Orbital angular momentum in Rashba, spin Hall and anomalous Hall effects

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Spin phenomena from orbital degree of freedom (orbital angular momentum) and its connection to Berry curvature

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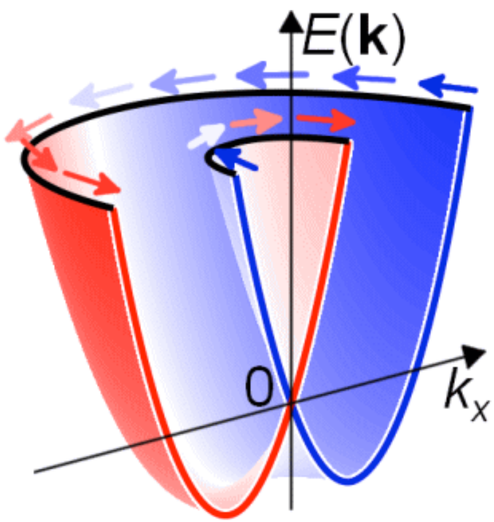
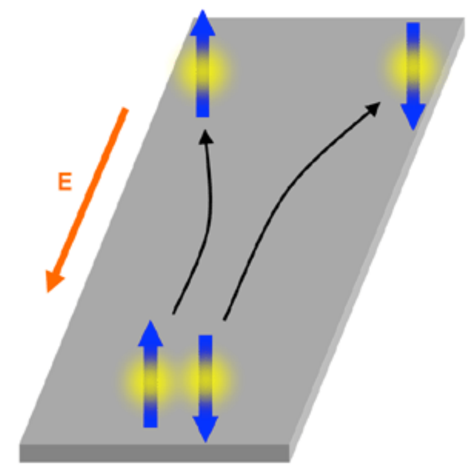
Spin phenomena

Rashba Effect



Spin Hall Effect

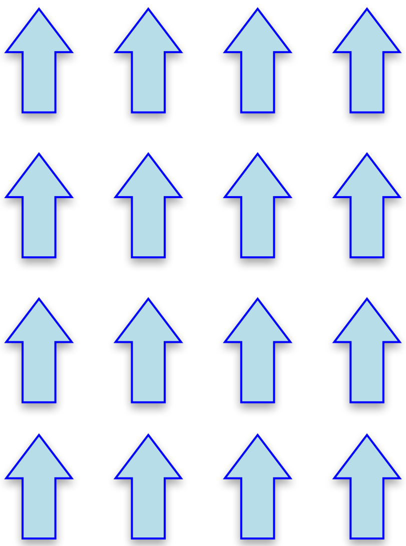


Orbital polarization (angular momentum) + Spin-orbit coupling

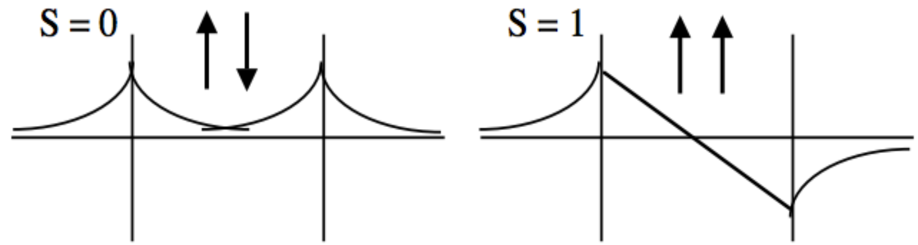
Electric vs magnetic

- Heisenberg Hamiltonian $\hat{H}_H = -J\vec{S}_1 \cdot \vec{S}_2$

Ferromagnet



Dipole-dipole interaction?



$$H_{\text{Coulomb}} = \frac{1}{2}\frac{1}{4\pi\epsilon_0}\int d^3r_1 d^3r_2 \frac{\rho(\mathbf{r}_1)\rho(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

➔ Coulomb interaction in combination with the exclusion principle

$$k_B T_c \sim z\,\frac{\mu_0}{4\pi}\frac{m_s^2}{a^3} = z\,\frac{\mu_0}{4\pi}\frac{g^2{\mu_B}^2}{4a^3} \cong \frac{\mu_0}{4\pi}\frac{e^2\hbar^2}{4m_e^2 a^3}$$

Factor of ~10^4 too small!

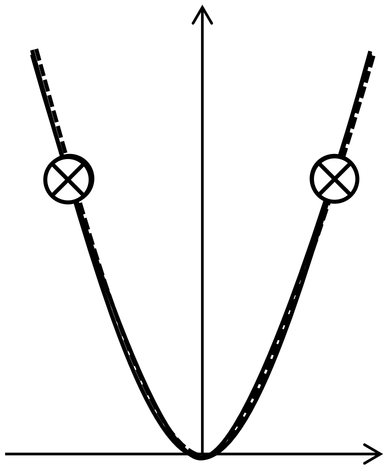
Lesson : $H_{\text{electric}} >> H_{\text{magnetic}}$

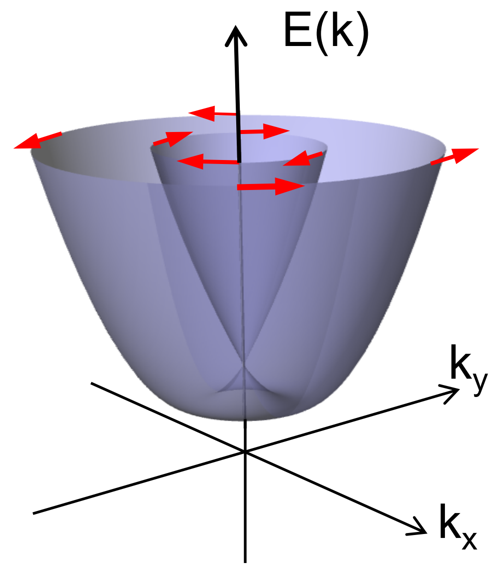
I. Rashba effect

II. Intrinsic spin Hall effect

III. Observation of hidden Berry curvature

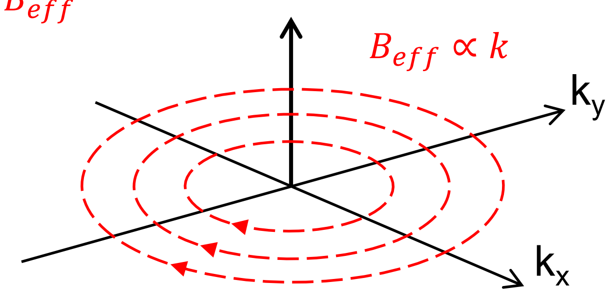
Rashba effects

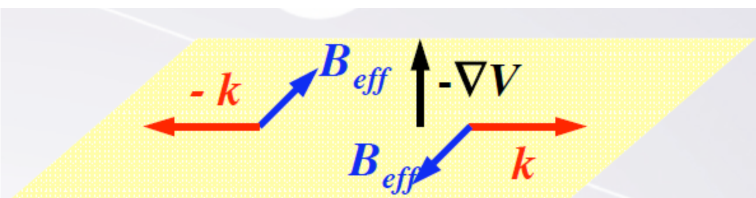




Rashba Hamiltonian JETP Lett. (1984)

$$\hat{H}_R = \underbrace{\alpha_R(\vec{k}\times\hat{z})}_{B_{eff}}\cdot\vec{\sigma}$$





Zeeman coupling

$$H_{SOC} \approx -\vec{\mu}_S\cdot\vec{B} = \alpha_R(\vec{e}_z\times\vec{p})\cdot\sigma$$

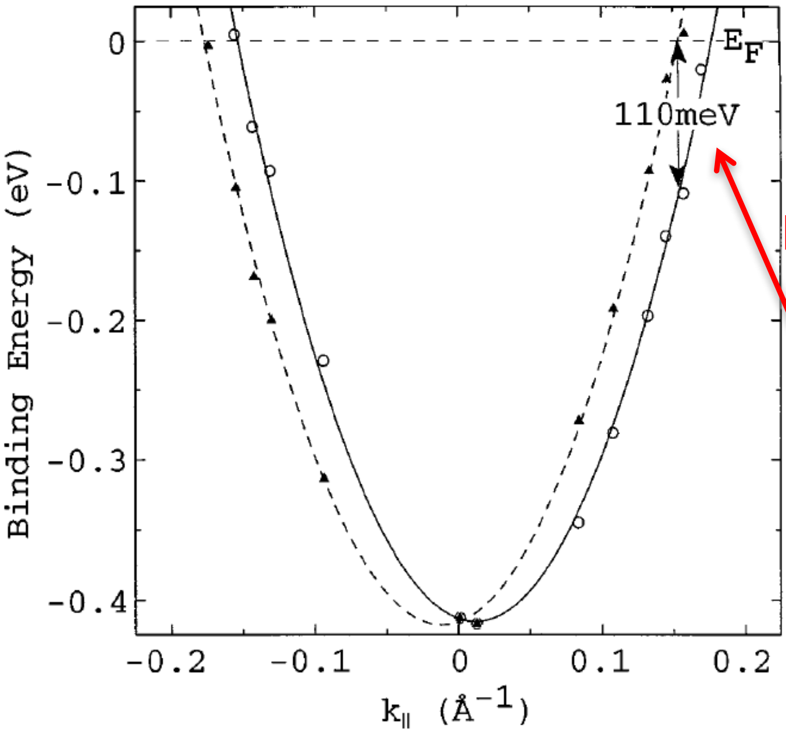
$$\vec{B}_{eff} = \frac{1}{c^2}\vec{v}\times\vec{E} = \frac{\hbar}{m^*c^2}\vec{k}\times\vec{E}$$ Relativistic effect

A ‘small’ problem in energy scale

VOLUME 77, NUMBER 16 PHYSICAL REVIEW LETTERS 14 OCTOBER 1996

Spin Splitting of an Au(111) Surface State Band Observed with Angle Resolved Photoelectron Spectroscopy

S. LaShell, B. A. McDougall, and E. Jensen
Physics Department, Brandeis University, Waltham, Massachusetts 02254
(Received 19 July 1996)



$$H_{\mathrm{SOC}} = (\hbar/4mc^2)(\nabla V \times \vec{p}) \cdot \vec{\sigma}$$

Factor of 10^5!

perpendicular to $\vec{k}_{\|}$ as shown in Fig. 1. The NFE matrix elements yield splittings proportional to k, and of order 10^{-6} eV.

Questions to answer

A proper model should explain…

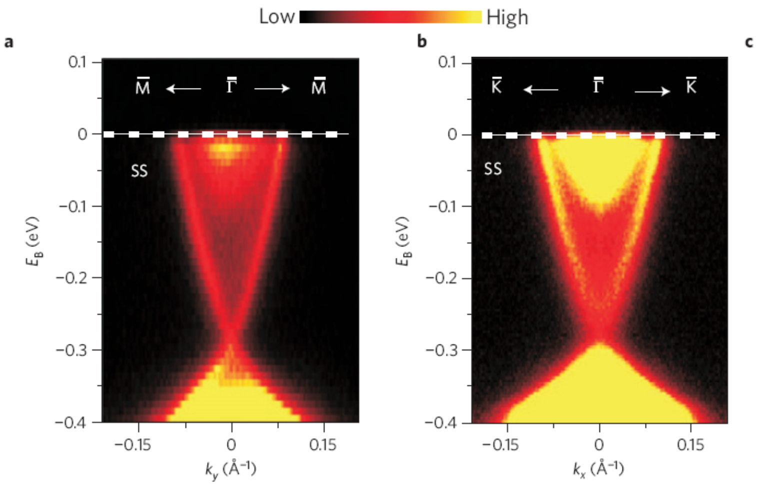
- Band splitting & spin degeneracy lifting
- Energy scale of the split
- Chiral spin structure (including chirality)
- The role of atomic SOC parameter α
- Asymmetric charge distribution
- Chiral orbital angular momentum structure

- Conventional interpretation explains only one of them!

$$H_{\mathrm{SOC}} = (\hbar/4mc^2)(\nabla V \times \vec{p}) \cdot \vec{\sigma}$$

Circular dichroism in ARPES

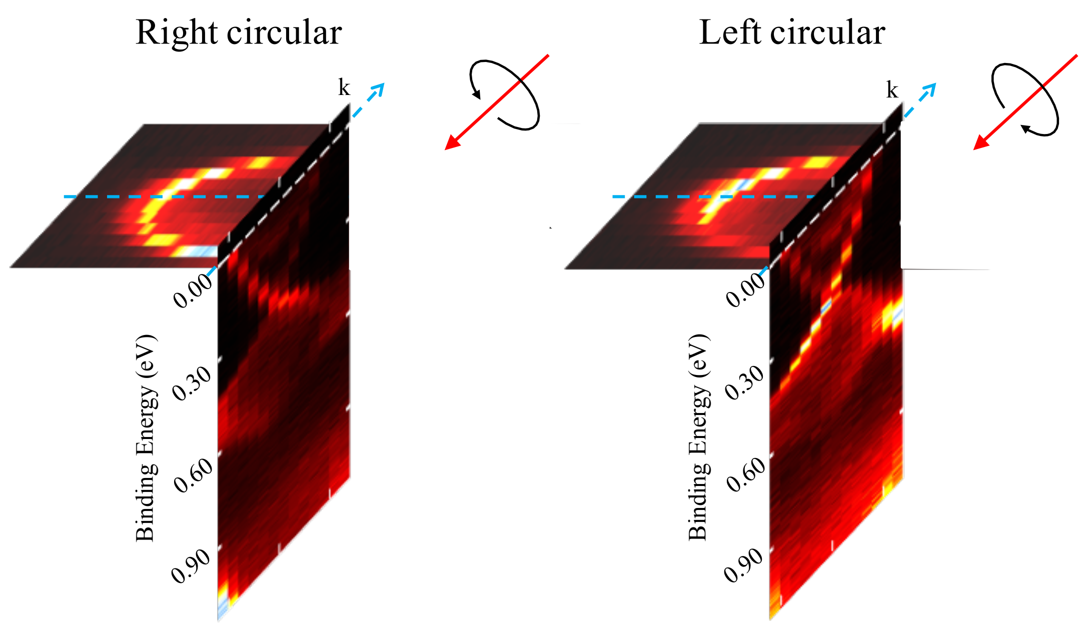
Bi_2Se_3 surface states



Nature Physics **5**, 398 (2009)

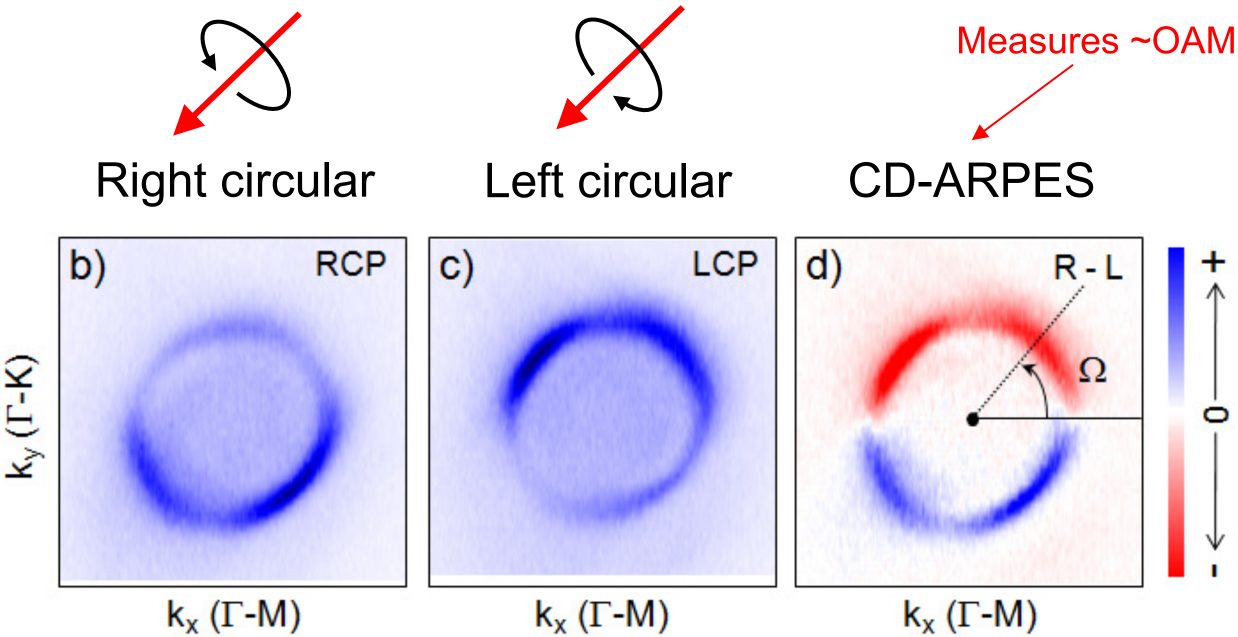
Rashba states
= Chiral spin states

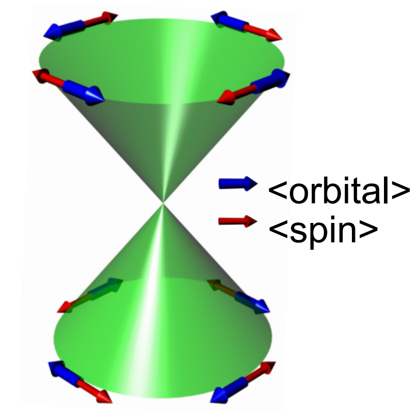
Bi_2Se_3 surface state data with two circular polarizations



S. R. Park et al, PRL **108**, 046805 (2012)

CD ARPES & Chiral OAM



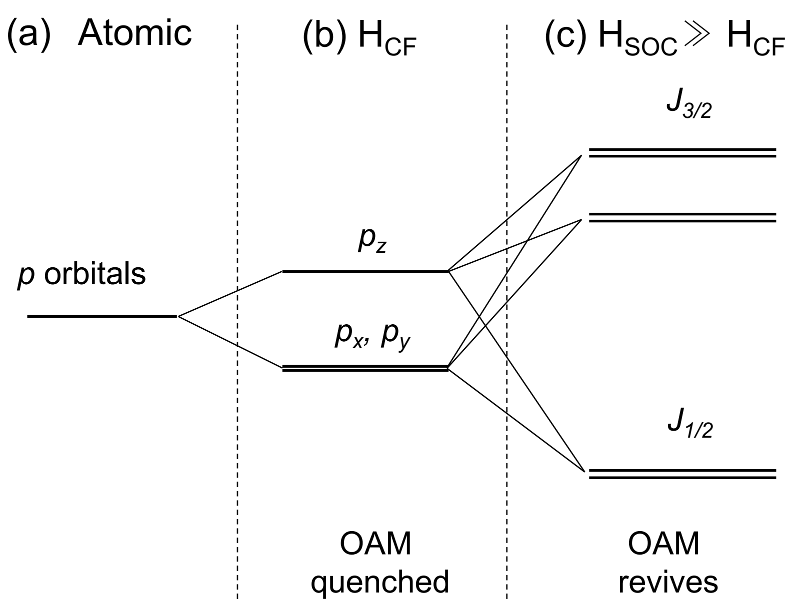


J=1/2

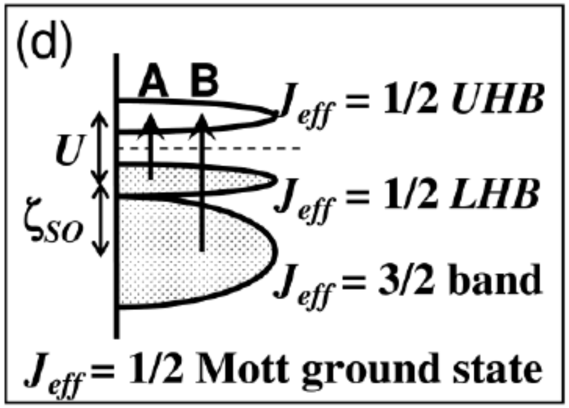
S. R. Park et al, PRL **108**, 046805 (2012)

OAM revives

With strong spin-orbit coupling



'J' state



PRL **101**, 076402 (2008)

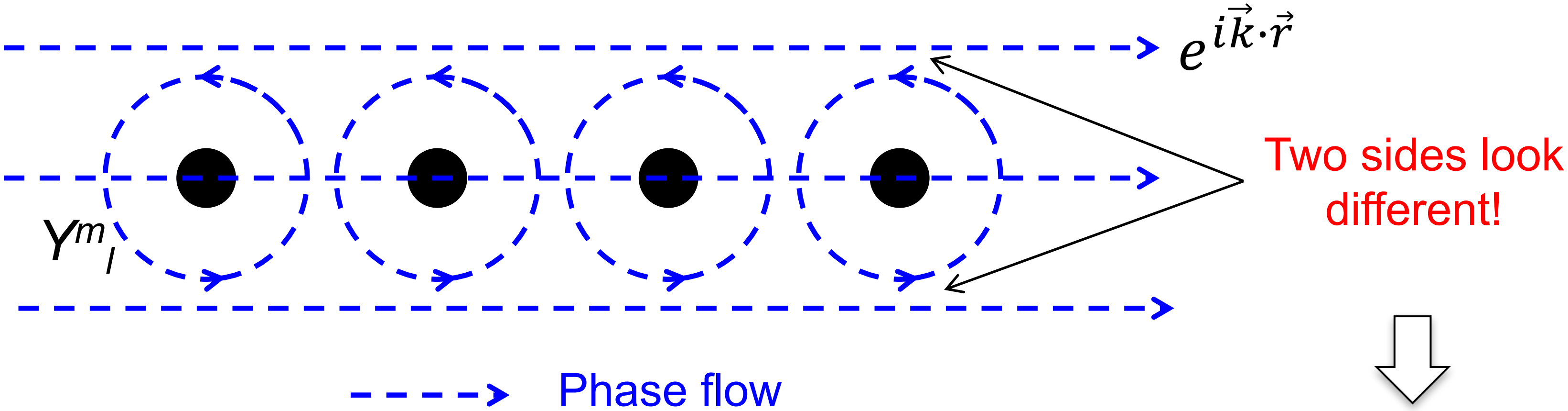
OAM in atomic orbital

Bloch state $$\psi(\boldsymbol{r}) \approx \frac{1}{\sqrt{N}} \sum_{\boldsymbol{R}_n} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_n} \; R(\boldsymbol{r}-\boldsymbol{R}_n)\, Y^m{}_l \; \xi_s$$

When we have both *L* & *k*…

$$\psi(\boldsymbol{r}) \approx \frac{1}{\sqrt{N}} \sum_{\boldsymbol{R_n}} e^{i\boldsymbol{k}\cdot\boldsymbol{R_n}} \; R(\boldsymbol{r} - \boldsymbol{R_n})\, Y^m{}_l \; \xi_s$$

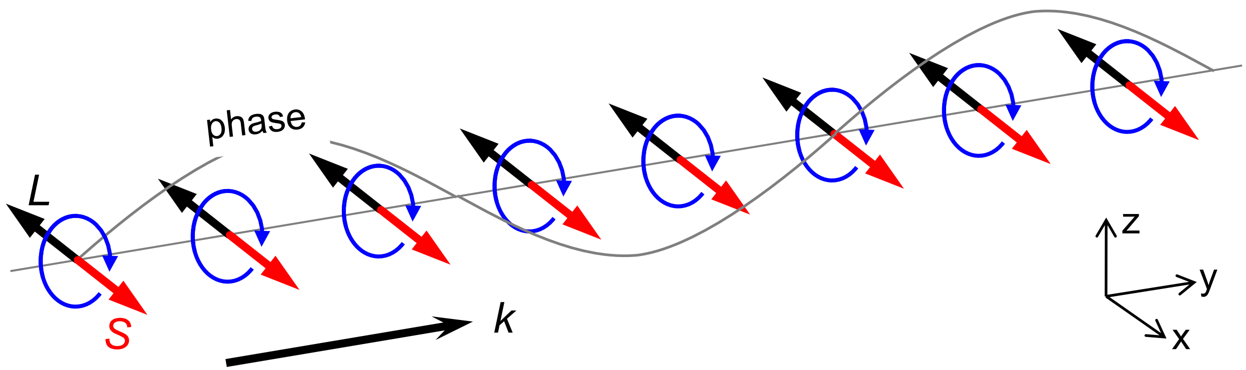
Bloch state in consideration = OAM + linear momentum

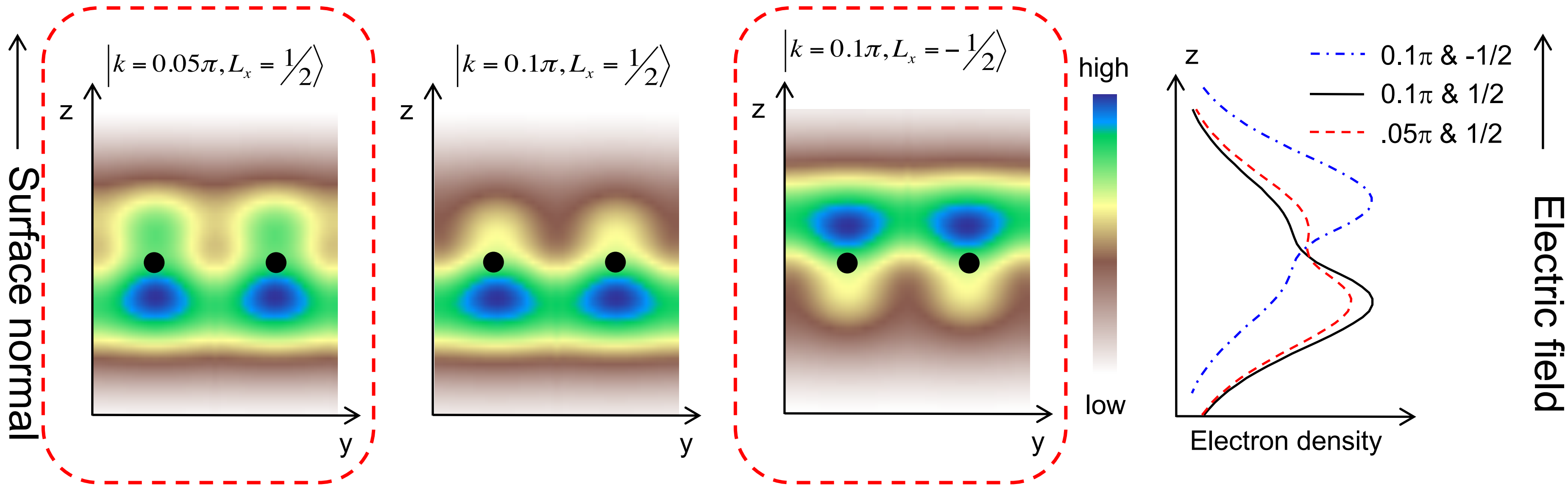


What does this to wave ftn?

Simulation

Asymmetric charge distribution





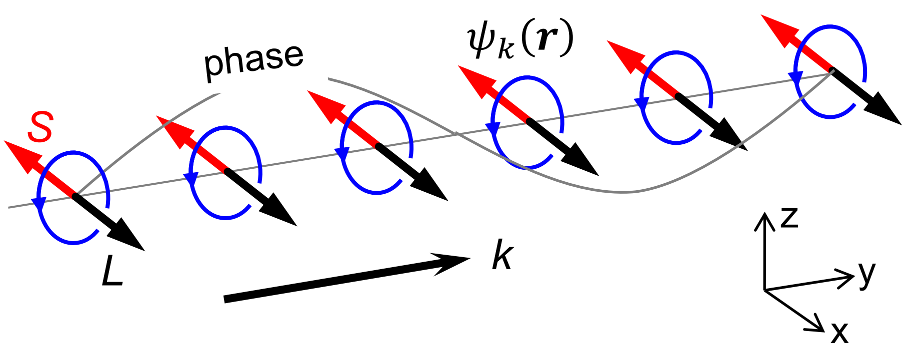
Combination of OAM & *k* results in an asymmetric charge distribution (electric polarization)

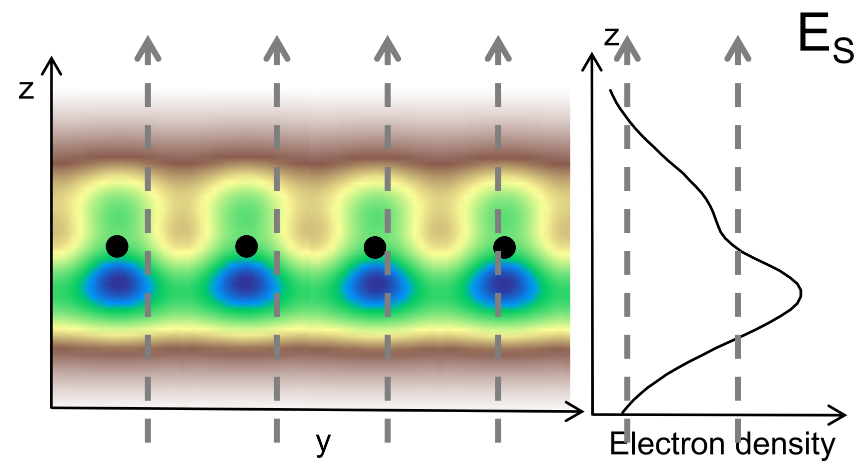
OAM induced large energy scale

Orbital angular momentum + Linear momentum → Asymmetric charge distribution

Asymmetric charge distribution + Electric field → **Electric energy**

Bloch state $\phi_{\mathbf{R}}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}} \psi_{\mathbf{k}}(\mathbf{r})$

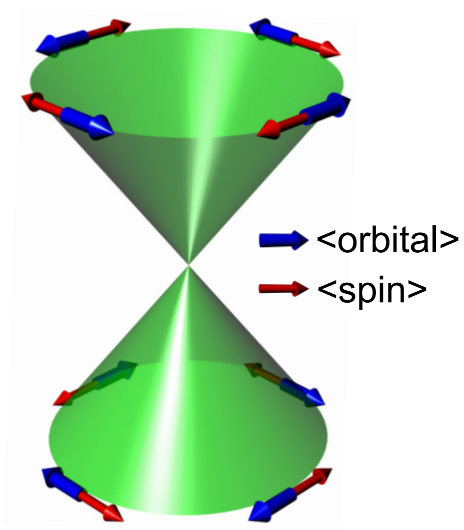


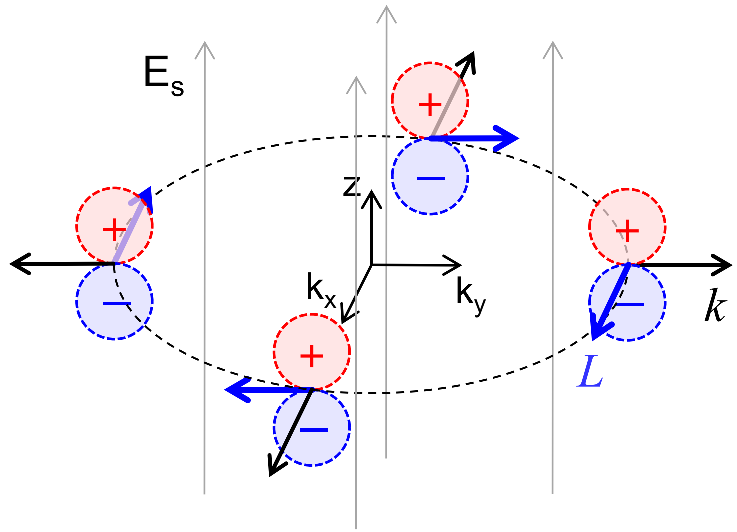


$$\hat{H}_L = -\alpha_L(\vec{L}\times\vec{k})\cdot\vec{E}_S$$

- Interference effect within a Bloch wave function
- $\psi_k(\boldsymbol{r})$ being *complex*

Chiral OAM & Rashba

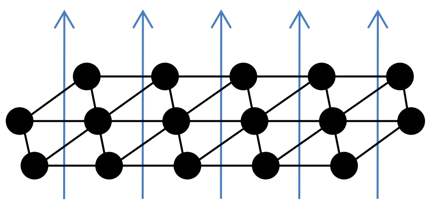


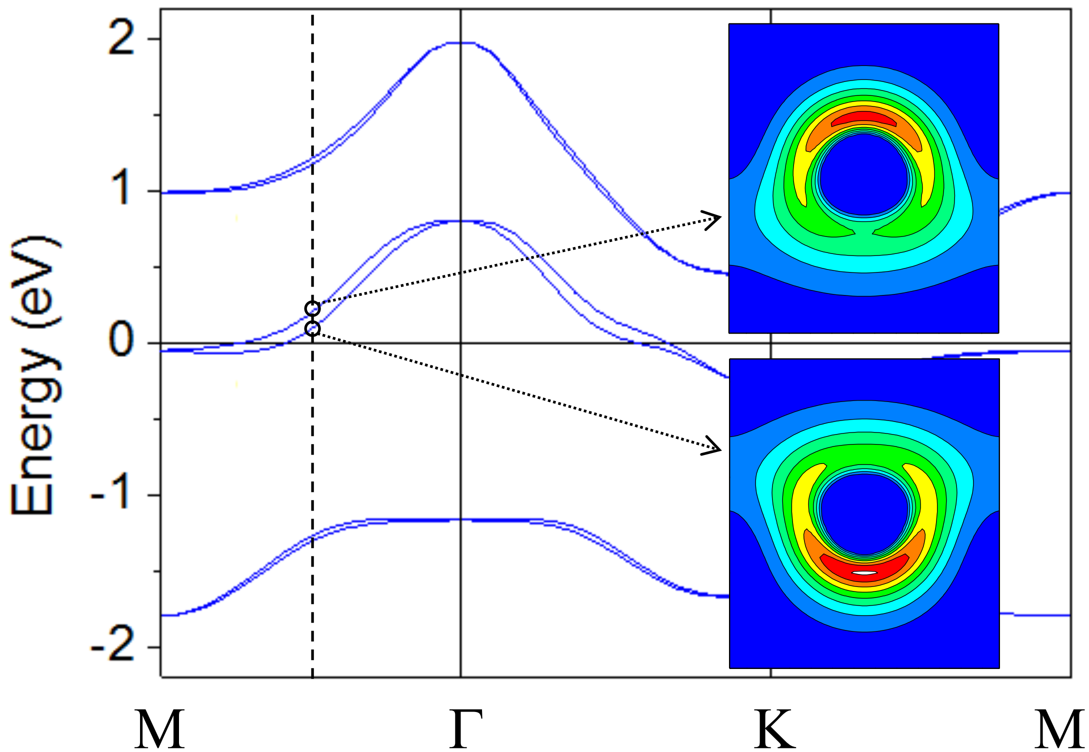


- Asymmetric charge ('electric polarization') determined by $\vec{p} \sim \vec{L} \times \vec{k}$
- Energy from $U = -\vec{p} \cdot \vec{E}_s \sim (\vec{L} \times \vec{k}) \cdot \vec{E}_s \sim (e\overset{o}{A}) \times (V / \overset{o}{A}) \sim eV$
- Chiral structure determined by OAM
- Spin chirality follows from SOC

LDA on single layer of Bi w/ external field

Single layer of Bi
with 3 V/A





J. S. Hong, et al., Scientific Reports 5, 13488 (2015)

LDA results reveal asymmetric charge distribution for Rashba states

OAM based Hamiltonian for Rashba effect

Conventional Rashba (spin)

$$\hat{H}_{Rashba} = \alpha_R(\hat{z}\times\vec{p})\cdot\underline{\hat{\sigma}}$$

spin

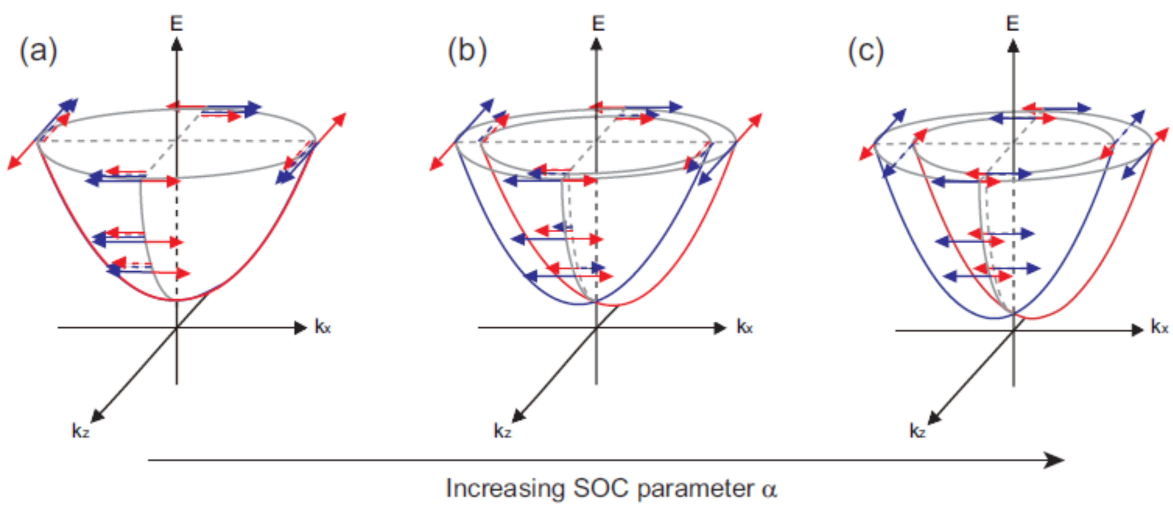
New Hamiltonian (orbital)

$$\hat{H}_L = -\vec{p}\cdot\vec{E}_S = -\alpha_L(\underline{\vec{L}}\times\vec{k})\cdot\vec{E}_S$$

OAM

$$\hat{H}_{eff} = \varepsilon_k + \alpha\vec{L}\cdot\vec{S} - \alpha_L(\vec{L}\times\vec{k})\cdot\vec{E}_S$$

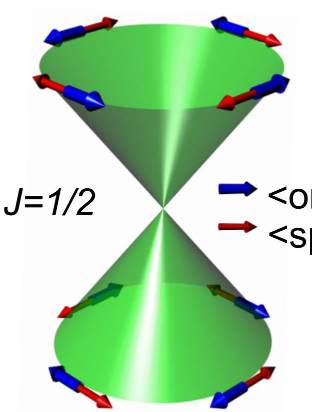
Crystal field + atomic SOC + Electrostatic



PRL 108, 046805 (2012);
PRB 85, 195402 (2012);
PRB 88, 205408 (2013)

Summary on Rashba

- Orbital angular momentum induces asymmetric charge distribution which can result in a large energy term
- Chiral OAM structure exists in Rashba states resulting from the energy term
- Spin chirality follows the OAM chirality through SOC
- OAM plays the essential role in Rashba effect.



Effective Hamiltonian

$$\hat{H}_R = \alpha_R(\vec{\sigma}\times\vec{k})\cdot\hat{z}$$

$$\Rightarrow$$

$$\hat{H}_L = -\alpha_L(\vec{L}\times\vec{k})\cdot\vec{E}_s \;+\; \lambda\vec{L}\cdot\vec{\sigma}$$

PRL **107**, 156803 (2011); PRL **108**, 046805 (2012); PRB **85**, 195402 (2012); PRB **88**, 205408 (2013)
Sci. Rep. 5, 13488 (2015); J. Electr. Spectr. Rel. Phenom, **201**, 6 (2015)

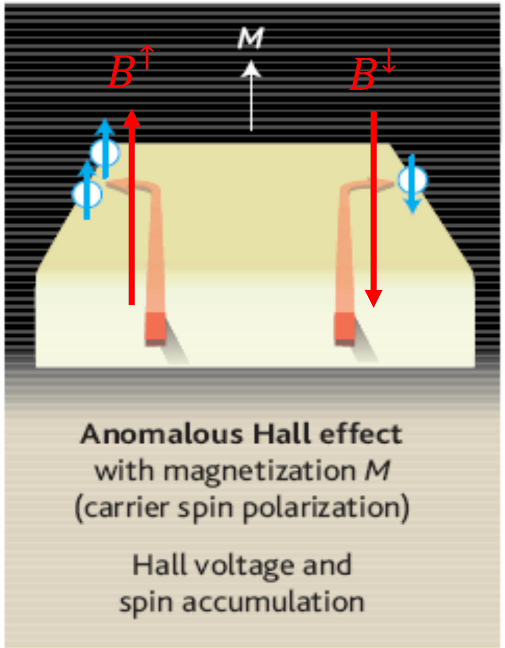
I. Rashba effect

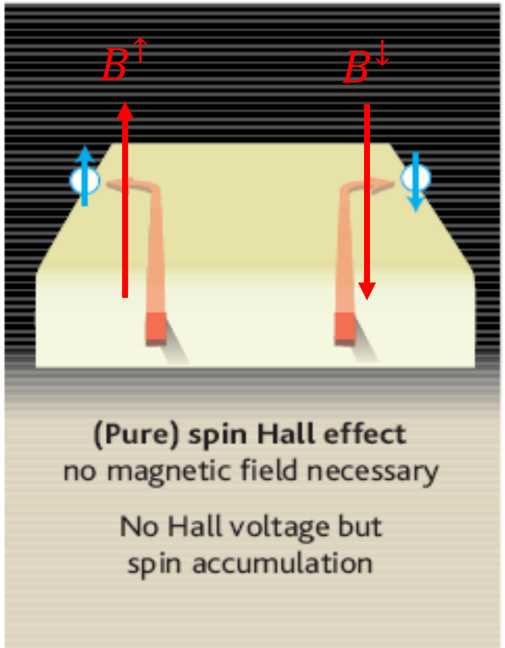
II. Intrinsic spin Hall effect

Is OAM important in other phenomena?

III. Observation of hidden Berry curvature

Anomalous and spin Hall effects





- Ferromagnetic system
- Hall effect without external B-field

- Non-magnetic metallic system
- Spin accumulation

Anomalous Hall effect

PHYSICAL REVIEW VOLUME 95, NUMBER 5 SEPTEMBER 1, 1954

Hall Effect in Ferromagnetics*

ROBERT KARPLUS,† *Department of Physics, University of California, Berkeley, California*

AND

J. M. LUTTINGER, *Department of Physics, University of Michigan, Ann Arbor, Michigan*

(Received May 21, 1954)

Both the unusually large magnitude and strong temperature dependence of the extraordinary Hall effect in ferromagnetic materials can be understood as effects of the spin-orbit interaction of polarized conduction electrons. It is shown that the interband matrix elements of the applied electric potential energy combine with the spin-orbit perturbation to give a current perpendicular to both the field and the magnetization. Since the net effect of the spin-orbit interaction is proportional to the extent to which the electron spins are aligned, this current is proportional to the magnetization. The magnitude of the Hall constant is equal to the square of the ordinary resistivity multiplied by functions that are not very sensitive to temperature and impurity content. The experimental results behave in such a way also.

- Evaluation of current operator
- Very general formula

REVIEWS OF MODERN PHYSICS, VOLUME 82, APRIL–JUNE 2010

Anomalous Hall effect

Naoto Nagaosa

Department of Applied Physics, University of Tokyo, Tokyo 113-8656, Japan and Cross-Correlated Materials Research Group (CMRG), and Correlated Ele Research Group (CERG), ASI, RIKEN, Wako, 351-0198 Saitama, Japan

Jairo Sinova

Department of Physics, Texas A&M University, College Station, Texas 77843- and Institute of Physics ASCR, Cukrovarnická 10, 162 53 Praha 6, Czech Re

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Condensed Matter Theory Laboratory, ASI, RIKEN, Wako, 351-0198 Saitama,

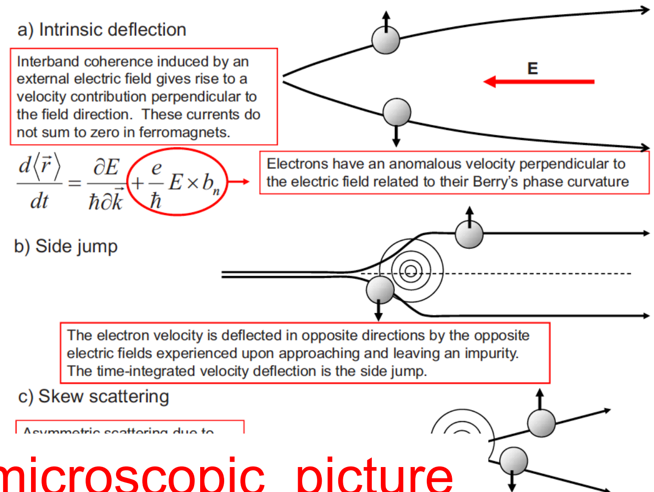
A. H. MacDonald

Department of Physics, University of Texas at Austin, Austin, Texas 78712-10

N. P. Ong

Department of Physics, Princeton University, Princeton, New Jersey 08544, U

(Published 13 May 2010)



- No true microscopic picture

- AHE in terms of Berry curvature

Issues in spin Hall effect

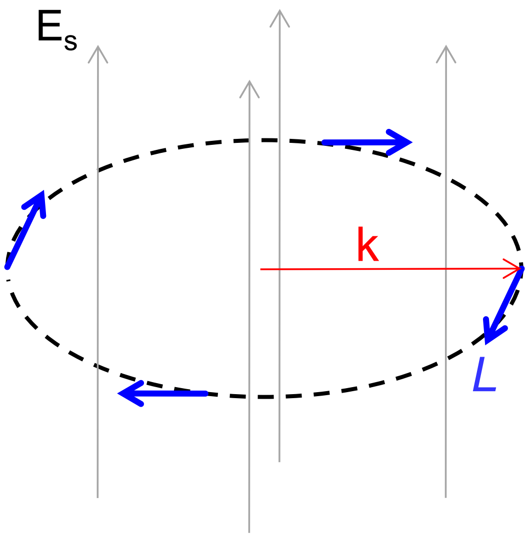
- Issues
  1. Role of SOC?
  2. Sign reversal issue? (Pt vs Ta)

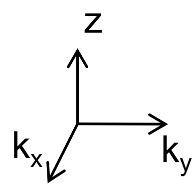
  ➔ Need a more intuitive picture

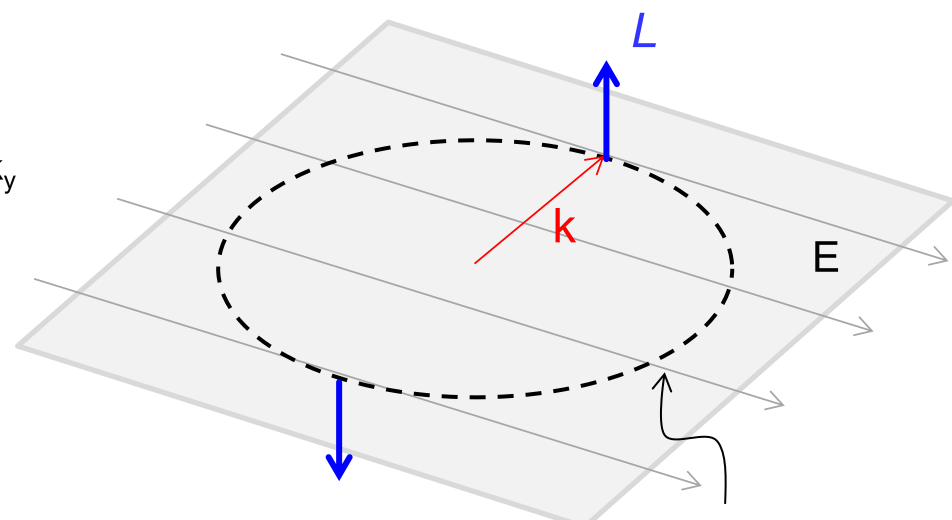
  ➔ OAM Hamiltonian can help

Rashba vs Spin Hall

- Rashba case
- Spin Hall case







Band is spin degenerate
Degeneracy lifted

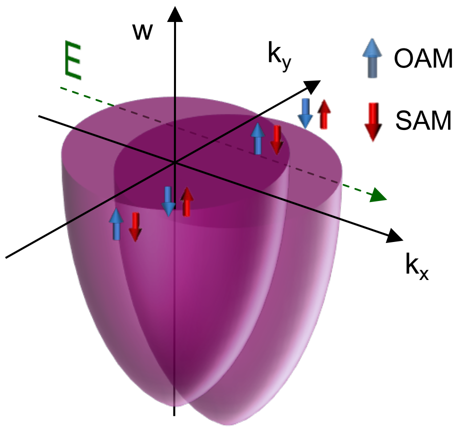
$$\hat{H}_L = -\alpha_L\left(\vec{L}\times\vec{k}\right)\cdot\vec{E}_S$$

Inversion symmetry breaking
from intrinsic field

Inversion symmetry breaking
applied field

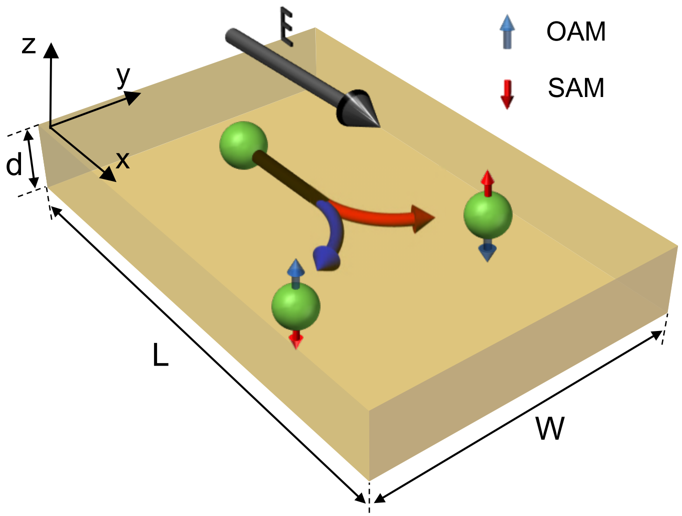
Spin Hall effect from the new Hamiltonian

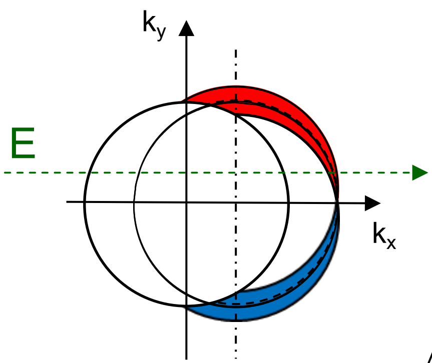
J = ½ case

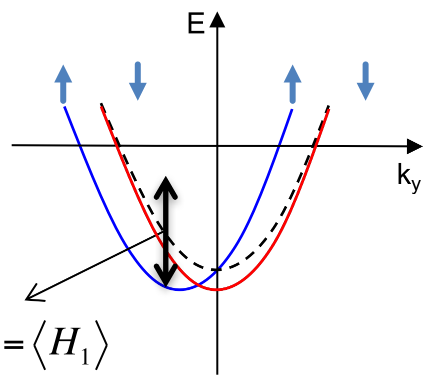


$$H_0 = \hbar^2 k^2 / 2m$$
$$+\alpha \vec{L} \cdot \vec{S}$$

$$H_1 = -\alpha_L (\vec{L} \times \vec{k}) \cdot \vec{E}_x$$







$$\Delta E = \langle H_1 \rangle$$

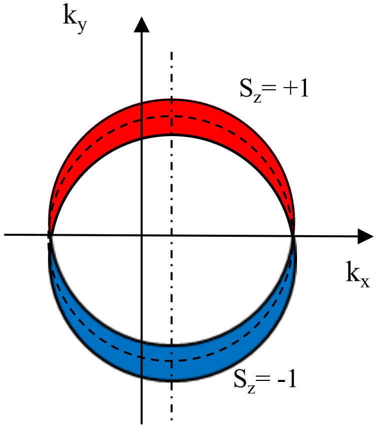
$$-\alpha_L (\vec{L} \times \vec{k}) \cdot \vec{E}_x$$

- causes OAM dependent transverse motion
- behaves like an effective magnetic field
- should be related to Berry curvature

* Spin Hall current is by-product due to SOC

SHE current (intuitive)

- J = ½ case



Spin current within dk_x :

$$\frac{n}{4\pi^2}\frac{2e\hbar k_y}{m_e}\Delta k_y dk_x = \frac{n}{4\pi^2}\frac{2e\hbar k_y}{m_e}2k_0 dk_x = \frac{ne\hbar k_0}{\pi^2 m_e}k_y dk_x$$

Total spin current :

$$j_y^{spin} = \frac{ne\hbar k_0}{\pi^2 m_e}\int_{-k_f}^{k_f} k_y\, dk_x = ne\hbar k_0 k_f^2/2\pi m_e \quad \leftarrow k_0 = \alpha_L m_e E_x/\hbar$$

$$= ne\alpha_L E_x k_f^2/2\pi$$

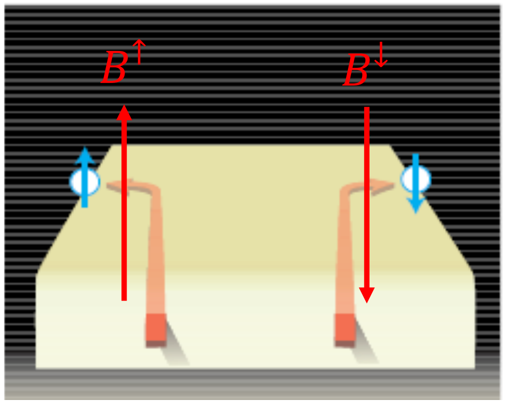
Spin Hall voltage :

$$V_y^{SH} = j_y^{spin}\rho_{yy}W = \frac{ne\alpha_L E_x k_f^2 \rho_{yy} W}{2\pi} = \frac{ne\alpha_L k_f^2 j_x \rho_{xx}\rho_{yy} W}{2\pi}$$

$$\approx ne\alpha_L k_f^2 W \rho^2 j_x \propto \rho^2$$ ← well known result from AHE

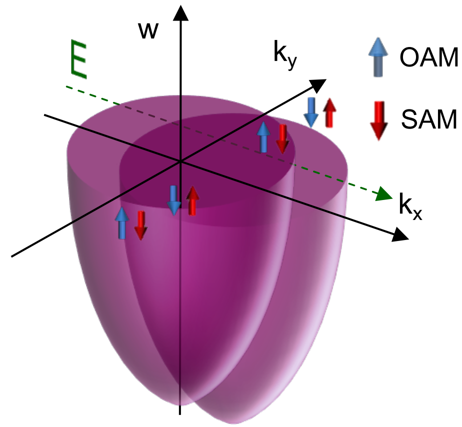
Connection to Berry phase - I

Spin Hall effect



Spin dependent effective B-field

OAM driven intrinsic spin Hall effect



$$H_0 = \hbar^2 k^2 / 2m$$
$$+\alpha \vec{L} \cdot \vec{S}$$

$$H_1 = -\alpha_L (\vec{L} \times \vec{k}) \cdot \vec{E}_x$$

- Equation of motion

$$\frac{d\mathbf{r}_c}{dt} = \boxed{\frac{1}{\hbar} \nabla_{\mathbf{k}} E_n (\mathbf{k}_c)} \boxed{- \frac{d\mathbf{k}_c}{dt} \times \mathbf{B}_n (\mathbf{k}_c)}$$

Anomalous velocity

Berry curvature

$$\psi_{n\mathbf{k}}(\mathbf{r}) = \boxed{e^{i\mathbf{k}\cdot\mathbf{r}}} \boxed{u_{n\mathbf{k}}(\mathbf{r})}$$

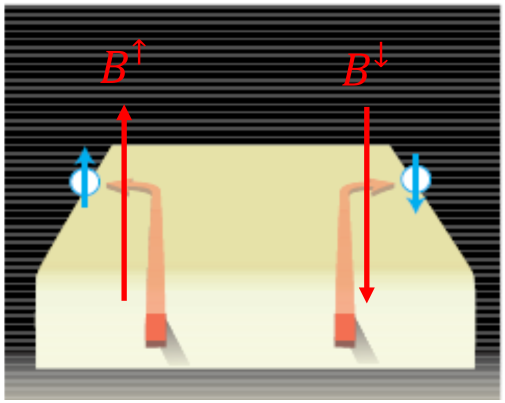
$$\frac{d\mathbf{k}_c}{dt} = -\frac{e\mathbf{E}}{\hbar}$$

This contains L

B_n related to OAM?

Connection to Berry phase - II

Spin Hall effect



Spin dependent effective B-field

Berry curvature

$$\vec{B}_n(\vec{k}) = \nabla_{\vec{k}} \times \vec{A}_n(\vec{k})$$

Berry connection

$$A_{ni}(\vec{k}) = -i\left\langle n\vec{k}\left|\frac{\partial}{\partial k_i}\right|n\vec{k}\right\rangle$$

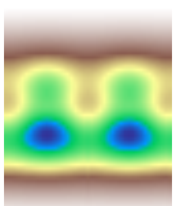
Hint

Theory of polarization of crystalline solids

R. D. King-Smith and David Vanderbilt

PRB 47, 1651 (1993)

$$P_{\parallel}^{(\lambda)} \sim \int_A d\mathbf{k}_{\perp} \sum_{n=1}^{M} \int_0^{|\mathbf{G}_{\parallel}|} dk_{\parallel} \underbrace{\left\langle u_{\mathbf{k}n}^{(\lambda)}\left|\frac{\partial}{\partial k_{\parallel}}\right|u_{\mathbf{k}n}^{(\lambda)}\right\rangle}_{\vec{A}(\vec{k})}$$



Dipole moment of asymmetric charge distribution (momentum dependent) $\vec{p} \sim \alpha_L \vec{L} \times \vec{k}$

Polarization $\vec{P} = \int \vec{p}\, d^3k \sim \int (\alpha_L \vec{L} \times \vec{k})\, d^3k$

$$\Rightarrow \vec{A}(\vec{k}) \sim \alpha_L \vec{L} \times \vec{k}?$$

Rigorous theory

Intrinsic Spin and Orbital Hall Effects from Orbital Texture

Dongwook Go,[1] Daegeun Jo,[1] Changyoung Kim,[2] and Hyun-Woo Lee[1,*]

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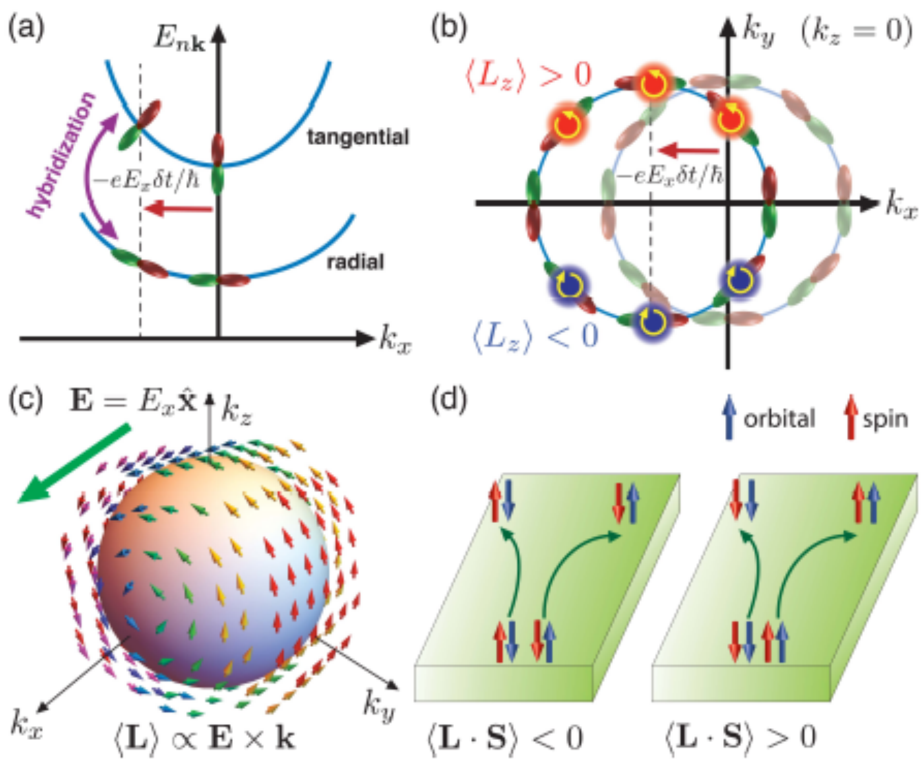
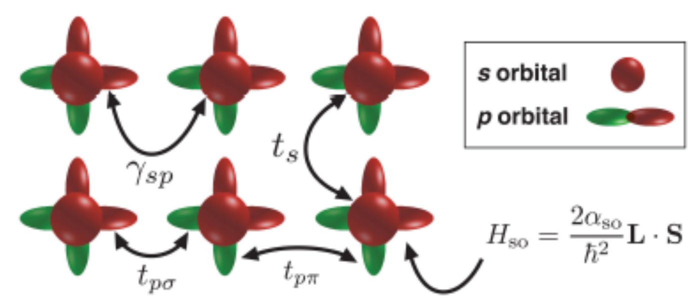
[2]*Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea*

(Dated: July 8, 2018)

*To appear in PRL, Aug 2018





$$\vec{A}(\vec{k}) \approx \lambda_p^s \vec{L} \times \vec{k}$$

$$\vec{B}(\vec{k}) \approx 2\lambda_p^s \vec{L}$$

Summary on SHE

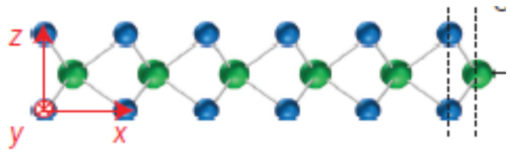
- OAM plays the key role in intrinsic SHE
- OHE is generated even when SOC=0
- OHE is more fundamental than SHE (SHE is a concomitant effect of OHE through SOC)
- Berry connection and curvature are directly related to $\vec{L}$

I. Rashba effect

II. Intrinsic spin Hall effect

III. Observation of hidden Berry curvature

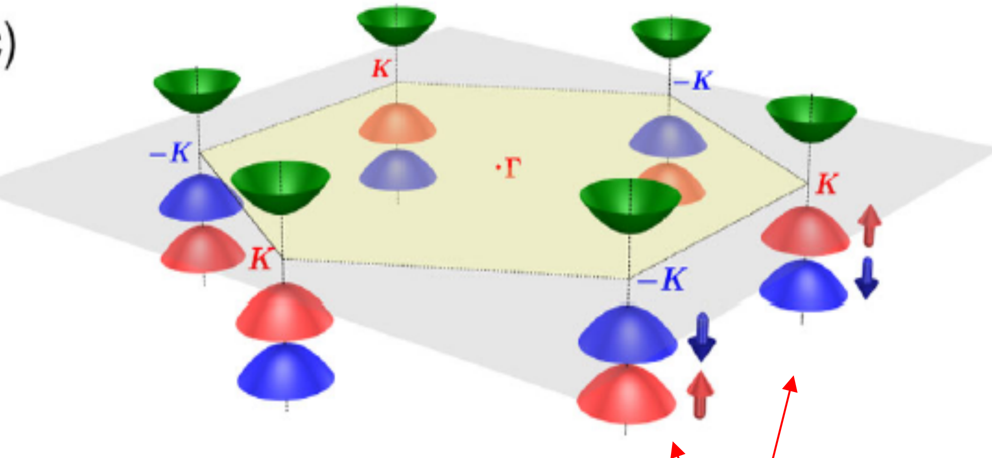
Spin & valley in 1ML TMDC

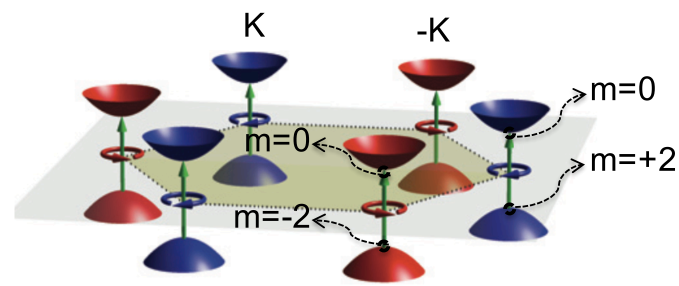


Xiao et al., PRL 108, 196802 (2012)

$$|\phi_v^\tau\rangle = \frac{1}{\sqrt{2}}(|d_{x^2-y^2}\rangle + i\tau|d_{xy}\rangle)$$

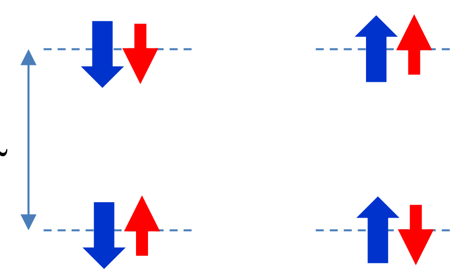
Orbital angular momentum!





Different valleys
What is ‘valley’?

$\lambda\vec{L}\cdot\vec{S}$ ➔ 2λ



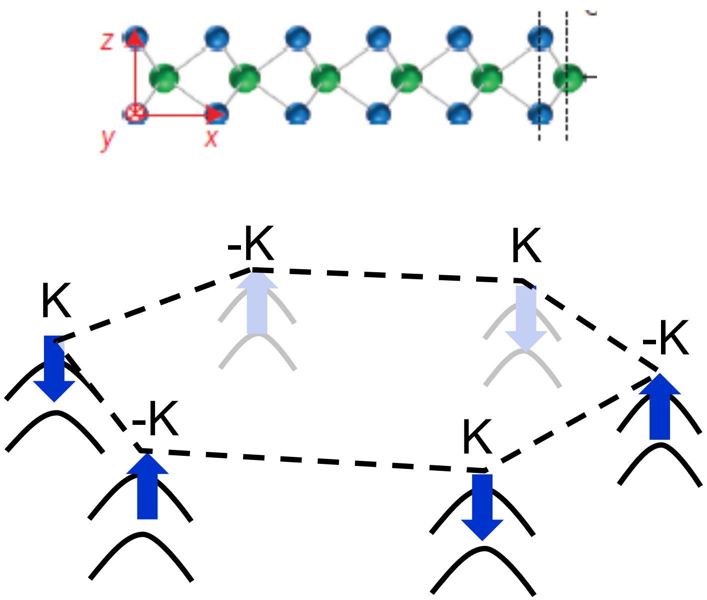
OAM
Spin

@ -K

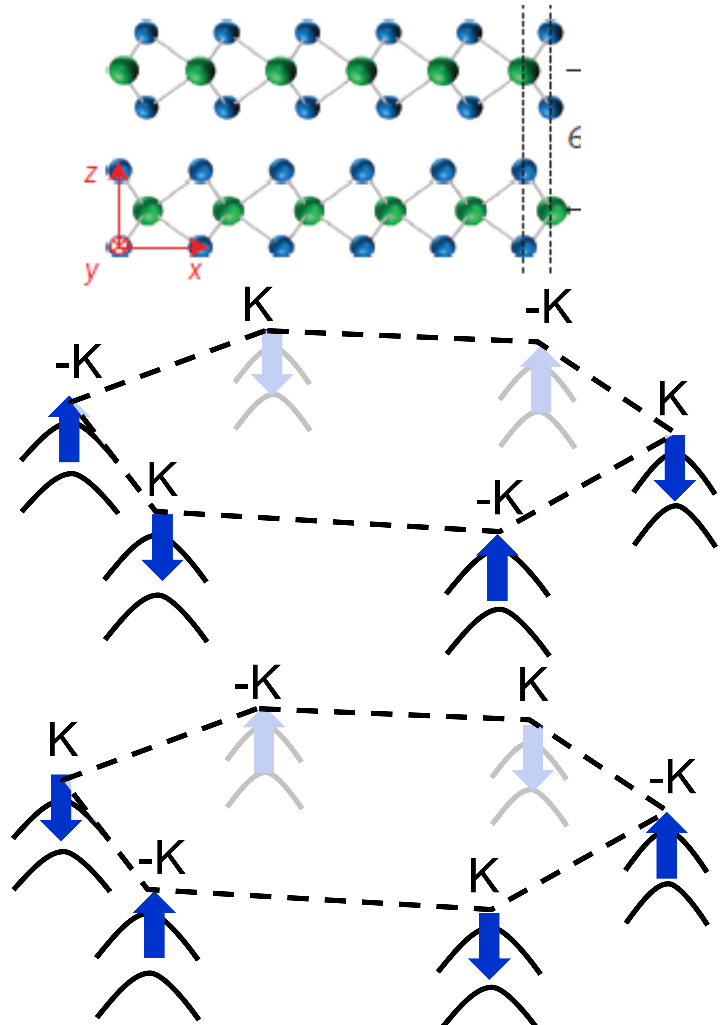
@ K

Valley, OAM & Berry curvature in TMDC

1 ML (no inversion)



2 ML (inversion)



Valley,
OAM &
Berry curvature

Berry curvature all but gone?

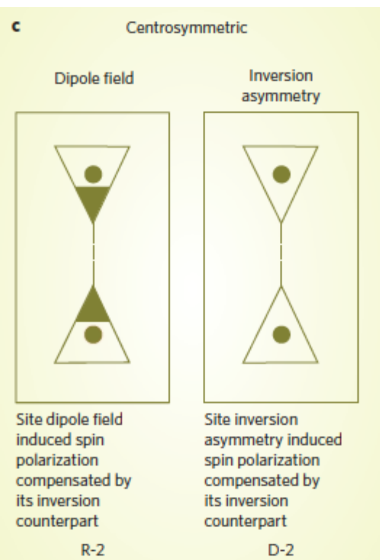
'Hidden' spin polarization & its observation

Prediction

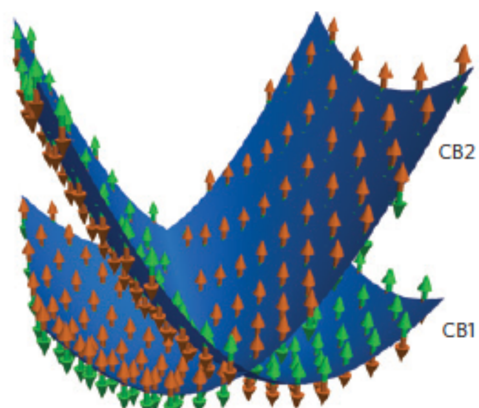
nature physics ARTICLES
PUBLISHED ONLINE: 13 APRIL 2014 | DOI: 10.1038/NPHYS2933

Hidden spin polarization in inversion-symmetric bulk crystals

Xiuwen Zhang[1,2,3†], Qihang Liu[1,4†], Jun-Wei Luo[3*], Arthur J. Freeman[4] and Alex Zunger[1*]



NaCaBi



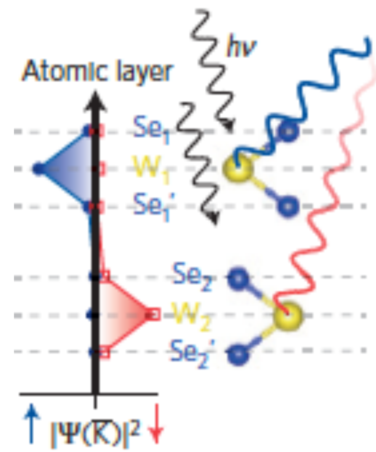
Observation

nature physics LETTERS
PUBLISHED ONLINE: 5 OCTOBER 2014 | DOI: 10.1038/NPHYS3105

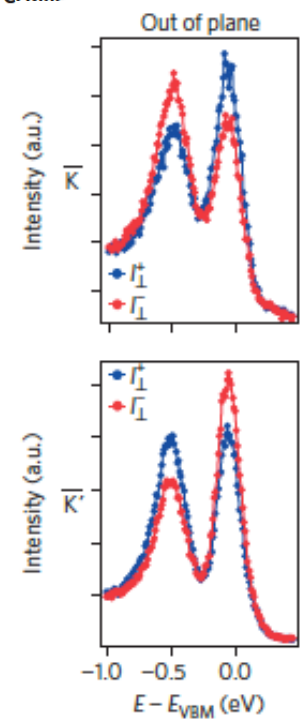
Direct observation of spin-polarized bulk bands in an inversion-symmetric semiconductor

J. M. Riley[1], F. Mazzola[2], M. Dendzik[3], M. Michiardi[3], T. Takayama[4,5], L. Bawden[1], C. Granerød[2], M. Leandersson[6], T. Balasubramanian[6], M. Hoesch[7], T. K. Kim[7], H. Takagi[4,5], W. Meevasana[8,9], Ph. Hofmann[3], M. S. Bahramy[10,11], J. W. Wells[2] and P. D. C. King[1*]

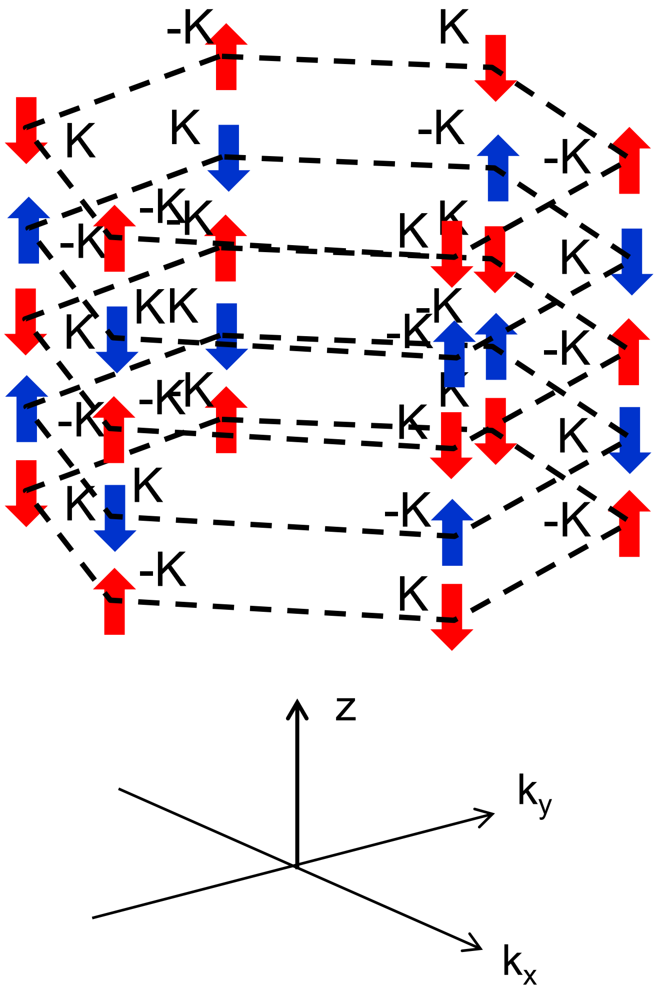
WSe_2



Preferentially looking at surface



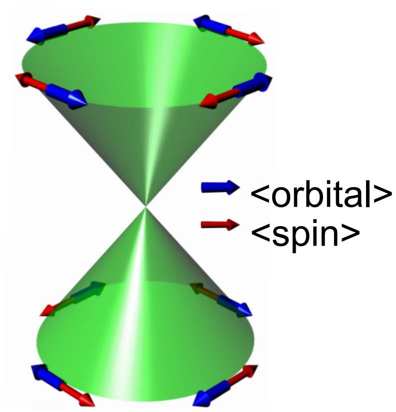
Hidden Berry curvature?



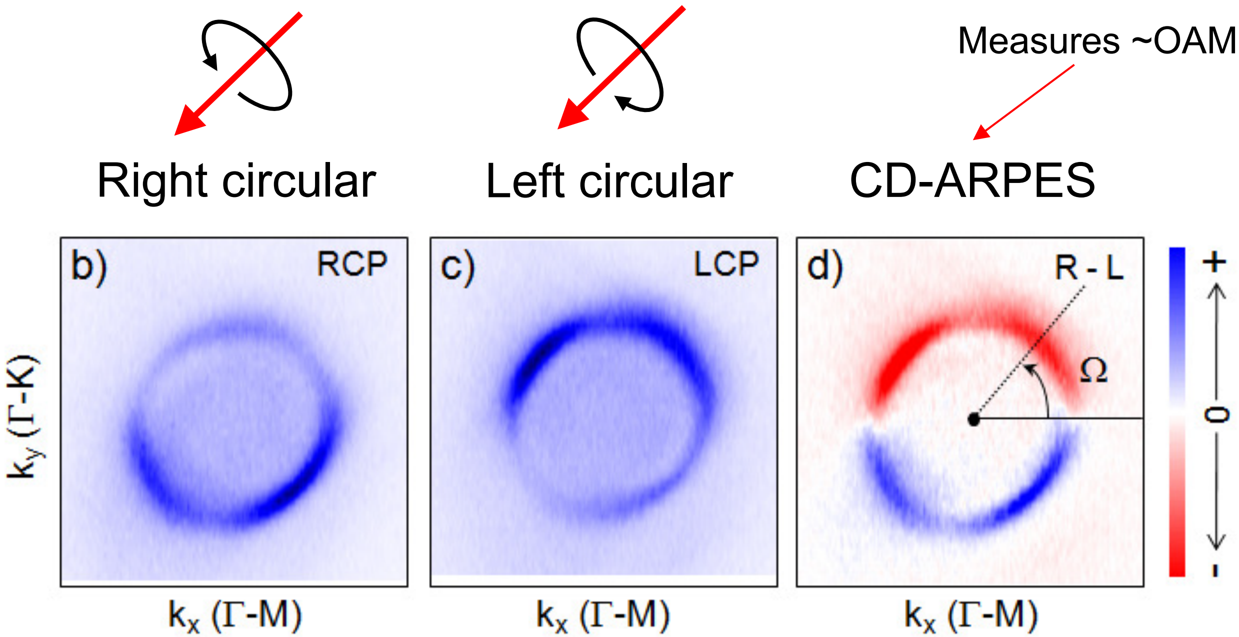
- ‘Hidden Berry curvature? (Berry curvature localized to a layer?)
- If so, can we observe it? How?
  ➔ CD-ARPES

Circular dichroism ARPES

Surface sensitive

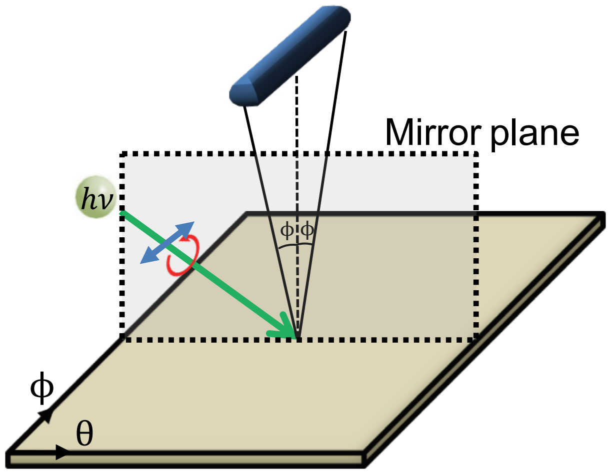


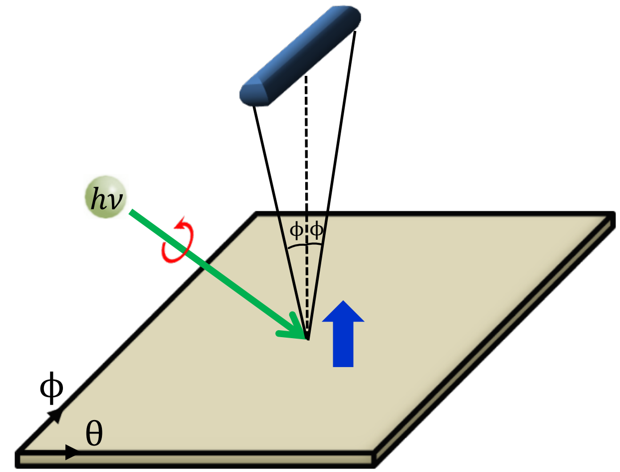
J=1/2



PRL **107**, 156803 (2011); PRL **108**, 046805 (2012); PRB **85**, 195402 (2012); PRB **88**, 205408 (2013)
Sci. Rep. 5, 13488 (2015); J. Electr. Spectr. Rel. Phenom, **201**, 6 (2015)

Two contributions





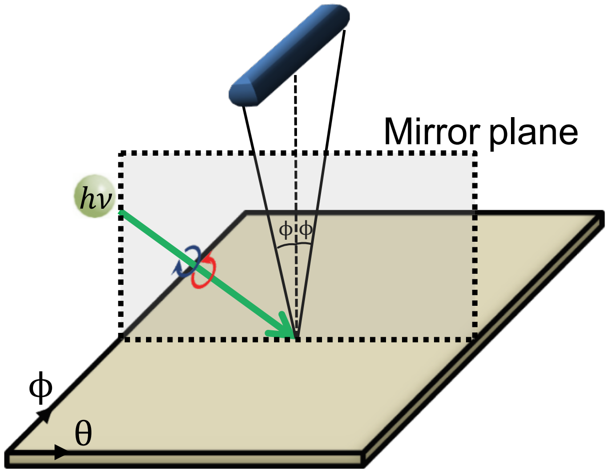
- Breaking mirror symmetry
- Geometrical contribution
- odd function of ϕ

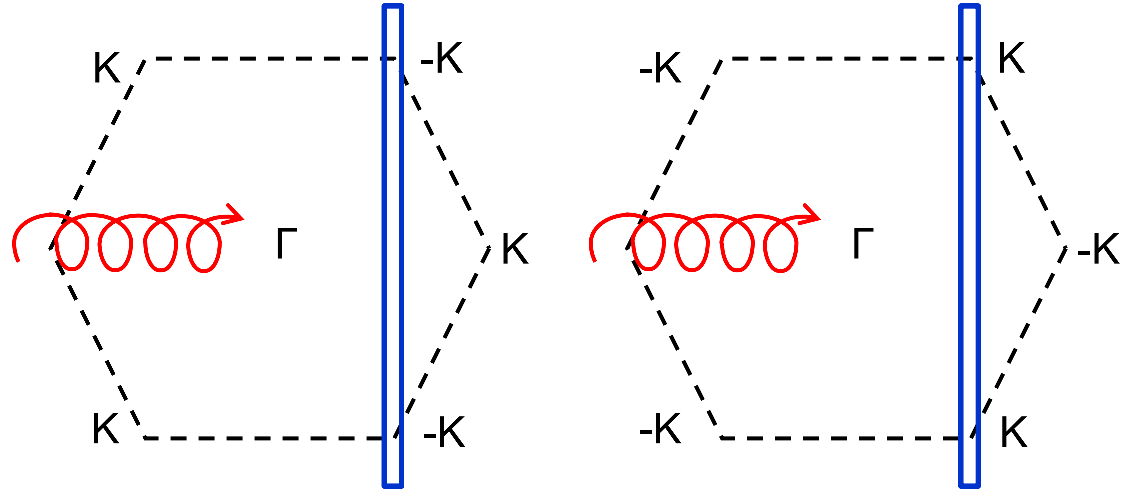
- Complexity of the wave function
- OAM contribution
- Proportional to OAM

⇧

Let's make this an even function

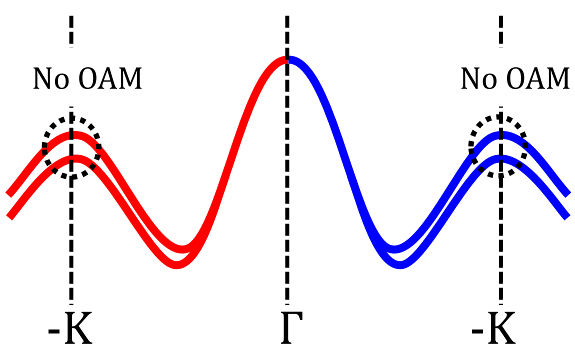
Expected CD pattern





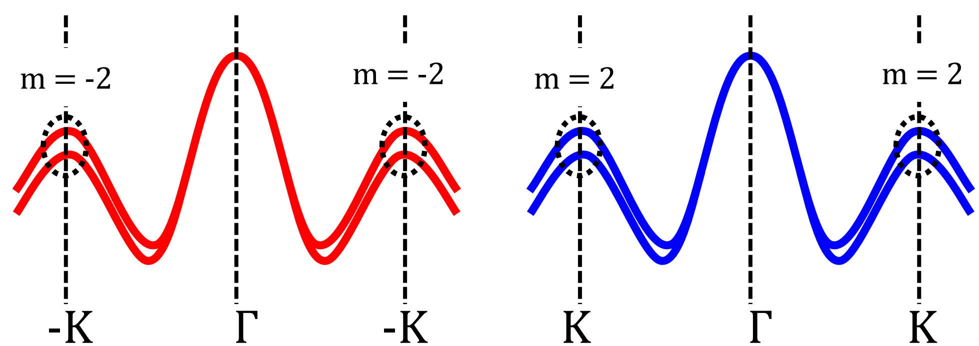
- Actual data contains both geometrical and OAM contributions

$CD = I_{RCP} - I_{LCP}$



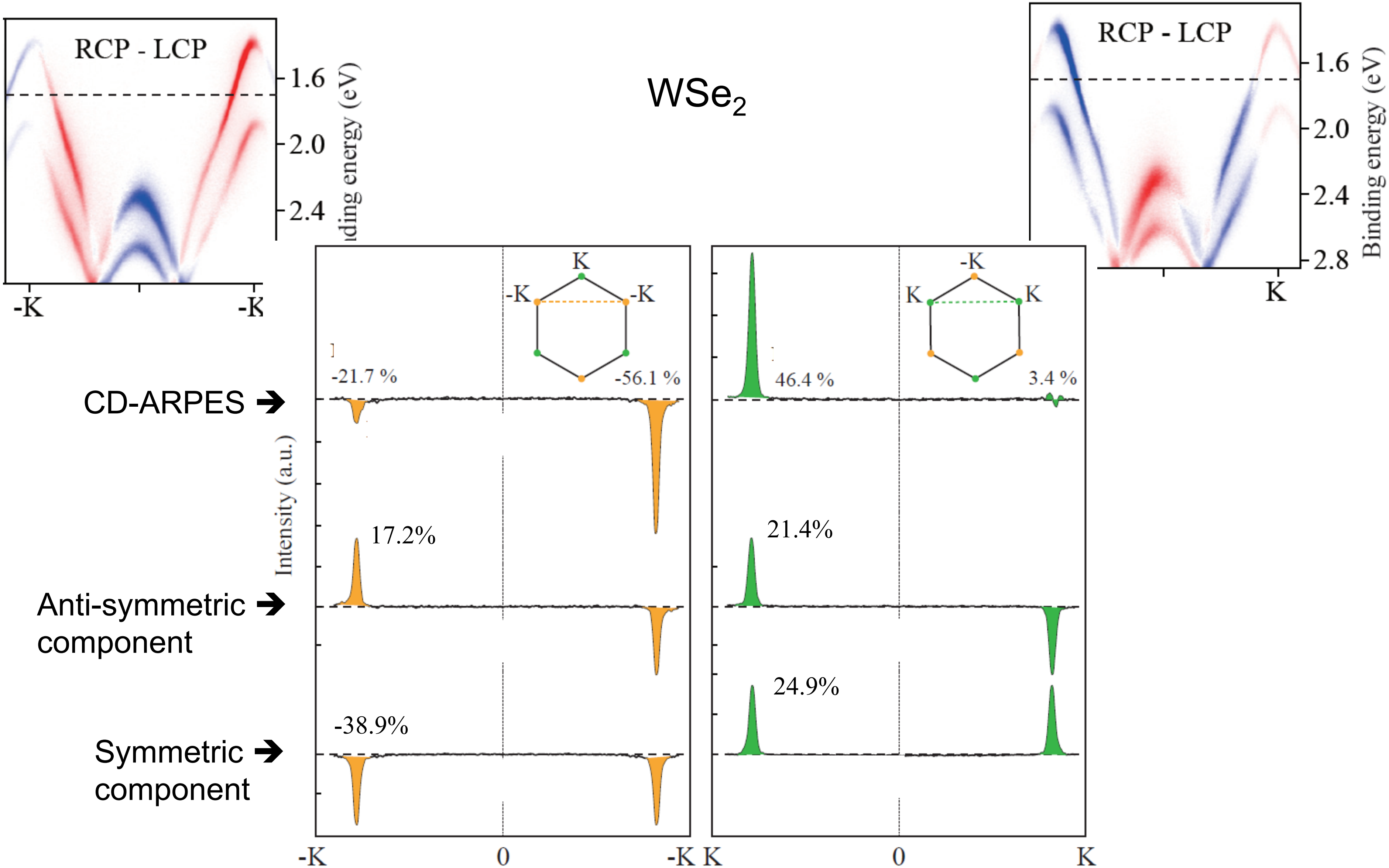
Geometrical contribution; odd function

$CD = I_{RCP} - I_{LCP}$

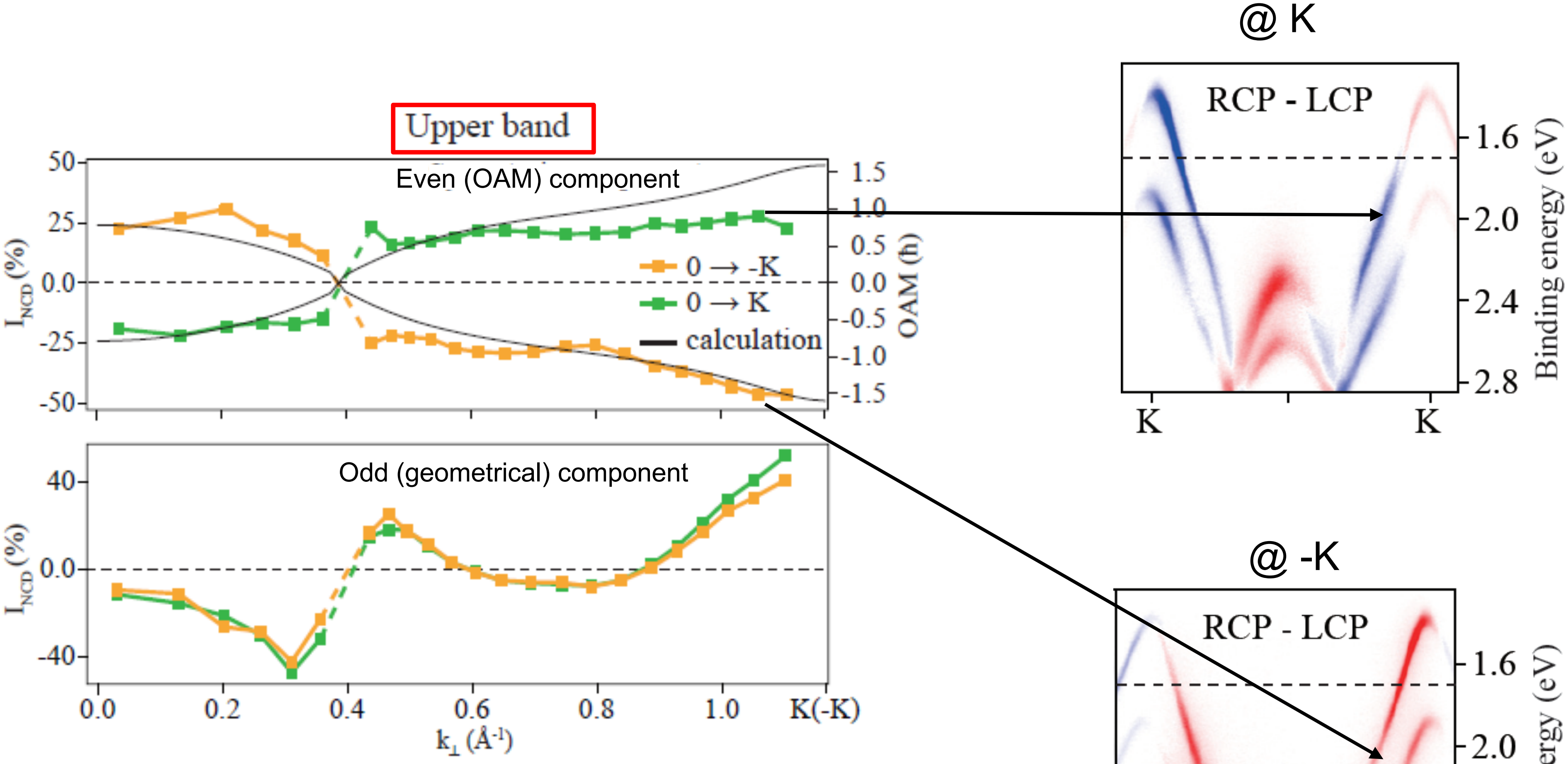


OAM contribution; even function

Extracting geometrical and OAM contributions

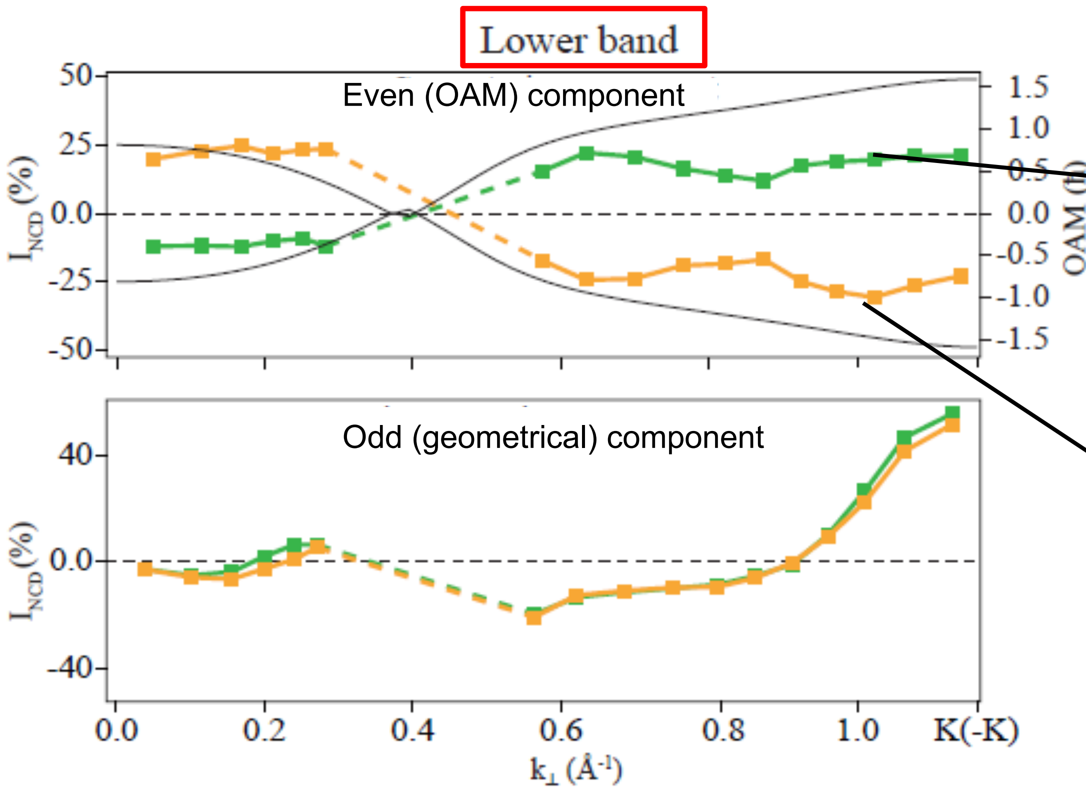


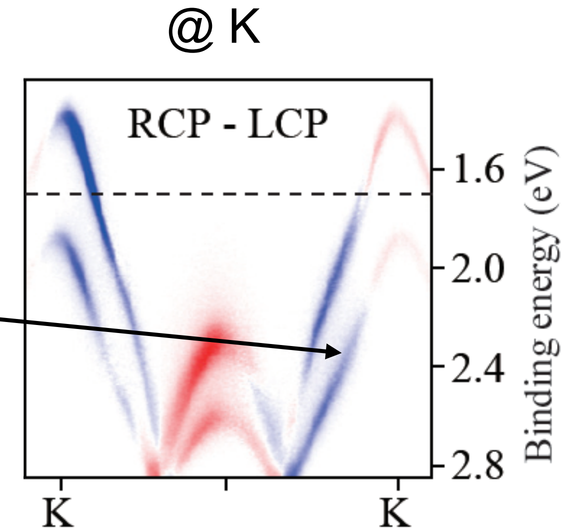
Even (OAM) and odd (geometrical) components

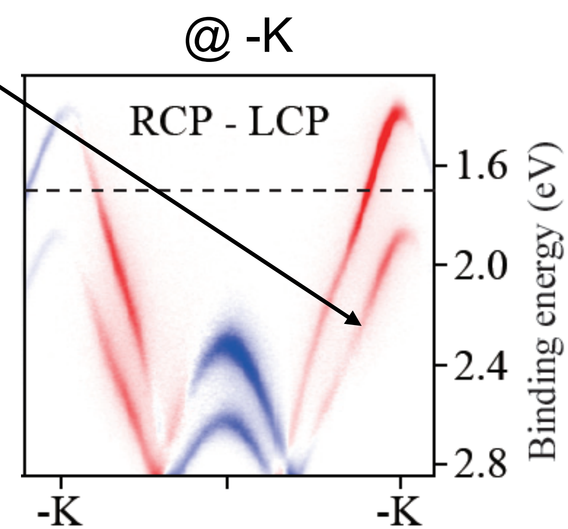


- Two different data sets (K-K and K'-K') show exactly same (opposite) behavior for odd (even) components

Even (OAM) and odd (geometrical) components



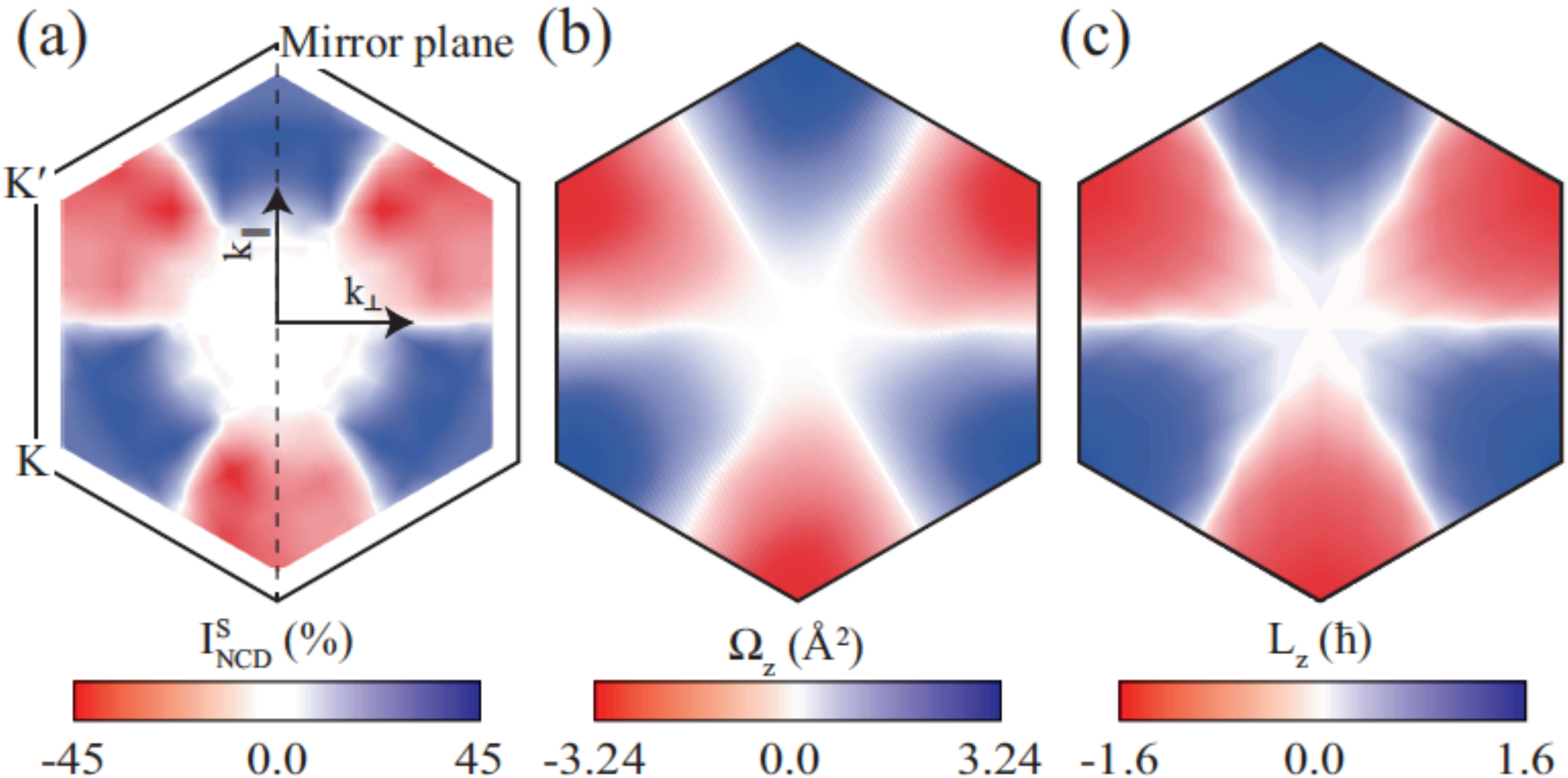




- We measured ~OAM by CD-ARPES
- Did we measure (hidden) Berry curvature?

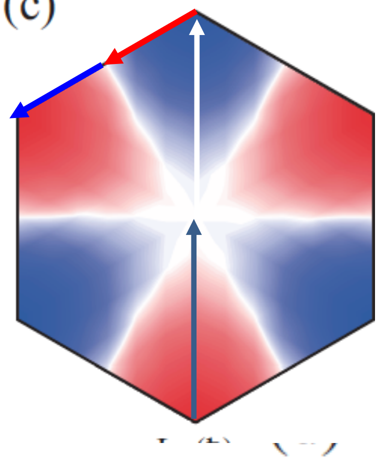
CD vs Berry curvature vs OAM

CD-ARPES (from surface layer) | Berry curvature (for 1 ML) | OAM (L_z) (for 1 ML)

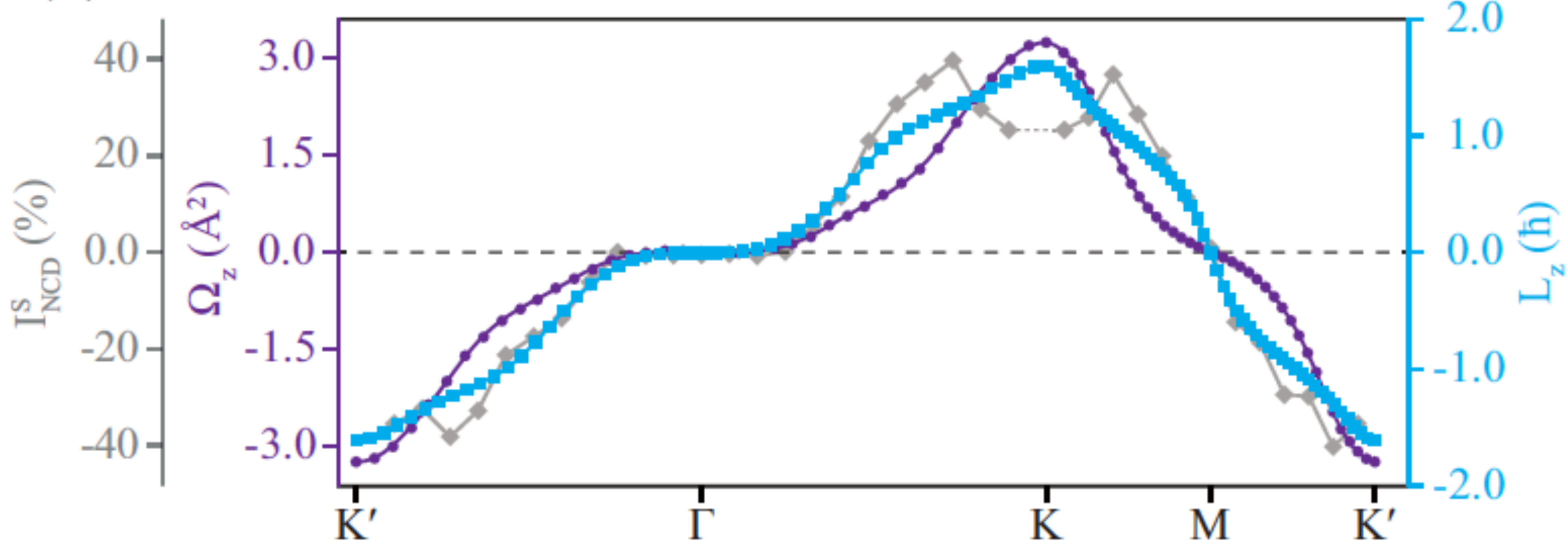


Along the high symmetry cuts

(c)



S. H. Cho et al, under review



Summary on ‘hidden’ Berry curvature

- Local nature of the Berry curvature (within a layer)
- ‘Hidden Berry curvature’ in inversion symmetric bulk
- OAM of the top-layer measured by CD-ARPES
- Similarity between CD, Berry curvature and OAM, indicating B
  erry curvature ~ OAM in this system
- Experimental measurement of hidden Berry curvature