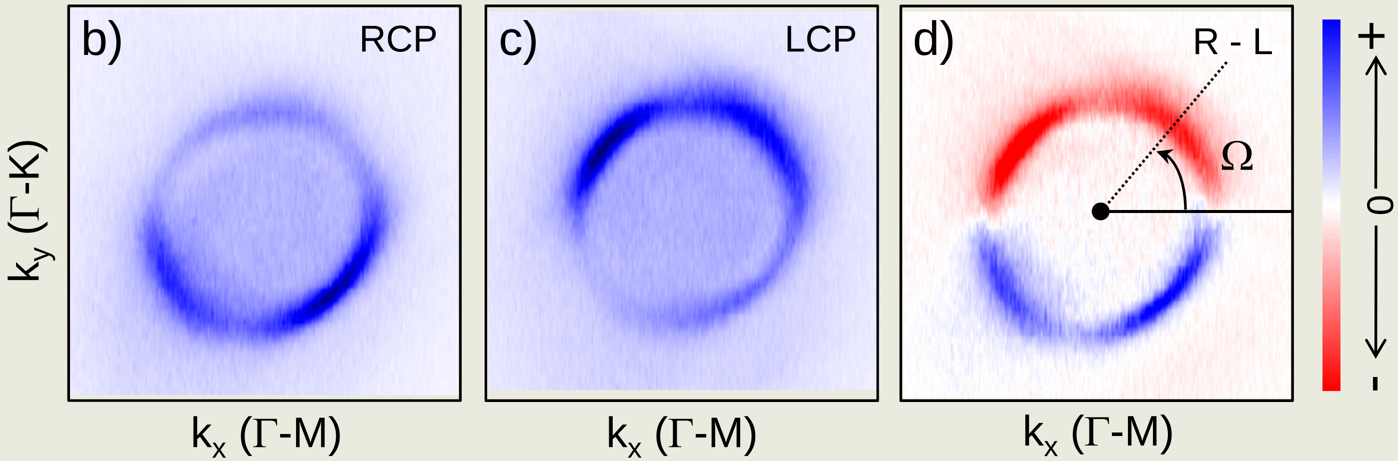


•PRB (2012) Yonsei group

Bi_2Se_3 (strong SOI)



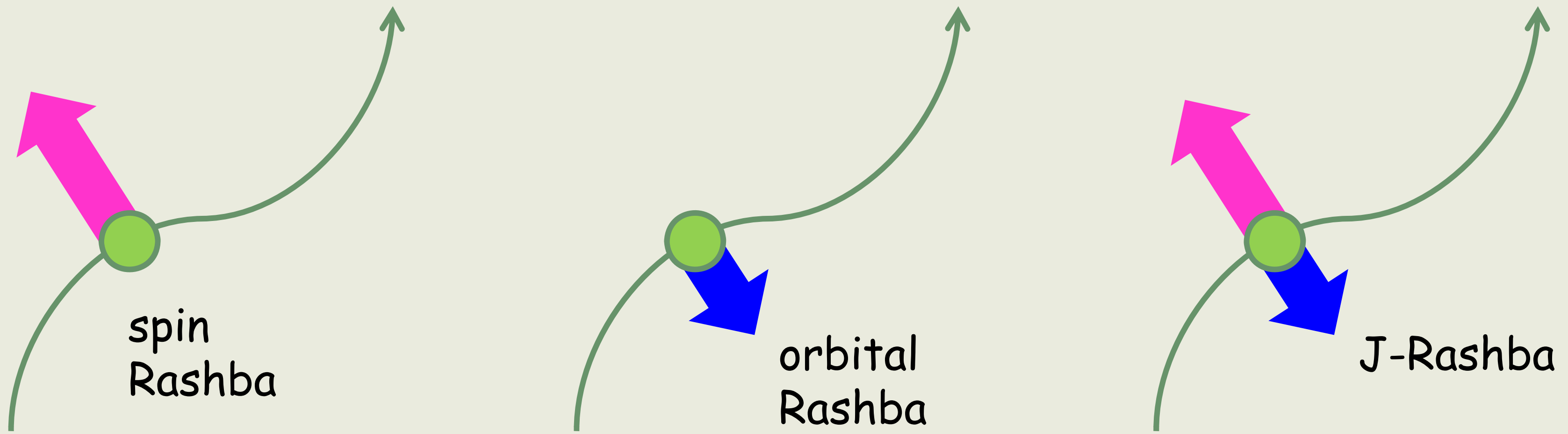
•MIT group, PRL (2011)



•Yonsei group, PRL (2012)

Since the first reports of circular dichroism on Bi_2Se_3 surface by MIT, Yonsei, Tokyo, another half-dozen PRL papers appeared on observation of CD on Bi_2Se_3 surface with varying interpretations

Practical question:
Is it spintronics, orbitronics, or J-tronics?



Next, I discuss other applications of orbital Rashba idea

I. ISB+Kondo: p-wave Kondo phase

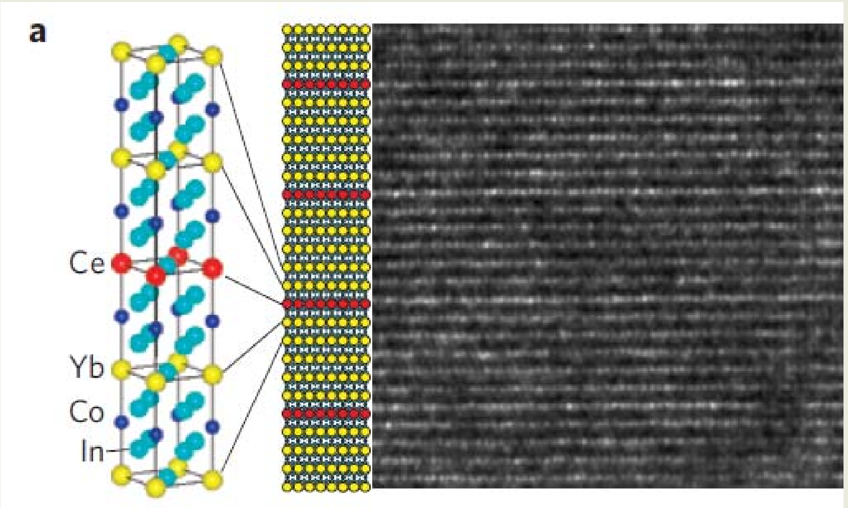
II. ISB+Hubbard interaction: orbital analogue of Dzyaloshinskii-Moriya interactioin

III. ISB+magnetism: OAM-dependent spin-transfer torque

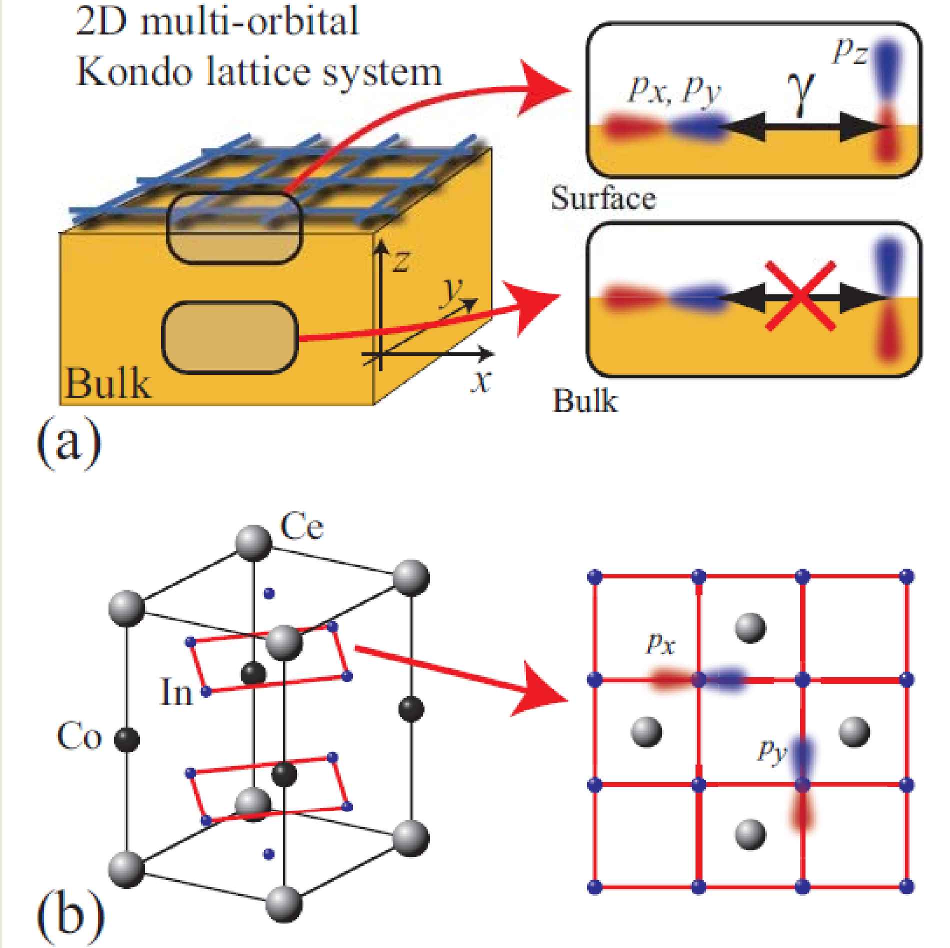
Application 1: Ultrathin Kondo lattice

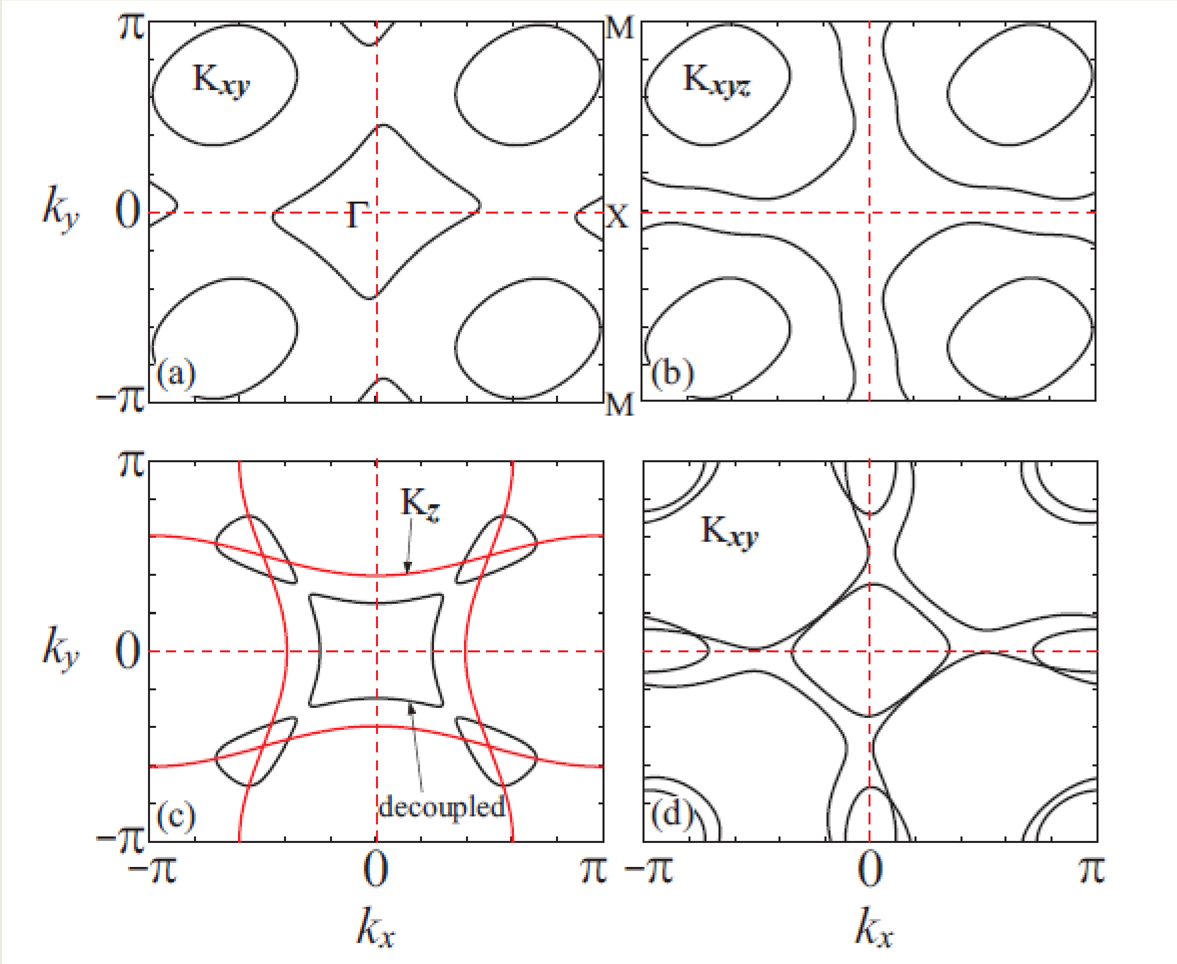
Emergent p-wave Kondo Coupling in Multi-orbital Bands with Mirror Symmetry Breaking

Jun Won Rhim[1] and Jung Hoon Han[2,3]



- Heavy-fermion heterostructure grown by Kyoto group





- •Over some parameter space we found Kondo-coupled band structure with only two-fold symmetry

- • Effective Kondo coupling has p-wave (not s-wave) symmetry due to nonzero ISB

Application 2: Orbital DM exchange

•Logic:

	Spin	Orbital
Inversion symmetry breaking	Spin Rashba effect	Orbital Rashba effect
ISB + strong interaction	Spin DM from superexchange	Orbital DM from multi-orbital superexchange

PHYSICAL REVIEW B, VOLUME 64, 212405

Order from disorder: Quantum spin gap in magnon spectra of $LaTiO_3$

G. Khaliullin

PHYSICAL REVIEW B **68**, 205109 (2003)

Theory of orbital state and spin interactions in ferromagnetic titanates

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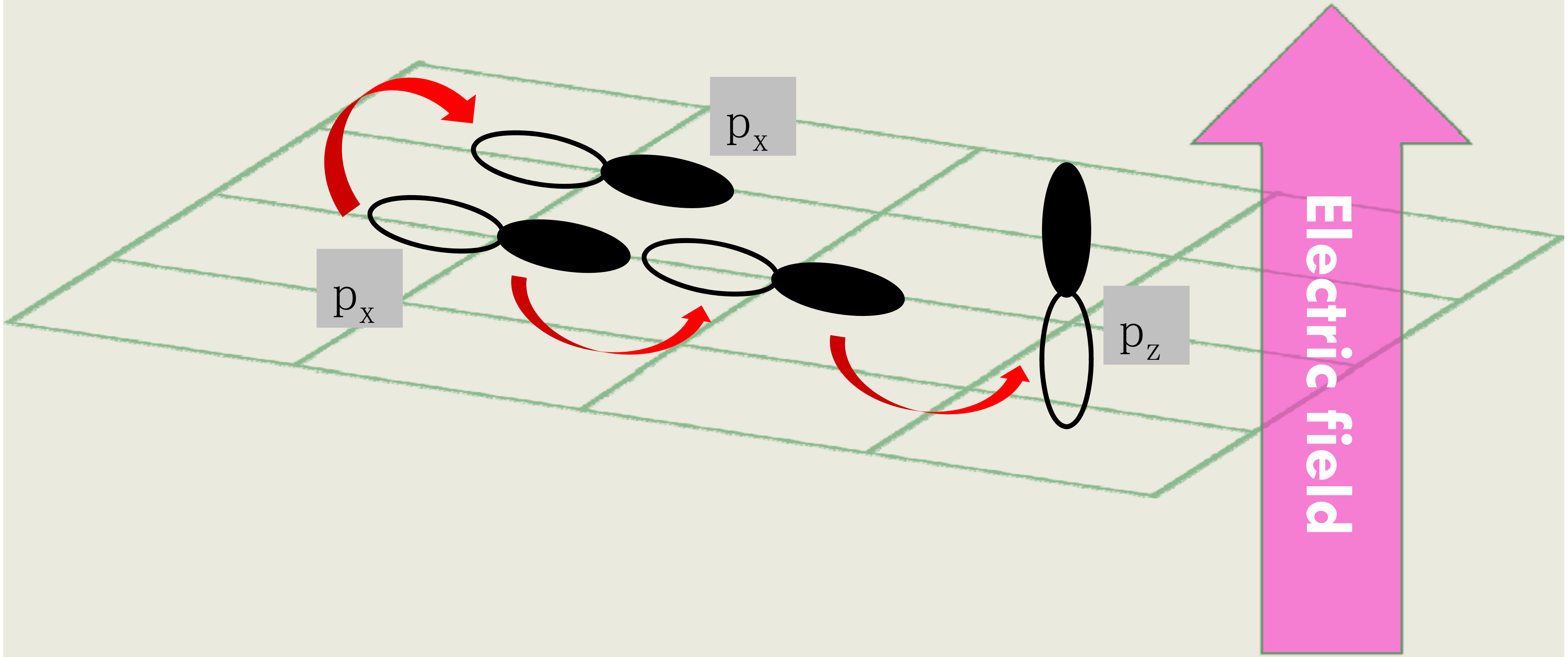
The Institute of Physical and Chemical Research (RIKEN), Saitama 351-0198, Japan

(Received 13 July 2003; published 24 November 2003)

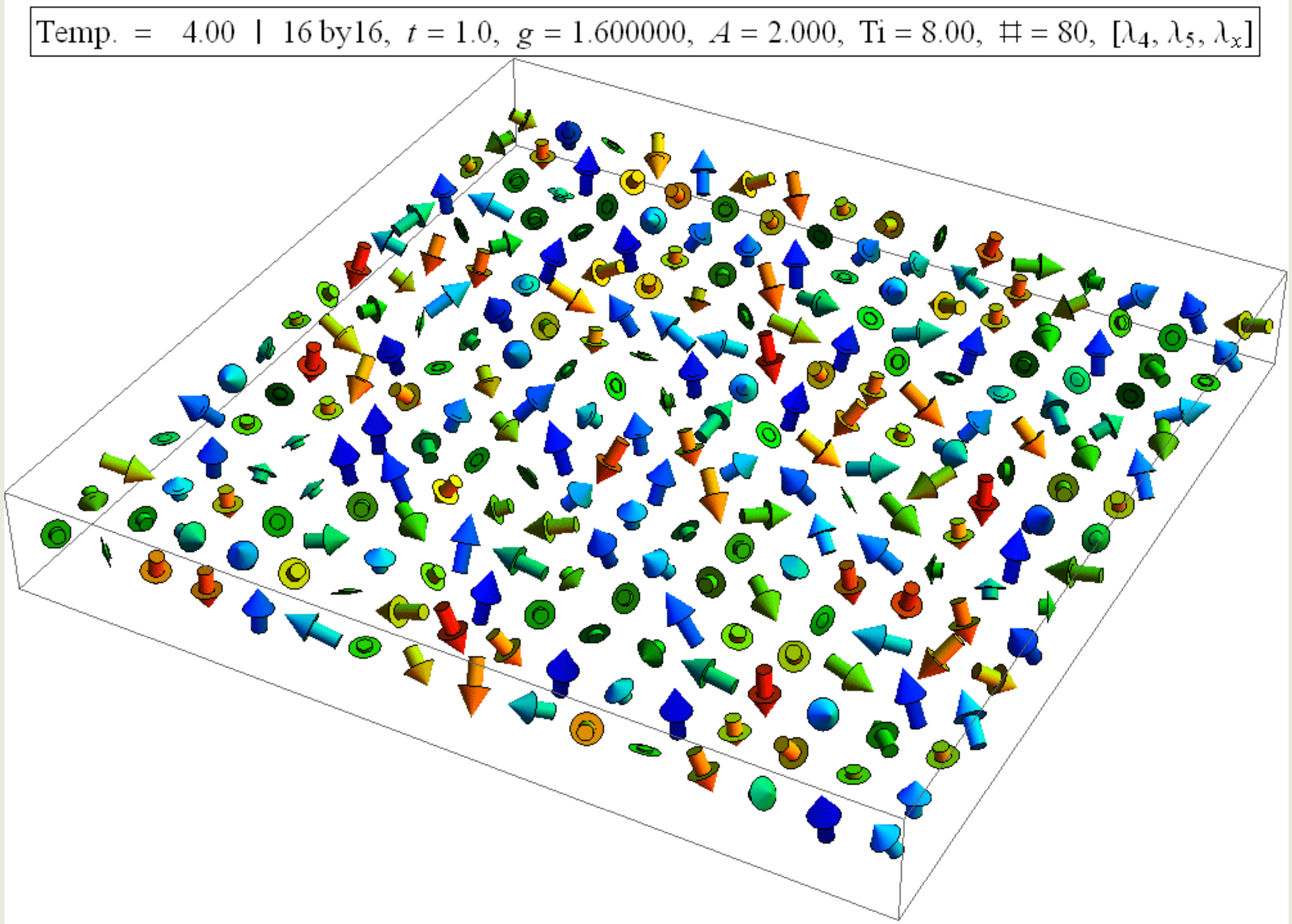
Same model as before



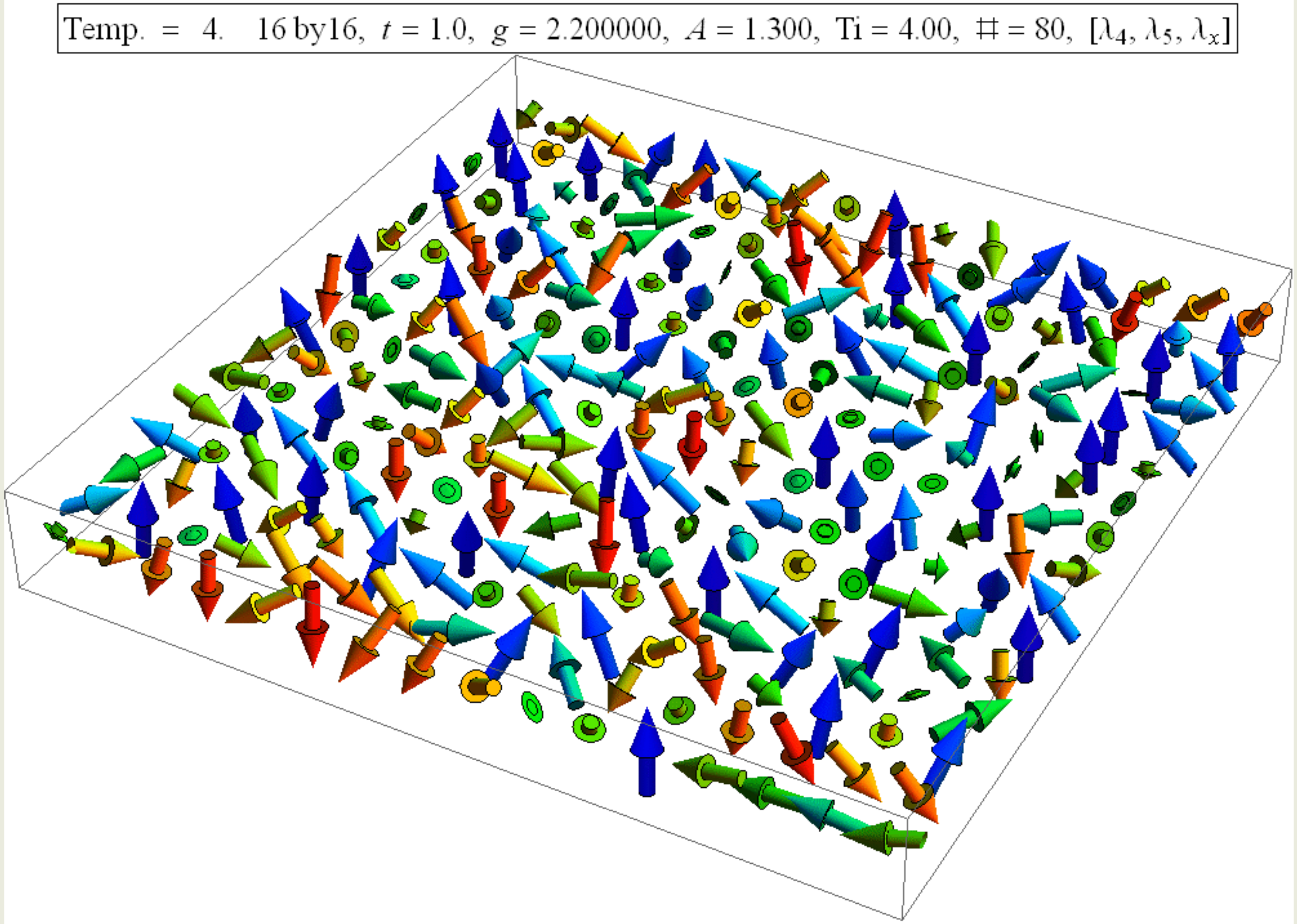
Add Hubbard interaction at every site and do superexchange calculation

Extension of Khaliullin's work to ISB situation

Orbital helix:

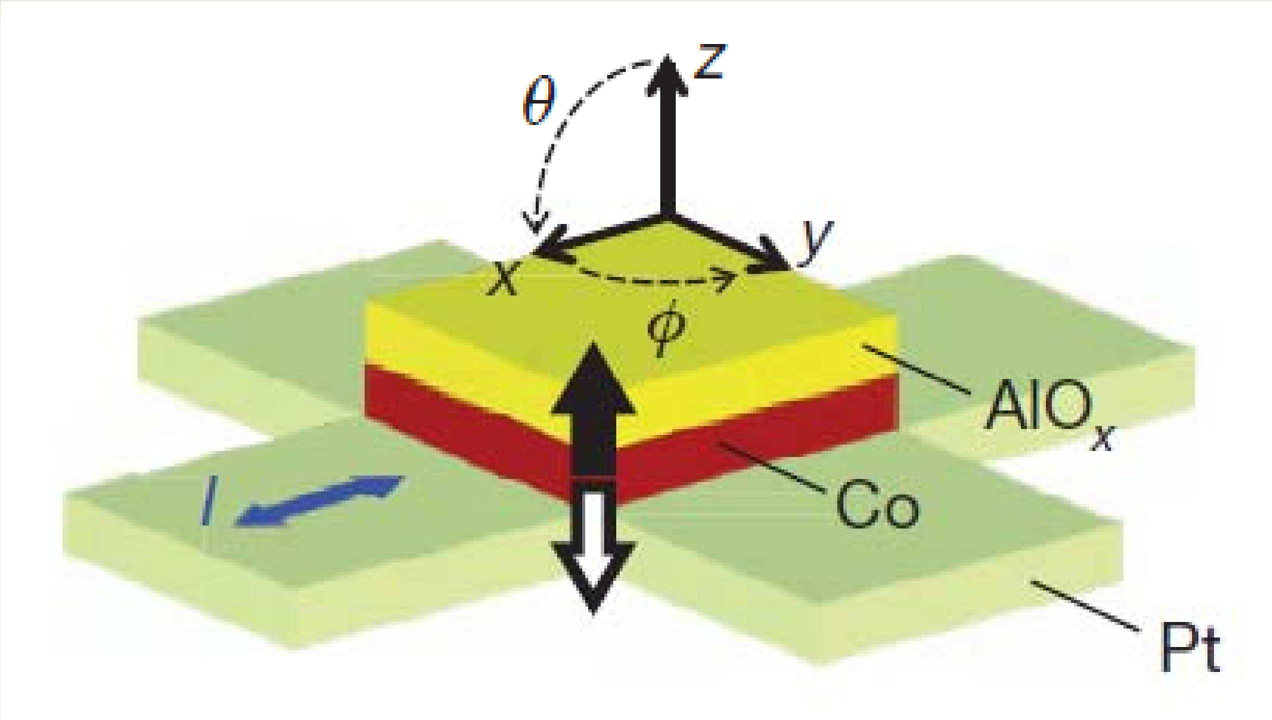


Orbital double-helix (~Skyrme crystal):



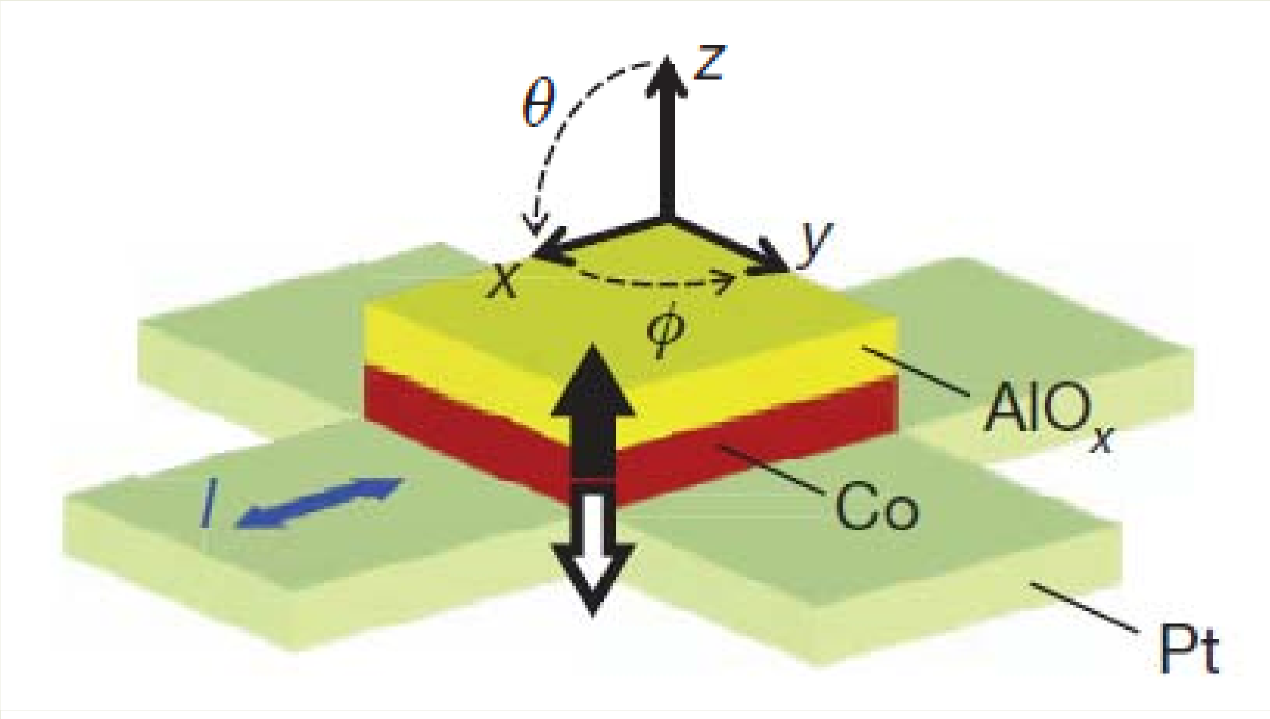
Application 1: Ultrathin Spintronics

• Atomic magnetic layer (< 1nm) between insulating and Pt layers (SPINTEC group, Cornell group)



• A new type of spin transfer torque due to Rashba effect proposed and detected (a blue ocean of spintronics!)

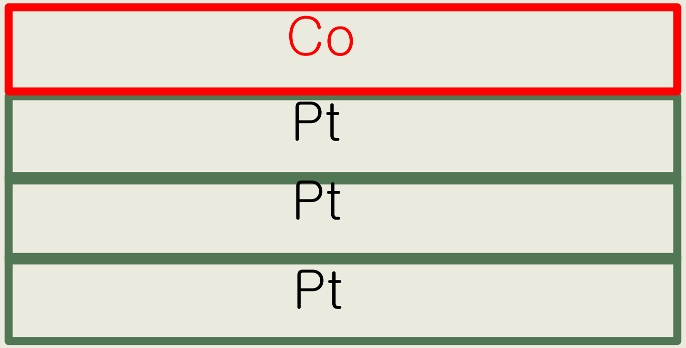
• Both the size and sign of STT vary greatly among samples (like Hall coefficients)



• We propose the notion of band-specific Rashba coefficient

•It is the Rashba coefficient that determines the sign of STT

LDA calculation for ultrathin magnet

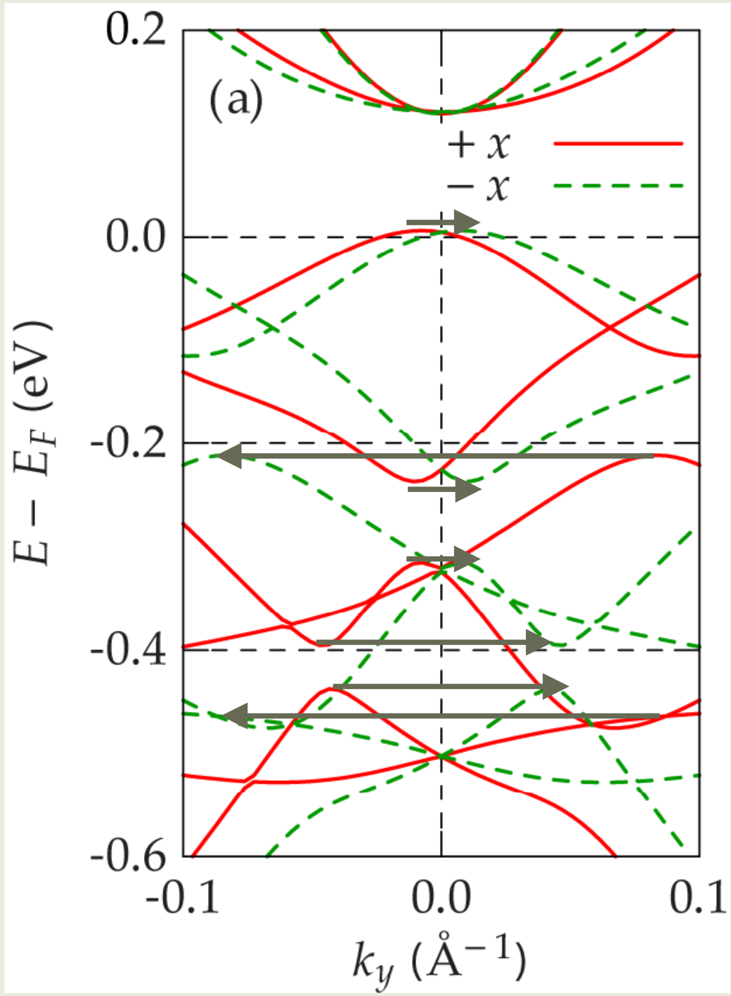


- Each band has its own sign of Rashba parameter

- Rashba parameter governs the sign/magnitude of STT

- Depending on which bands cross the Fermi level, different STT will be found (lot like the problem of Hall effect in multi-band system)

1 Co- 3 Pt



JH Park et al. PRB 87, 041301(R) (2013)

Summary & Outlook

- Direct consequence of inversion symmetry breaking in multi-orbital bands is orbital Rashba effect resulting in chiral OAM structure in k-space

- Spin Rashba follows from splitting of spin degeneracy in pre-existing chiral OAM bands due to spin-orbit interaction (very different picture from conventional free-electron theory of Rashba)

- Origin of SOI is still relativity, but origin of Rashba is non-relativistic (contrary to many existing statements)

- "Detection" of chiral OAM confirmed by CD-ARPES

- There can be many interesting consequences of chiral OAM