Rashba and Dresselhaus Effects & Spin Transport

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Spin-orbit driven magnetic phenomena

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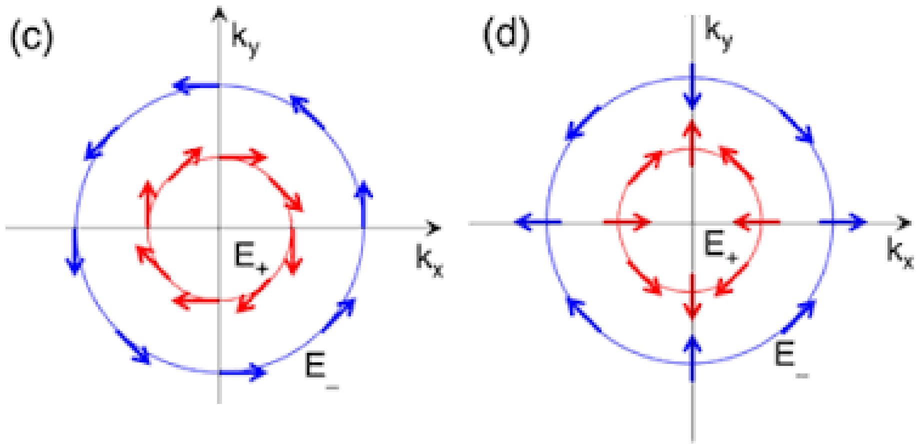
Outline –

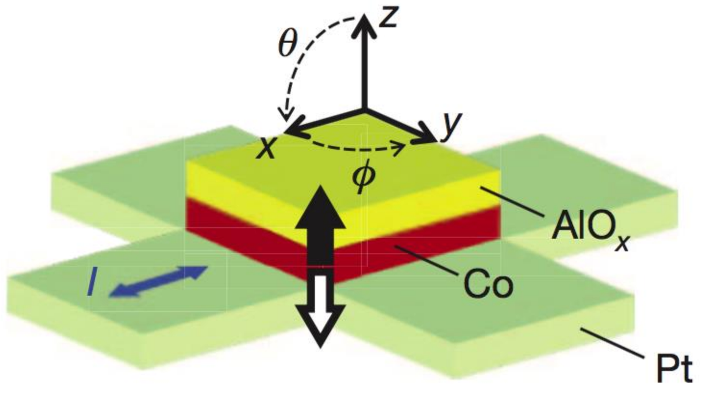
- Introduction – Spin-orbit driven magnetic phenomena
- Theory approaches for spin-orbit driven magnetic phenomena in 3D and 2D solids
- Rashba spin-orbit coupling – theory
- Dresselhaus spin-orbit coupling – theory
- Rashba & Dresselhaus spin-orbit coupling – experimental observation & deeper understanding
- Orbital Rashba effect, spin/orbital Hall effect & spin/orbital Rashba-Edelstein effect
- Implications for spin & orbital transport & spin-orbit driven magnetic phenomena

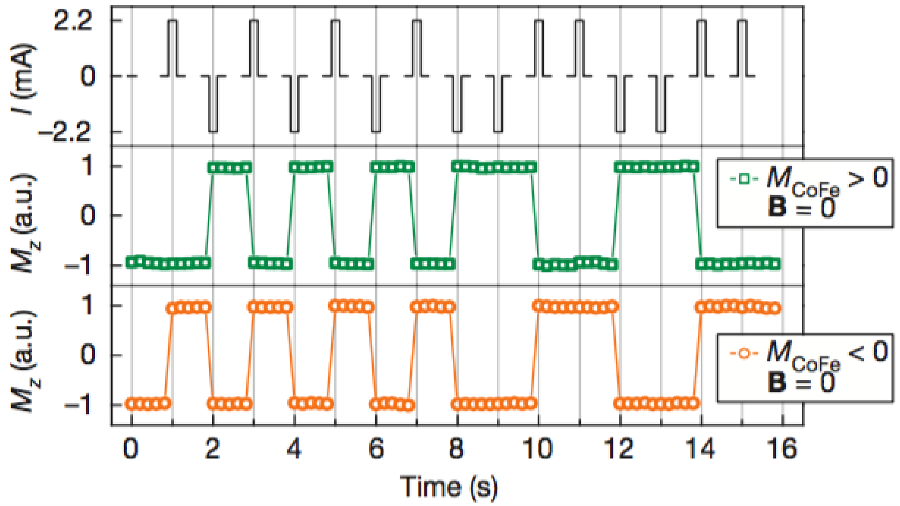


Rashba Dresselhaus

Introduction – Discovery of spin-orbit torques (SOTs)

Magnetization switching with current-induced SOT





Attributed to the spin Hall effect <u>or</u> Rashba effect

Caused by relativistic spin-orbit interaction in Pt metal

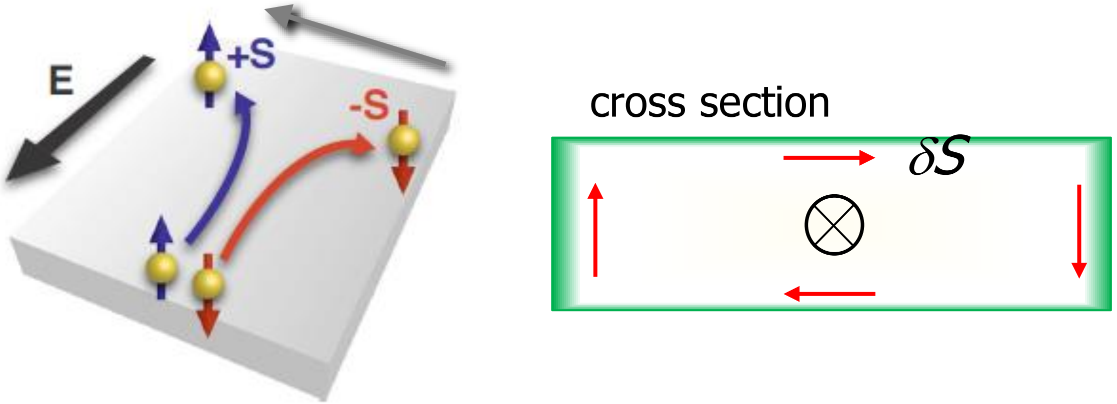
Miron et al, Nature Mater. **9**, 230 (2010)

Miron et al, Nature **476**, 189 (2011)

Liu et al, Science **336**, 555 (2012)

Review: Manchon et al, Rev. Mod. Phys. **91**, 035004 (2019)

Spin Hall effect – transverse spin current



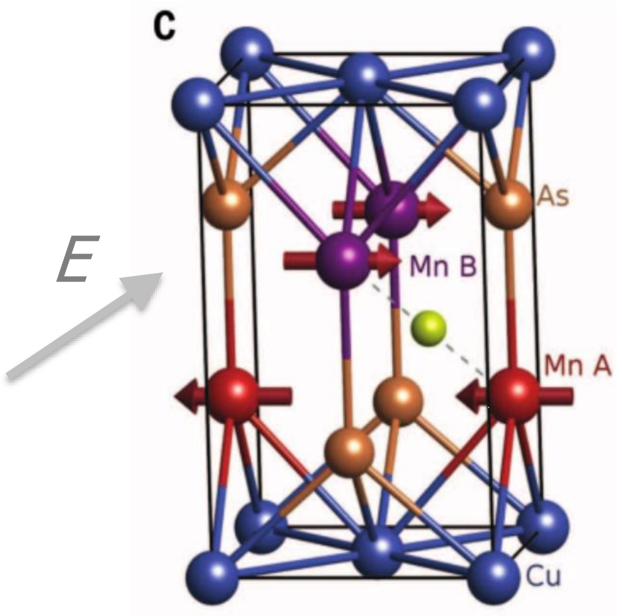
Hirsch, PRL **83**, 1834 (1999)

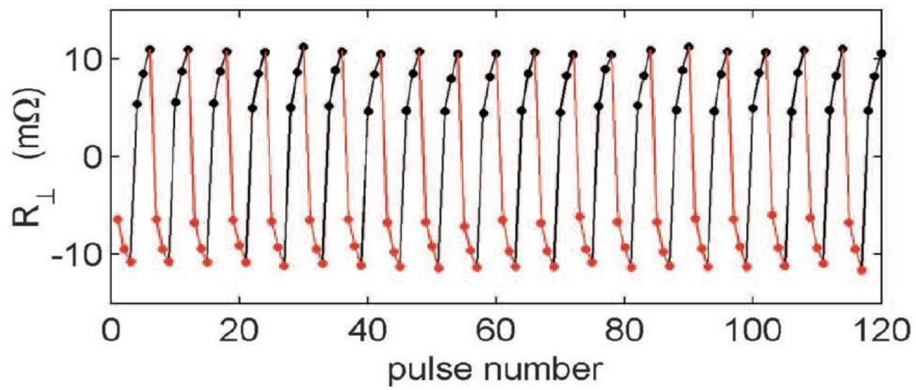
Introduction – Discovery of local spin-orbit torque

Antiferromagnets with special symmetry properties

Attributed to staggered SOTs caused by Rashba-Edelstein effect

CuMnAs



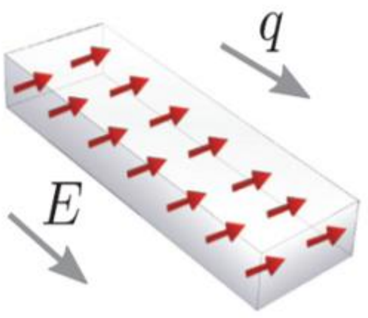


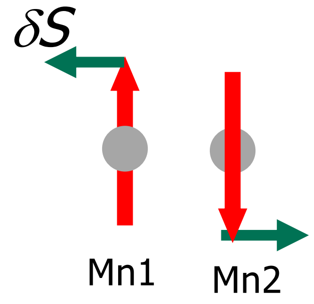
Wadley et al, Science **351**, 587 (2016)

Zelezny et al, PRB **95**, 014403 (2017)

Atomic spin Rashba-Edelstein effect – transverse spin polarization

(relativistic)



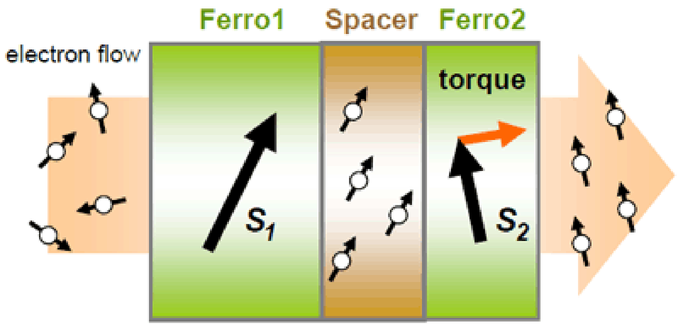


Review: Manchon et al, Rev. Mod. Phys. **91**, 035004 (2019)

Edelstein, Solid State Comm. **73**, 233 (1990)

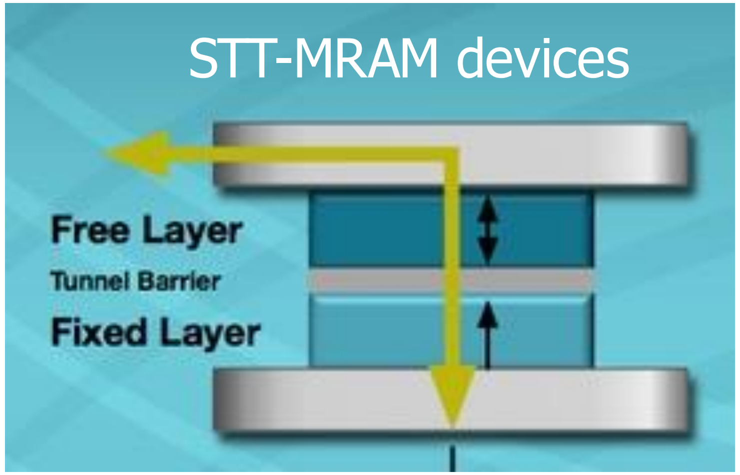
Spin-orbit torque driven devices vs. spin-transfer torque driven devices

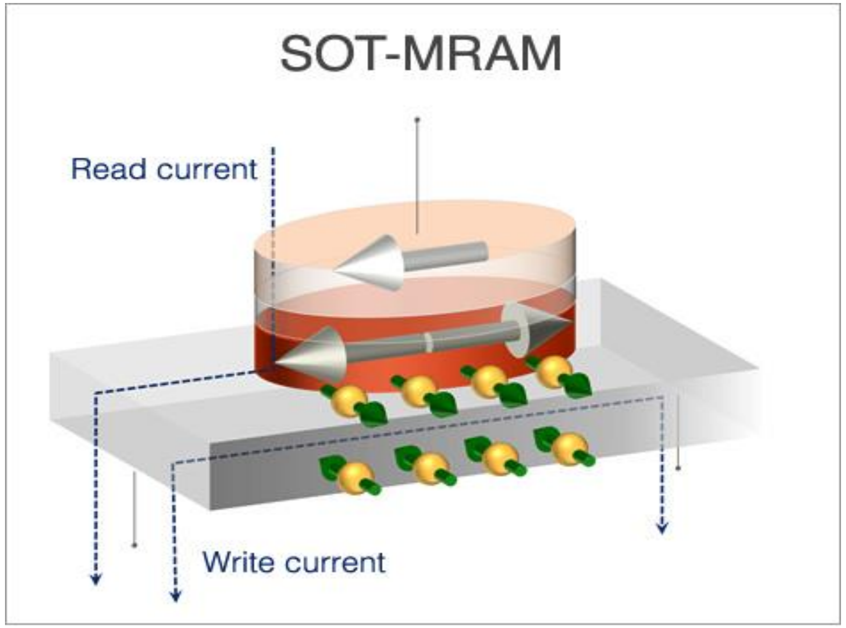
Spin-transfer torque driven switching



Longitudinal spin-polarized current

Slonczewski, JMMM **159**, L1 (1996)





Transversal pure spin current

Hirsch PRL **83**, 1834 (1999) (SHE)

Miron et al, Nature **476**, 189 (2011)

Theoretical explanations - A

Consider periodic solids in 2-dim. or in 3-dimensions

Different ways to treat electronic structure and induced spin transport

A) All electron Hamiltonian

Density-functional theory (effective single-particle Hamiltonian)

$$\hat{H} = \sum_i \frac{p_i^2}{2m} + V_{e-e} + V_{e-N} \Longrightarrow \hat{H}_{DFT} = -\frac{\hbar^2\nabla^2}{2m} + \int \frac{n(r')}{|r-r'|} dr' + V_{xc}[n] + V_{e-N}$$

Kohn-Sham equation: $\hat{H}|\psi_{nk}\rangle = \varepsilon_{nk}|\psi_{nk}\rangle$ with $n(r) = \sum_{nk\ occ} |\psi_{nk}|^2|$

Calculate electron band structure ε_{nk} and quantities like induced spin polarization $\delta\boldsymbol{S}$ and induced spin current $\boldsymbol{j}_S$

Advantage: very accurate, materials' specific numbers. Disadvantage: low physical insight

Consider periodic solids in 2-dim. or in 3-dimensions

B) Effective low-energy or continuum models

$\hat{\mathcal{H}}(k)|u_{nk}\rangle = \varepsilon_{nk}|u_{nk}\rangle$ Few bands, considered in parts of *k*-space (Brillouin zone)

<u>Steps:</u> Lattice periodicity: $V(\boldsymbol{r} + \boldsymbol{R}_i) = V(\boldsymbol{r})$ For all lattice vectors $\boldsymbol{R}_i$

Bloch's theorem: $\psi_{nk}(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}} u_{nk}(\boldsymbol{r})$ where u_{nk} is a periodic function, $u_{nk}(\boldsymbol{r} + \boldsymbol{R}_i) = u_{nk}(\boldsymbol{r})$

Substitute in Schrödinger-type equation: $\hat{H}|\psi_{nk}\rangle = \varepsilon_{nk}|\psi_{nk}\rangle$

$$\hat{H}\left|e^{ik\cdot r}u_{nk}\right\rangle = \varepsilon_{nk}e^{ik\cdot r}\left|u_{nk}\right\rangle \Rightarrow \underbrace{e^{-ik\cdot r}\hat{H}e^{ik\cdot r}}_{\hat{\mathcal{H}}(k)}|u_{nk}\rangle = \varepsilon_{nk}|u_{nk}\rangle$$

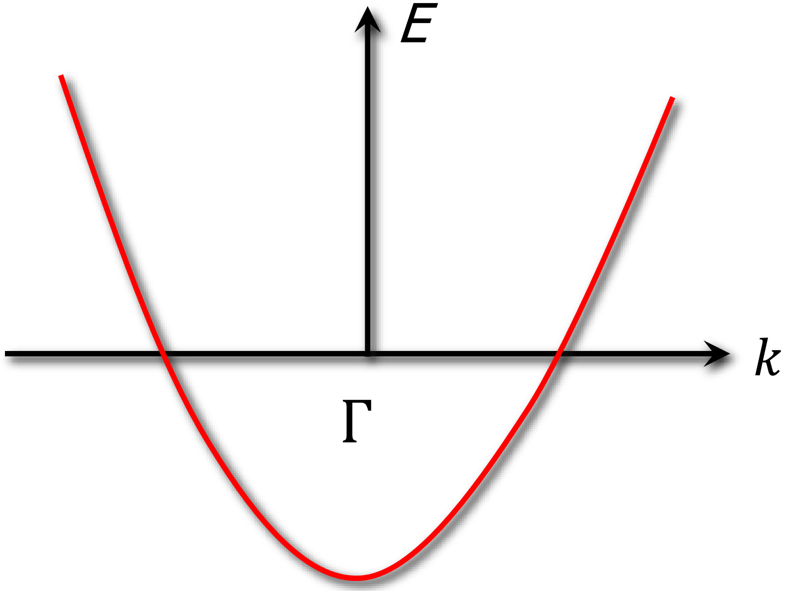
$$\hat{\mathcal{H}}(k) \longrightarrow \hat{\mathcal{H}}(k)|u_{nk}\rangle = \varepsilon_{nk}|u_{nk}\rangle$$

Low-energy model approach

Typical form of the Hamiltonian: $\hat{\mathcal{H}}(\boldsymbol{k}) = \dfrac{\hbar^2 k^2}{2m} + F(\boldsymbol{k})$

In k-space - 1st Brillouin zone

(itinerant electrons)



Parabolic band around center of BZ

<u>Common procedure:</u>

1) include degrees of freedom in $\hat{\mathcal{H}}(\boldsymbol{k})$ such as spin

$$\hat{\mathcal{H}}(\boldsymbol{k}, \hat{\boldsymbol{\sigma}}) \quad [\hat{\boldsymbol{S}} = \frac{\hbar \hat{\boldsymbol{\sigma}}}{2}]$$

2) Obtain eigenenergies & analyze typical effects

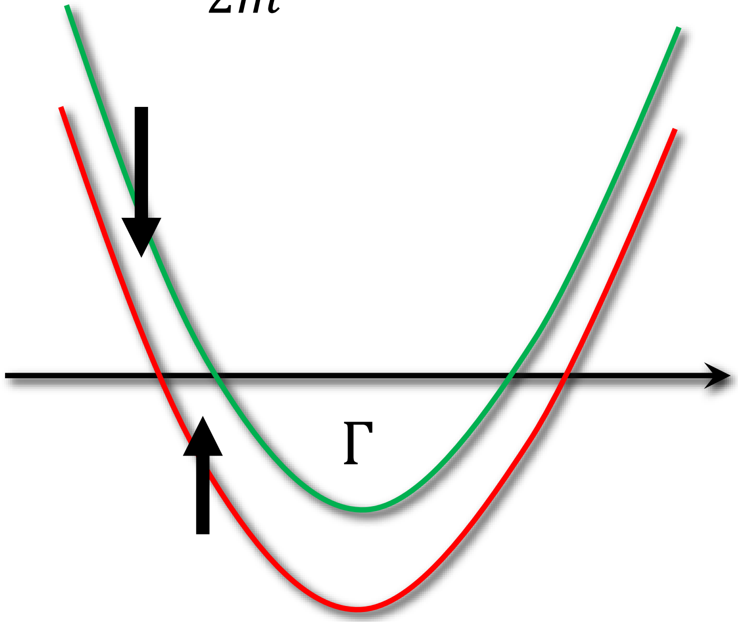
Advantage: simple insight in low-energy physics. Disadvantage: not accurate nor materials' specific

Improvements – use tight-binding bands, or bands fitted to DFT calculations

Low-energy Hamiltonians: Some warm-up examples

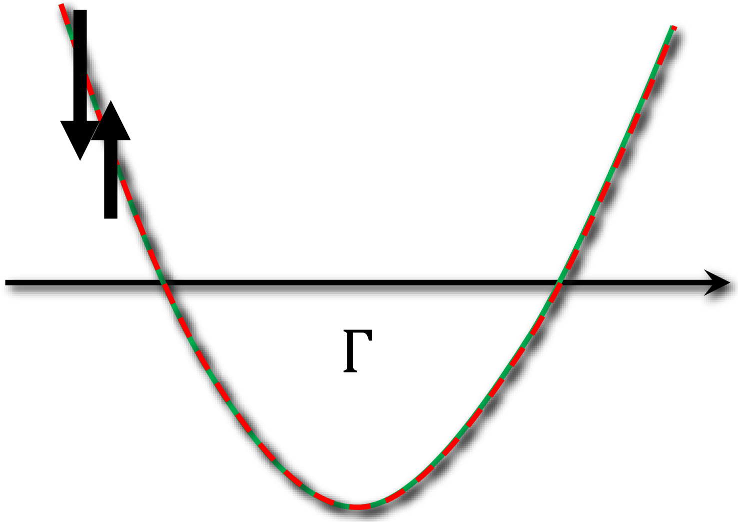
Pauli spin matrices: $\sigma_0 = \mathbb{I},\ \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$$\hat{\mathcal{H}} = \frac{\hbar^2 k^2}{2m^*}\sigma_0 + M_0\sigma_z$$



Simple ferromagnet

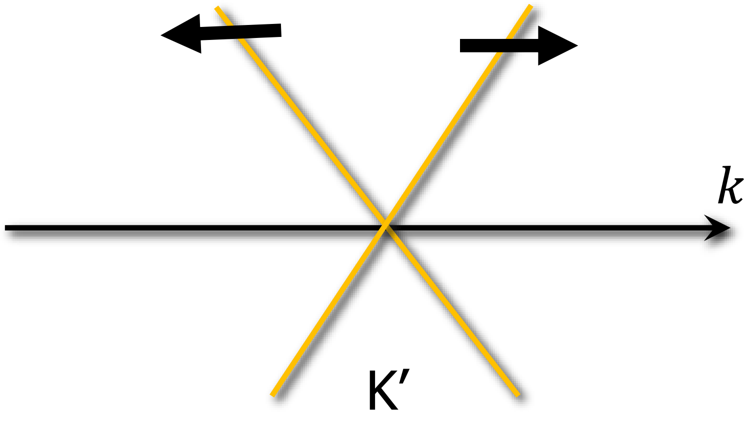
$$\hat{\mathcal{H}} = \frac{\hbar^2 k^2}{2m^*}\sigma_0$$



Nonmagnetic metal

(Or AFM with spin degeneracy)

$$\hat{\mathcal{H}} = \hbar v_F(\sigma_x k_x + \sigma_y k_y)$$



“Dirac” material

Next:
Include spin-orbit coupling

Atomic spin-orbit interaction

Coupling of the electron spin with effective magnetic field due to electron orbital motion:

$$H_{S.O.} \propto -\vec{\mu} \cdot \vec{B}_{eff} \quad and \quad B_{eff} = -\frac{1}{c^2} \vec{v} \times \vec{E} \quad and \quad \vec{E} = -\frac{\partial \Phi}{\partial r} = -\frac{\partial \Phi}{\partial r} \frac{\partial \vec{r}}{\partial r} = -\frac{1}{-e} \frac{\partial V}{\partial r} \frac{\vec{r}}{r}$$

Gives: $$H_{S.O.} \propto \vec{S} \cdot (\vec{r} \times \vec{v}) \frac{1}{r} \frac{\partial V}{\partial r} \propto \frac{1}{r} \frac{\partial V}{\partial r} (\vec{S} \cdot \vec{L}) \qquad \vec{\mu}_s = -2 \left(\frac{e}{2m_e} \right) \vec{S} \qquad \vec{L} = \vec{r} \times \vec{p}$$

With precise prefactor: $$\boxed{\hat{H}_{S.O.} = \frac{1}{2m^2c^2} \frac{1}{r} \frac{\partial V}{\partial r} (\vec{S} \cdot \vec{L})}$$ or $$\widehat{H}_{S.O.} = \xi (\widehat{\boldsymbol{L}} \cdot \widehat{\boldsymbol{S}})$$

Total Hamiltonian: $$\hat{H} = \hat{H}_0 + \hat{H}_{S.O.}$$

(small because $1/c^2$ is small)

BUT: provides the coupling of spin to orbital motion and therefore to the lattice !

Basic symmetry properties

$$\hat{\mathcal{H}}(\boldsymbol{k},\boldsymbol{\sigma})|u_{n\boldsymbol{k}\sigma}\rangle = \varepsilon_n(\boldsymbol{k},\sigma)|u_{n\boldsymbol{k}\sigma}\rangle$$ (spin quantum number)

1) Time reversal operation $\mathcal{T}$: $t \to -t, \quad p \to -p, \quad S \to -S$

For spin-1/2 systems: $\hat{\boldsymbol{S}} \to \mathcal{T}^{-1}\hat{\boldsymbol{S}}\mathcal{T} = -\hat{\boldsymbol{S}}$

Gives: $\hat{\mathcal{T}} = i\sigma_y K \Rightarrow \hat{\mathcal{T}}^2 = -\mathbb{I}$ (K : complex conjugation)

<u>Time reversal:</u> $[\hat{\mathcal{H}},\hat{\mathcal{T}}] = 0 \Rightarrow \hat{\mathcal{T}}|u_{nk\sigma}\rangle$ Is eigenstate at same eigenenergy $\boxed{\varepsilon_n(-\boldsymbol{k},-\sigma) = \varepsilon_n(\boldsymbol{k},\sigma)}$

2) Spatial inversion operation $\mathcal{P}$: $x \to -x, \quad p \to -p, \quad S \to S, \quad L \to L$

If $[\hat{\mathcal{H}},\mathcal{P}] = 0 \Rightarrow \mathcal{P}|u_{nk\sigma}\rangle$ Is eigenstate at same eigenenergy $\boxed{\varepsilon_n(-\boldsymbol{k},\sigma) = \varepsilon_n(\boldsymbol{k},\sigma)}$

<u>Both time and inversion symmetry $\mathcal{PT}$:</u> $\boxed{\varepsilon_n(\boldsymbol{k},-\sigma) = \varepsilon_n(\boldsymbol{k},\sigma)}$

(Kramers degeneracy)

Low-energy models: Rashba and Dresselhaus spin-orbit coupling

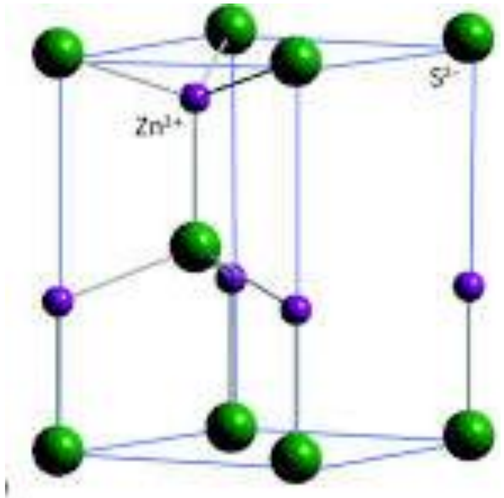
Rashba spin-orbit coupling

Originally proposed for semiconductors with wurtzite structure (ZnS, CdS)

(time rev.symmetry, no inversion symmetry, hexagonal)

$$H_{S.O.} \propto -\vec{\mu} \cdot \vec{B}_{eff} \quad \Rightarrow \frac{-g\mu_B}{2mc^2} \hat{\boldsymbol{\sigma}} \cdot (\boldsymbol{p} \times \boldsymbol{E})$$

$$\boldsymbol{E} = E_0 \hat{z}$$



Emmanuel Rashba
(1927 – 2025)

$$\Rightarrow \quad H_{R-SO} = \alpha\,(\hat{\boldsymbol{z}} \times \boldsymbol{p}) \cdot \hat{\boldsymbol{\sigma}}$$

Or: $$H_{R-SO} = \alpha_R (\hat{\boldsymbol{z}} \times \boldsymbol{k}) \cdot \hat{\boldsymbol{\sigma}}$$

With $\alpha = \frac{g\mu_B E_0}{2mc^2}$ the Rashba spin-orbit constant – R-SOC works like a *k*-dependent magnetic field

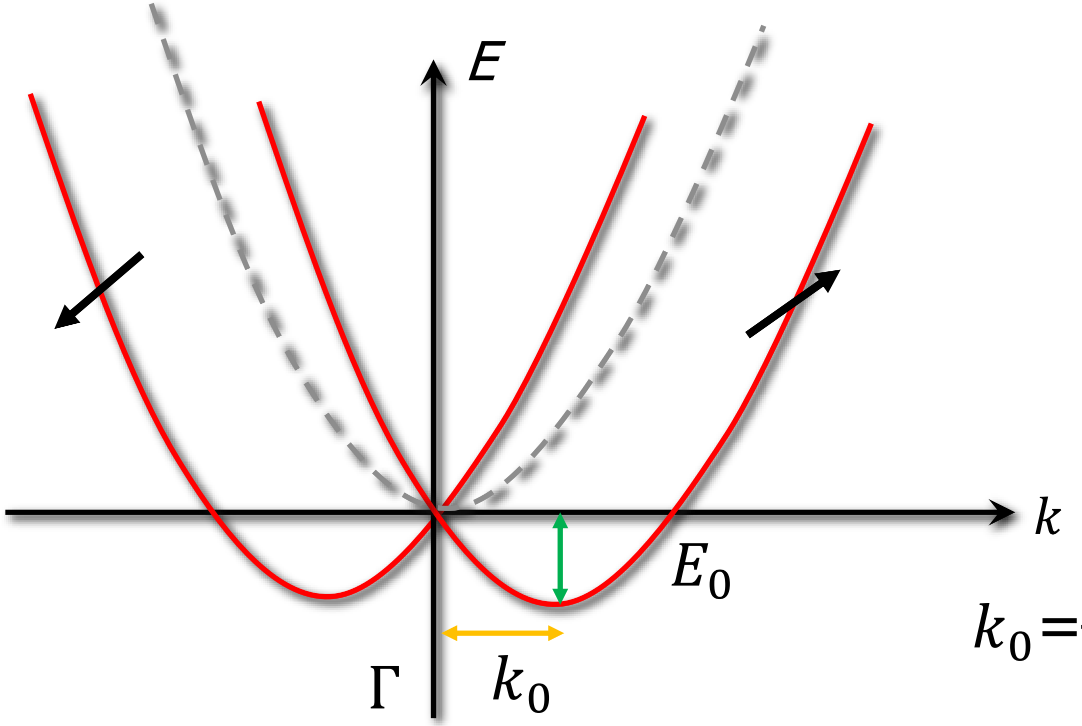
Rashba & Shekla, Fiz. Tverd. Tela CP **2**, 62 (1959)

Bychkov-Rashba spin-orbit coupling

2nd proposal for Rashba spin-orbit coupling: 2 dim. systems – surfaces or 2D electron gas at interfaces

$$\mathcal{H}(\boldsymbol{k},\boldsymbol{\sigma}) = \frac{\hbar^2 k^2}{2m^*} + \alpha(\boldsymbol{\sigma}\times\boldsymbol{k})\cdot\hat{\boldsymbol{z}}$$

$$H_{R-SO} = \alpha(k_x\sigma_y - k_y\sigma_x)$$



Energy dispersions:

$$\varepsilon_\pm = \frac{\hbar^2 k^2}{2m^*} \pm \alpha k$$

$$k_0 = \frac{\alpha m^*}{\hbar^2}$$

$$E_0 = -\frac{m^*\alpha^2}{2\hbar^2}$$

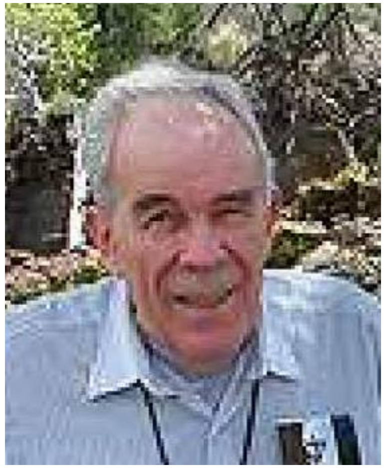
And: spin texture of energy bands (discussed later)

Bychkov & Rashba, JETP Lett. **39**, 78 (1984)

Dresselhaus spin-orbit coupling

Consider now a different crystal structure (zinc blende) e.g. GaAs

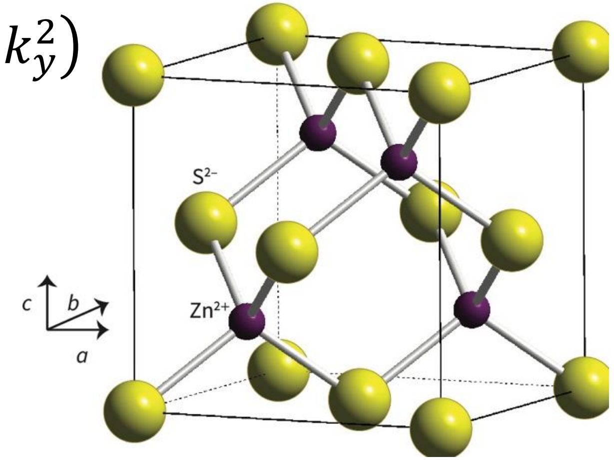
(time reversal, no inversion symmetry, cubic)



Gene Dresselhaus (1929 – 2021)

Proposed low-energy Hamiltonian – 3-dim.:

$$H_{D-SOC} = \gamma_D[\sigma_x k_x(k_y^2 - k_z^2) + \sigma_y k_y(k_z^2 - k_x^2) + \sigma_z k_z(k_x^2 - k_y^2)$$



Energy shifts: $\varepsilon_\pm =$

$$\pm\gamma_D[k^2(k_x^2k_y^2 + k_y^2k_z^2 + k_z^2k_x^2) - 9k_x^2k_y^2k_z^2]^{1/2}$$

2-dim. systems: $[\langle k_z\rangle = 0, \langle k_z^2\rangle \neq 0]$

$$H_{D-SOC} = \beta(\sigma_x k_x - \sigma_y k_y)$$

And cubic term: $H_{D-SOC}^{(3)} = \xi k_x k_y(k_y\sigma_x - k_x\sigma_y)$

Dresselhaus, Phys. Rev. **100**, 580 (1955)

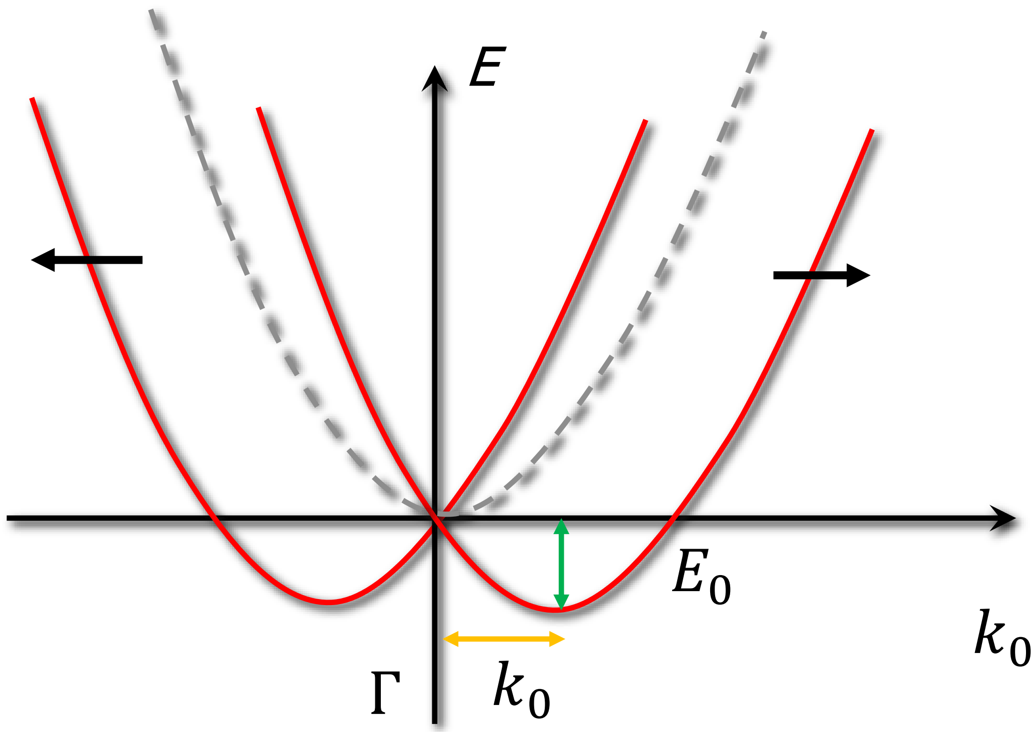
Dresselhaus spin-orbit coupling

Hamiltonian for 2-dim. electron gas system: $$\mathcal{H} = \frac{\hbar^2 k^2}{2m^*} + \beta(\sigma_x k_x - \sigma_y k_y)$$

Energy dispersions: $$\varepsilon_\pm = \frac{\hbar^2 k^2}{2m^*} \pm \beta k$$

Same as for Rashba spin-orbit coupling!

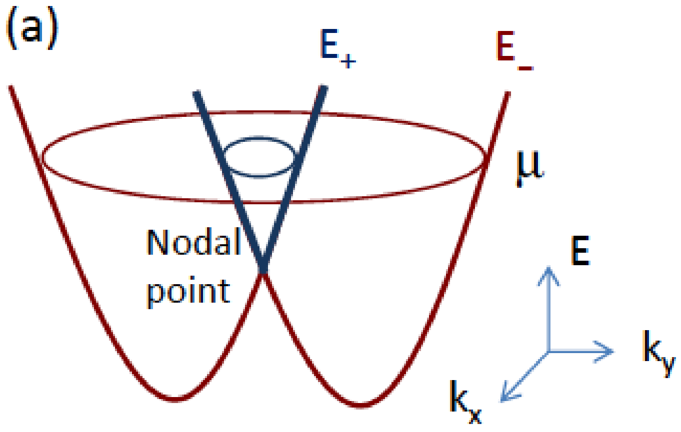
But spin textures are not the same!



$$k_0 = \frac{\beta m^*}{\hbar^2}$$

Spin textures or "spin-momentum locking"

Same energies



$$\boldsymbol{B}_R(\boldsymbol{k})\cdot\hat{\boldsymbol{\sigma}} = \alpha(k_y,-k_x,0)\cdot\hat{\boldsymbol{\sigma}}$$

"*k*-dependent Zeeman field"

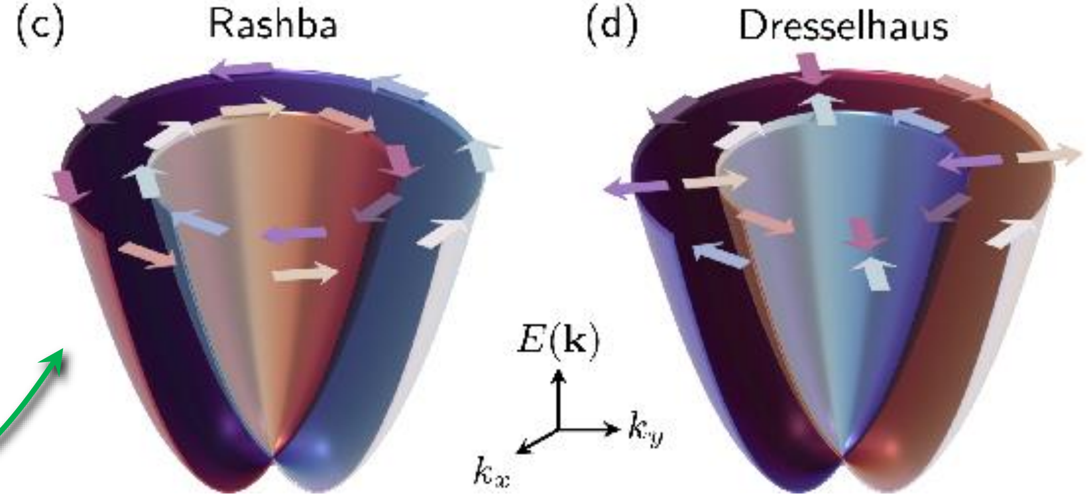
Time-rev. symmetry present

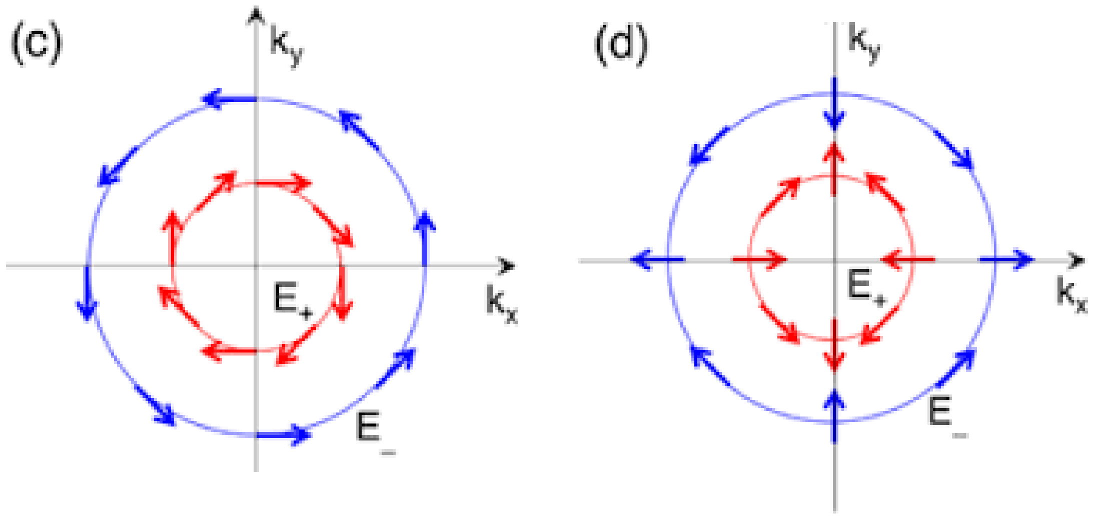
$$\boxed{\varepsilon_n(-\boldsymbol{k},-\sigma) = \varepsilon_n(\boldsymbol{k},\sigma)}$$

Spatial inversion broken:

$$\boxed{\varepsilon_n(-\boldsymbol{k},\sigma) \neq \varepsilon_n(\boldsymbol{k},\sigma)}$$

Different spin textures





So far, all low-energy model theory.

Figure removed.

What about experiments?

$$\varepsilon_{\pm} = \frac{\hbar^2 k^2}{2m^*} \pm \alpha k$$

Best for free-electron
type materials
in 2-dimensions

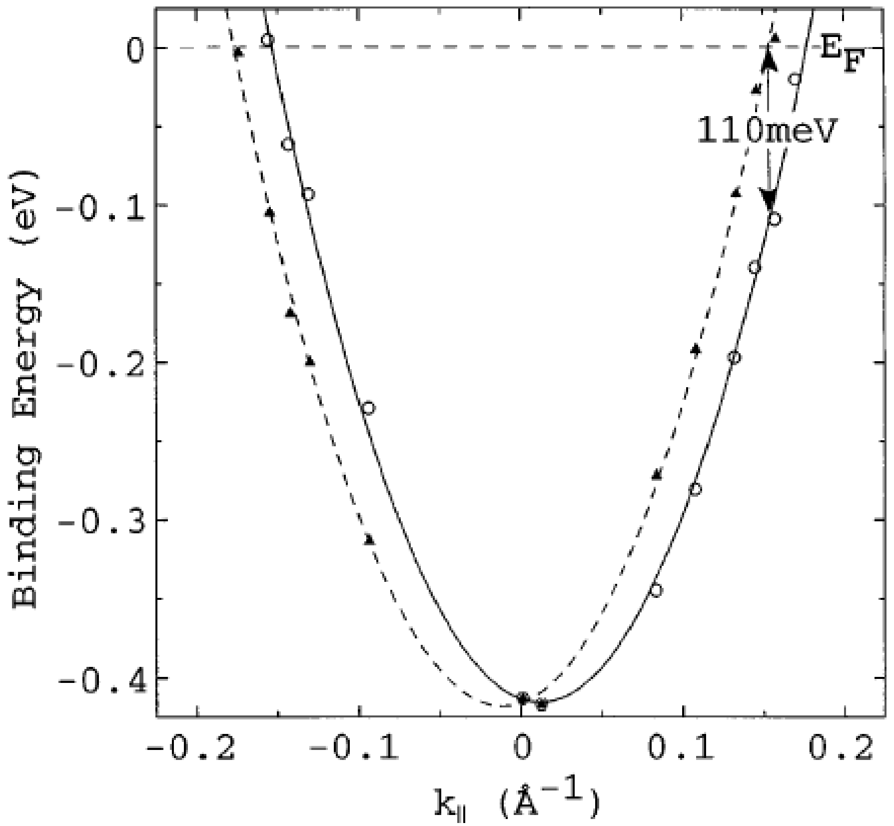
α in units eV Å
large for heavy materials (large SOC)

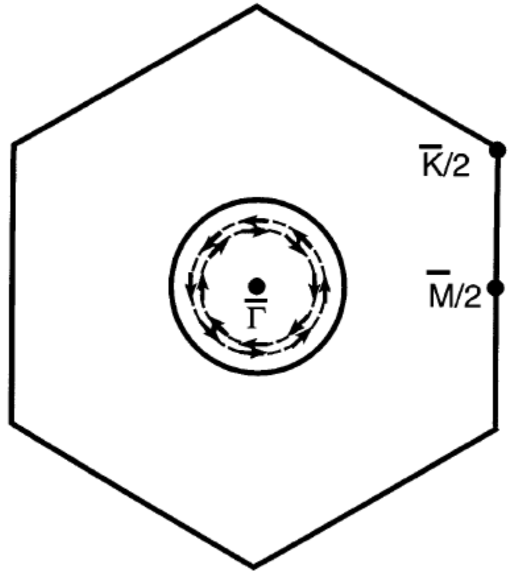
Angular resolved photoemission experiments (ARPES)

Surface state of Au(111)

$$\varepsilon_{\pm} = \frac{\hbar^2 k^2}{2m^*} \pm \alpha_R k$$

$$\alpha_R = \frac{\hbar^2 k_0}{m^*}$$



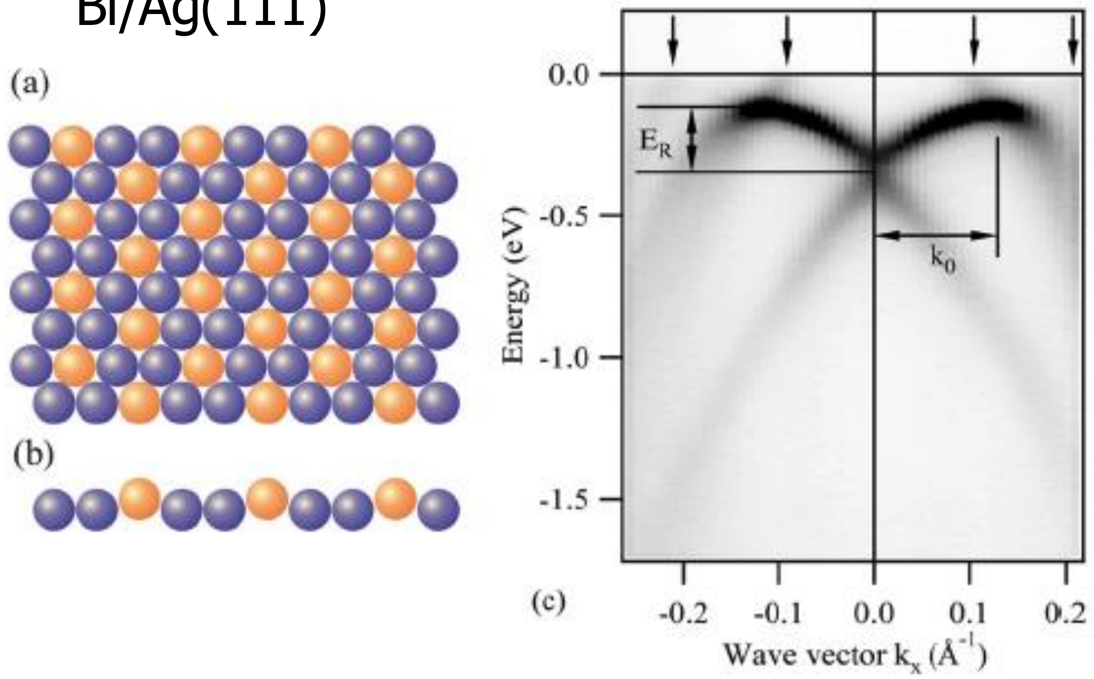


Energy splitting of 0.11 eV

LaShell et al, PRL **77,** 3419 (1996)

ARPES on other materials

Bi/Ag(111)



Size of Rashba parameter $\alpha_R = \frac{\hbar^2 k_0}{m^*}$

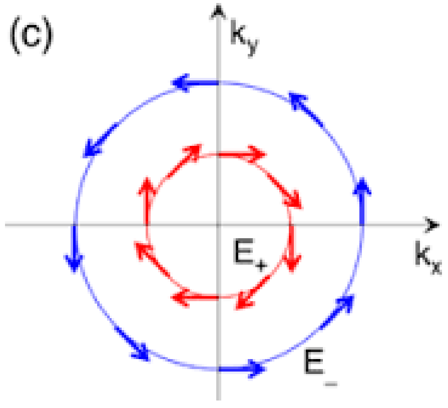
Material	E_R (meV)	k_0 (Å^{-1})	α_R (eV Å)	Reference
InGaAs/InAlAs heterostructure	<1	0.028	0.07	[4]
Ag(111) surface state	<0.2	0.004	0.03	[5,6]
Au(111) surface state	2.1	0.012	0.33	[6,7]
Bi(111) surface state	~14	~0.05	~0.56	[8]
Bi/Ag(111) surface alloy	200	0.13	3.05	This work

Giant Rashba spin-splitting observed

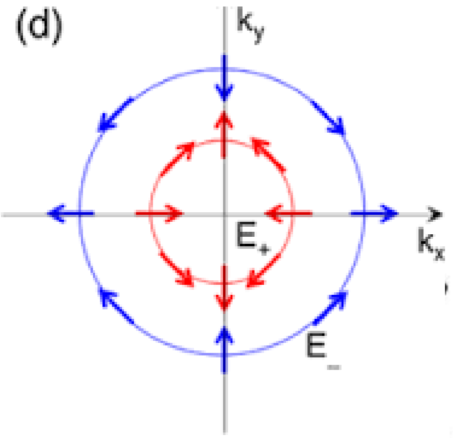
Ast et al, PRL **98**, 186807 (2007)

What about the spin texture?

Rashba - type spin texture observed with spin-polarized ARPES on (bulk) BiTeI



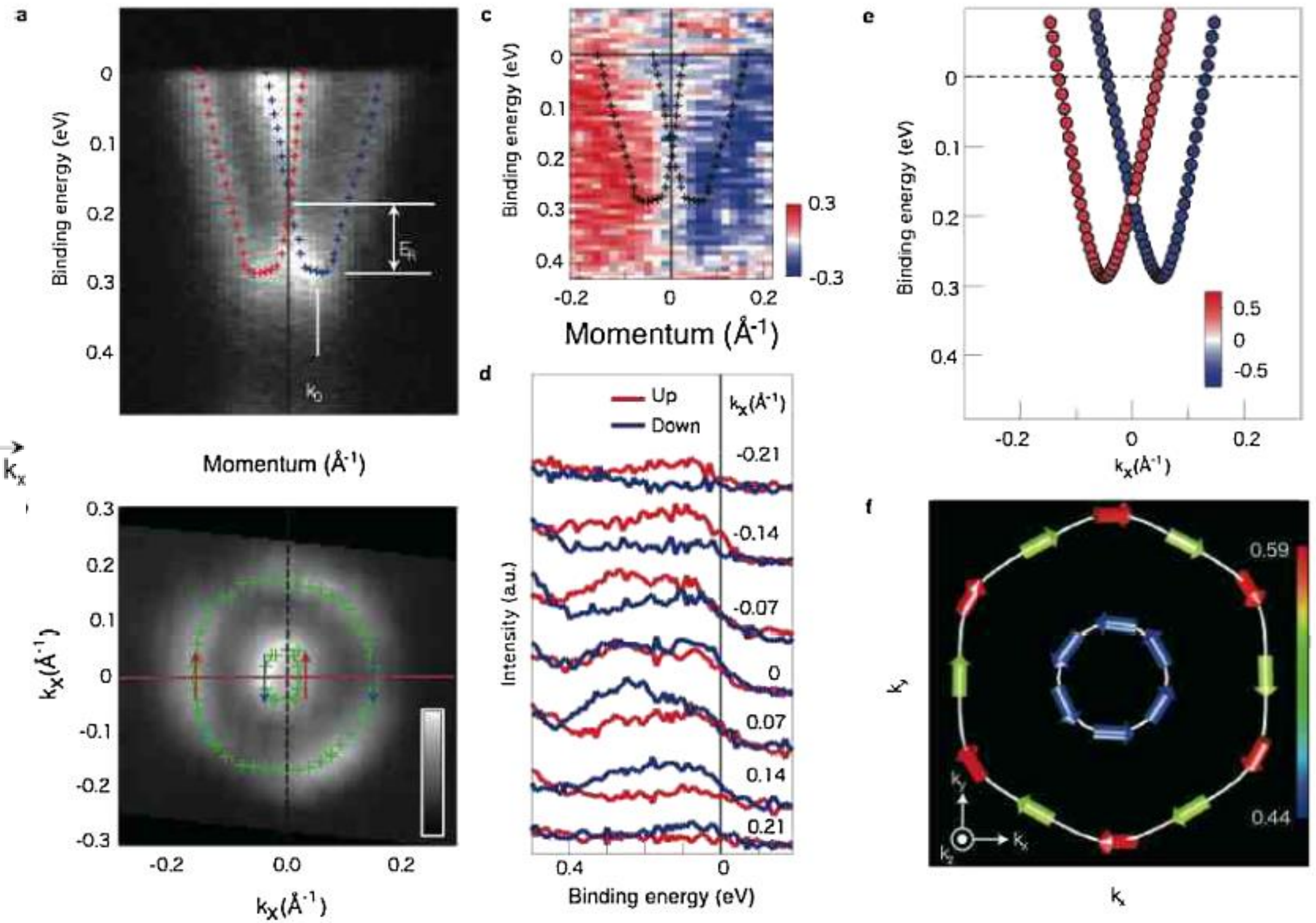
Rashba



Dresselhaus

SP-ARPES

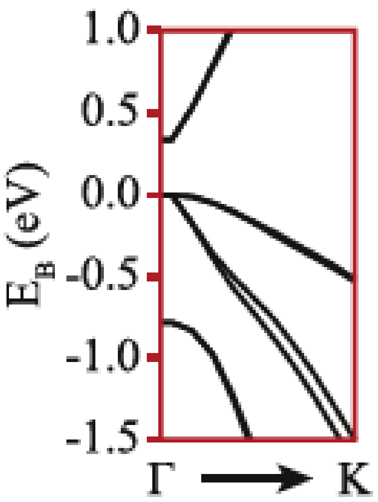
Theory



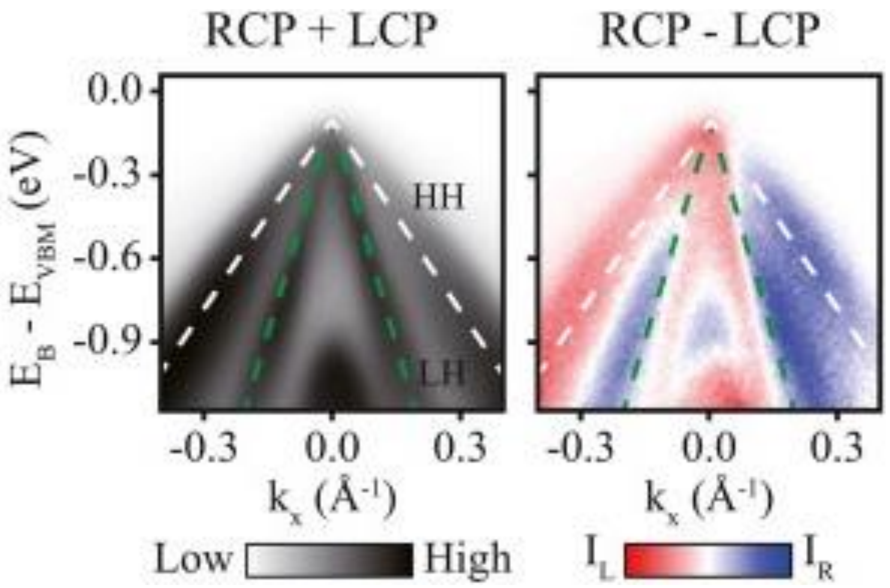
Ishizaka et al, Nature Mater. **10**, 521 (2011)

Dresselhaus spin texture - observation

Zinc-blende InSb



Using circular dichroism in ARPES



Cho et al, Curr. Appl. Phys. **30**, 96 (2021)

➢ Most materials have a combination of Dresselhaus & Rashba spin textures

Is all understood?

Back to the Rashba parameter – consider Au

$$H_{S.O.} \propto \frac{-g\mu_B \hbar}{2mc^2} \hat{\boldsymbol{\sigma}} \cdot (\boldsymbol{k} \times \boldsymbol{E}) \qquad \alpha = \frac{g\mu_B E_0}{2mc^2}$$

$\nabla V \sim \Phi/\lambda_F$ ~ 1 eV/Å

Fermi wavelength: ~5 Å, Φ~4.3 eV ⟹ $\Delta E_{shift} \sim \alpha_R k$

Energy splitting of 10^{-6} eV, measured 0.11 eV !

⟹ The effect is too small, potential gradient is still dominated by the Coulomb nuclear field

Free-electron approximation is insufficient, need a tight-binding model with orbitals.

3-orbitals per Au atom – p_x, p_y, and p_z

With inversion symmetry: p_x and p_y don't hybridize with p_z

But with broken inversion symmetry $V(z)$ gives hybridization $\underline{\gamma} = \langle p_z(\boldsymbol{R})|V|p_n(\boldsymbol{R}+\boldsymbol{x})\rangle$ $(n = x,y)$

Petersen & Hedegård, Surf. Sci. **459**, 49 (2000)

Tight-binding approach

Unperturbed Hamiltonian: $$H_0 = \sum t_{\alpha\beta}(\boldsymbol{R}_i - \boldsymbol{R}_j)|p_\alpha(\boldsymbol{R}_i),\sigma\rangle\langle p_\beta(\boldsymbol{R}_j),\sigma|$$

Add SOC Hamiltonian: $$H_{\mathrm{SOC}} = \alpha \boldsymbol{L}\cdot\boldsymbol{S} = \frac{\alpha}{2}(L^+\sigma^- + L^-\sigma^+ + L^z\sigma^z)$$

In 6-orbital basis:

$$H_{\mathrm{SOC}} = \frac{\alpha}{2}\begin{pmatrix} 0 & -i & 0 & 0 & 0 & 1 \\ i & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & -1 & i & 0 \\ 0 & 0 & -1 & 0 & i & 0 \\ 0 & 0 & -i & -i & 0 & 0 \\ 1 & i & 0 & 0 & 0 & 0 \end{pmatrix}$$

Effective, low energy Hamiltonian around Γ

$$H_{\mathrm{eff}} = \begin{pmatrix} -6\delta + (\frac{3}{2}\delta + 9\gamma^2/w)k^2 & -\underline{6i(k_x - ik_y)}\alpha\gamma/w \\ \underline{6i(k_x + ik_y)\alpha\gamma/w} & -6\delta + (\frac{3}{2}\delta + 9\gamma^2/w)k^2 \end{pmatrix}$$

$\Rightarrow$ $$\alpha_R = 6\,\alpha\,\gamma/w$$

Hopping size, band width

Atomic SOC

Effect of ISB

Gives much larger energy splitting

Petersen & Hedegård, Surf. Sci. **459**, 49 (2000)

More general derivation

Orbital splitting due to ISB $\Rightarrow$ *Orbital* Rashba effect $\Rightarrow$ With SOC – gives spin Rashba effect

Procedure: tight-binding Hamiltonian for t_{2g} 3d-orbitals

$$H_{\mathrm{TB}} = H_{t_{2g}} + H_{\mathrm{ISB}} + H_{\mathrm{ex}} + H_{\mathrm{SOI}}$$

$$H_{\mathrm{SOI}} = \lambda_{\mathrm{so}} \sum_{i,\sigma,\sigma'} \mathbf{C}^{\dagger}_{i,\sigma} \mathbf{L} \cdot (\boldsymbol{\sigma})_{\sigma,\sigma'} \mathbf{C}_{i,\sigma'}$$

$$\mathbf{C}^{\dagger}_{i,\sigma} = (c^{\dagger}_{i,xy,\sigma}, c^{\dagger}_{i,yz,\sigma}, c^{\dagger}_{i,zx,\sigma})$$

$$H_{\mathrm{ISB}}(\mathbf{k}) = -\gamma \sum_{\sigma} \mathbf{C}^{\dagger}_{\mathbf{k},\sigma} [\mathbf{L} \cdot \mathbf{R}(\mathbf{k}) \times \hat{z}] \mathbf{C}_{\mathbf{k},\sigma}$$

$$\mathbf{R}(\mathbf{k}) \equiv 2[\sin(k_x a_L)\hat{x} + \sin(k_y a_L)\hat{y}]$$

$\boxed{\propto (\boldsymbol{k} \times \hat{z}) \cdot \boldsymbol{L}}$ "orbital Rashba effect" $\longrightarrow$ SOI $\longrightarrow$ $\mathbf{L} \cdot \boldsymbol{\sigma} \sim m\mathbf{R}(\mathbf{k}) \times \hat{z} \cdot \boldsymbol{\sigma}$

(around Γ)

$$\bar{\alpha}_{\mathrm{R}} (\mathbf{k} \times \hat{z}) \cdot \boldsymbol{\sigma}$$

$$\bar{\alpha}_{\mathrm{R}} \equiv (\lambda_{\mathrm{so}} a_L)(\gamma / t_1)$$

Park et al, PRL **107**, 156803 (2011)

Park et al, PRB **87**, R041301 (2013)

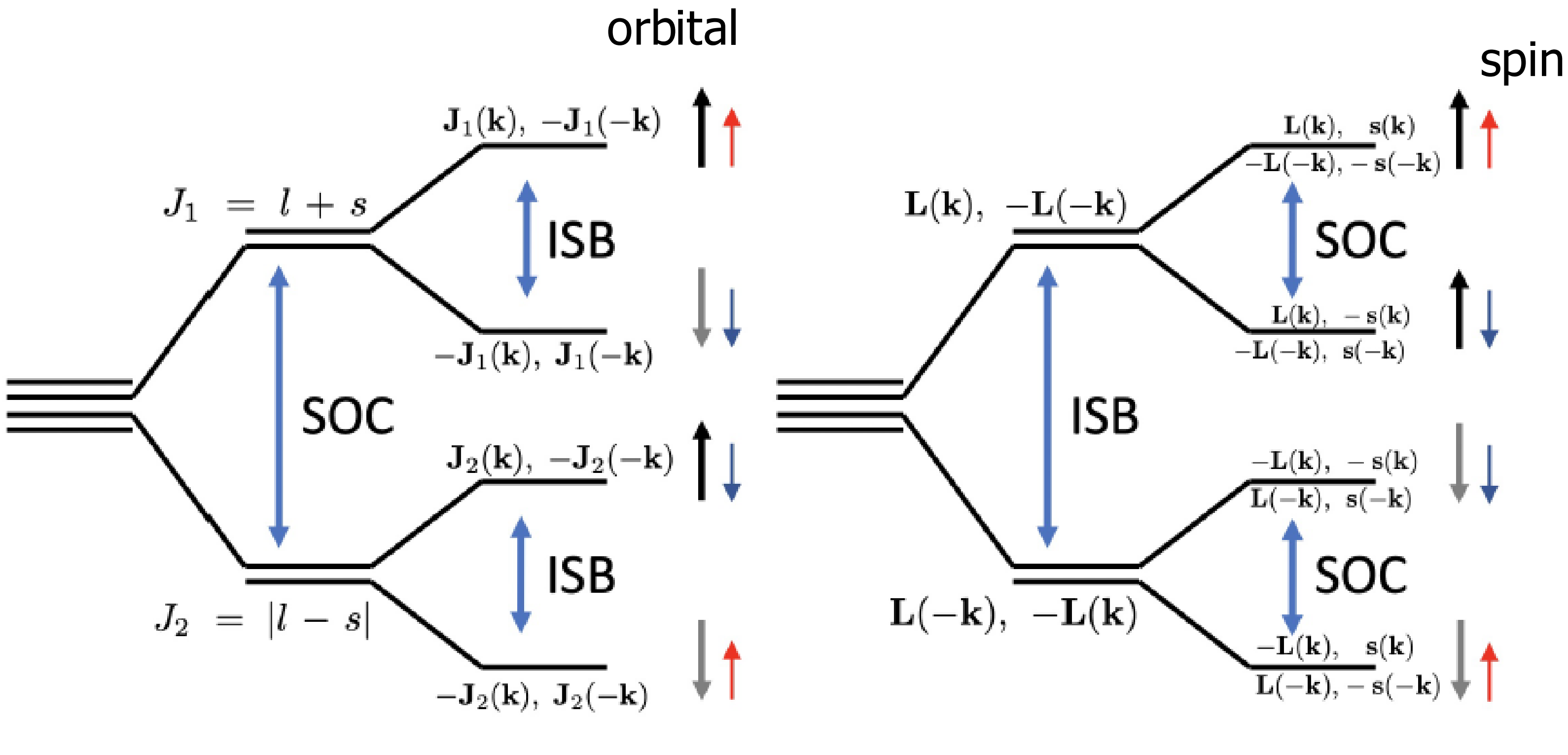
Summarizing

What is the dominating energy scale?

Inversion-symmetry breaking
vs. spin-orbit coupling

Splitting of orbitals due to
ISB leading term

$$L(\boldsymbol{k}) \neq L(-\boldsymbol{k})$$



Conventional Rashba effect

SOC splitting ~ meV

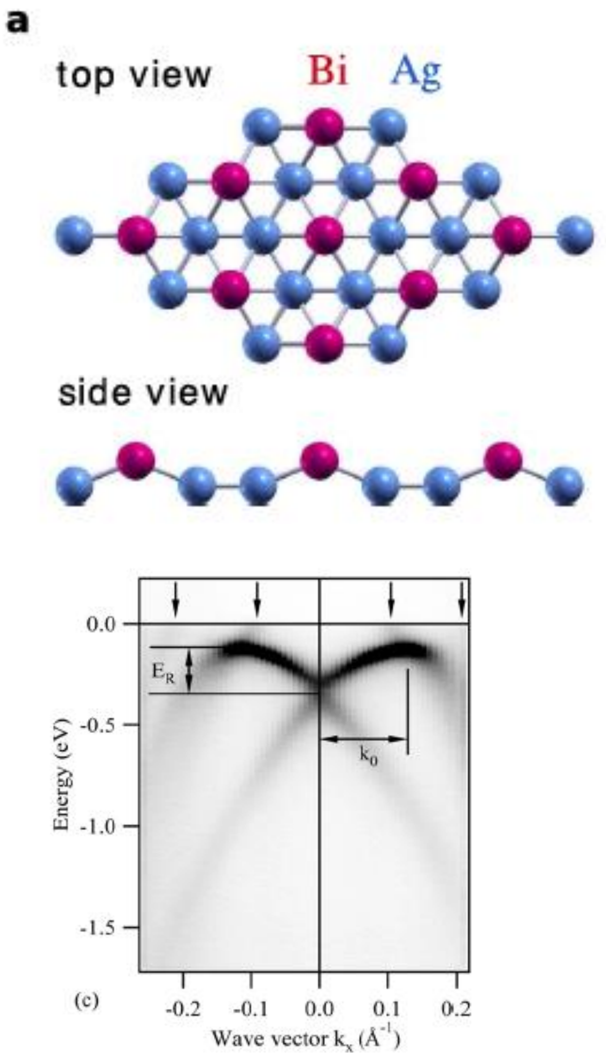
Orbital Rashba effect

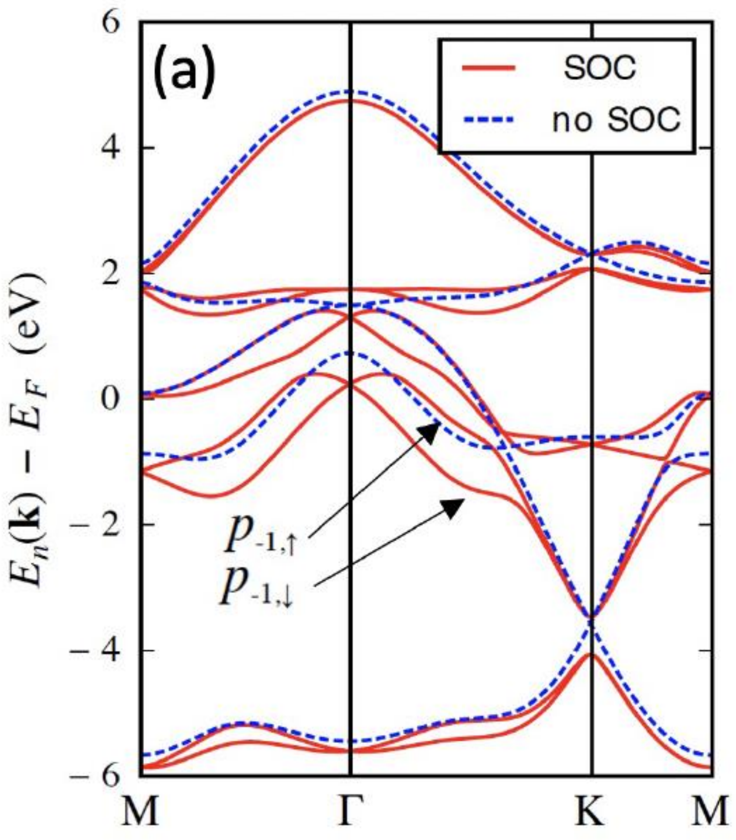
ISB splitting $\lesssim$ eV

Bihlmayer et al, Nature Rev. Phys. **4**, 642 (2022)

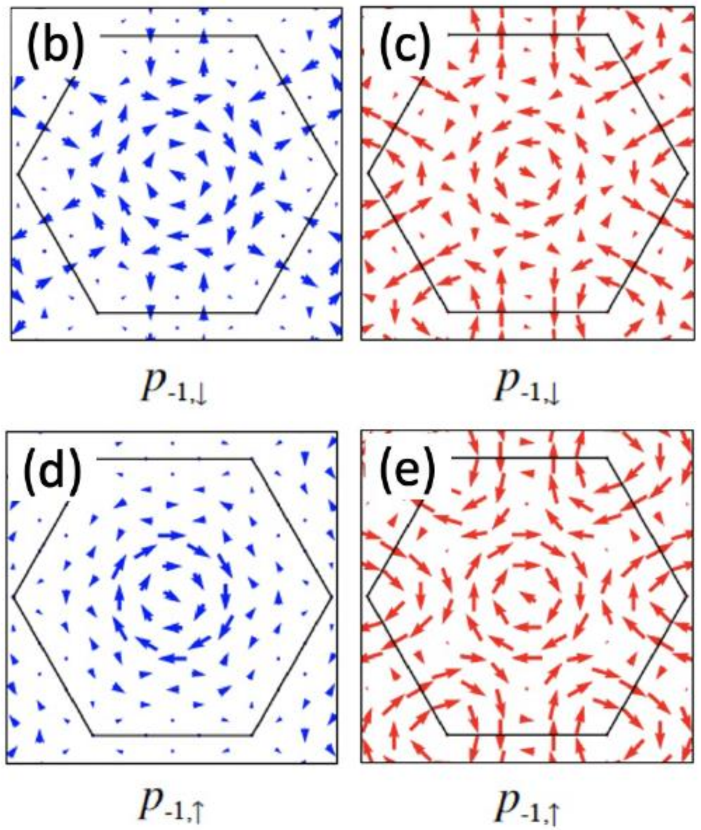
Ab initio calculations

Monolayer hexagonal Ag_2Bi





Orbital spin texture



Go et al, Sci. Rep. **7**, 46742 (2017)

Orbital ang. momentum texture present without SOC

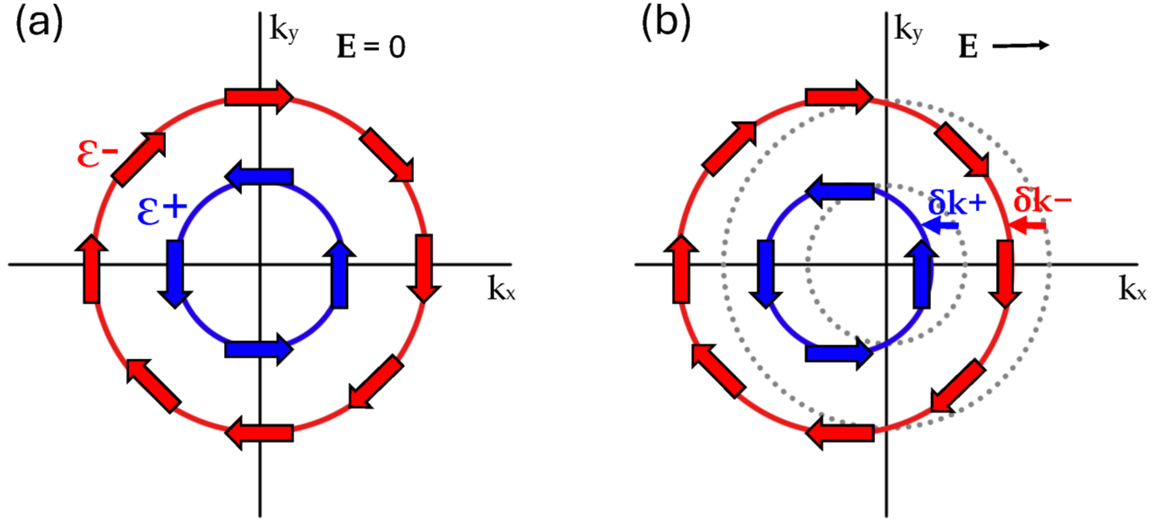
Applications – Edelstein effect (or Rashba-Edelstein effect)

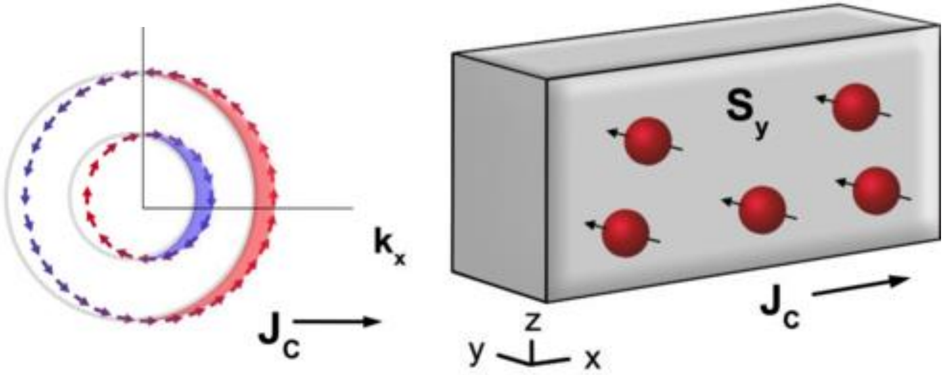
Influence of applied electric field: $\widehat{H} = \widehat{H}_o - |e|\vec{r}\cdot\vec{E}$ $\longrightarrow$ $\varepsilon'_{nk\sigma} = \varepsilon_{nk\sigma} + \Delta\varepsilon_{nk\sigma}$

1st order pert. theory: $\Delta\varepsilon_{nk\sigma} = -|e|\vec{E}\cdot\langle\vec{r}\rangle_{nk\sigma} \approx -|e|\vec{E}\cdot\tau\langle\vec{v}\rangle_{nk\sigma} \approx -|e|\vec{E}\cdot\tau\frac{\hbar}{m}\langle\vec{k}\rangle_{nk\sigma}$ (constant relaxation time approximation)

k-space Hamiltonian: $\mathcal{H} \cong \frac{\hbar^2 k^2}{2m} - |e|\frac{\hbar\tau}{m}\vec{E}\cdot\vec{k} \approx \frac{\hbar^2}{2m}(\vec{k} - \frac{|e|\tau}{\hbar}\vec{E})^2$

$\delta\boldsymbol{k}$ – shift in k-space



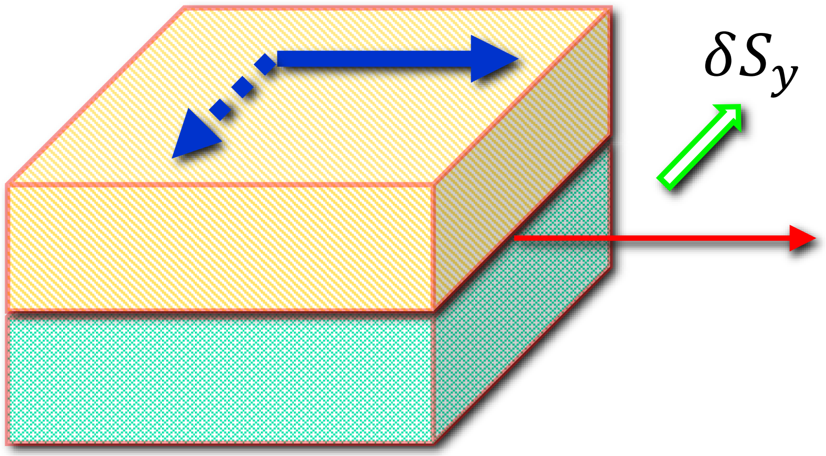


(spin) Edelstein effect: Leads to net, non-zero transv. spin-polarization $\delta S_y \perp E_x$; $\delta S \propto -|e|E\,\tau/\hbar k_0$

Edelstein, Solid State Commun. **173**, 233 (1990)

Applications: Spin-orbit torque switching models

In-plane magn. easy axis

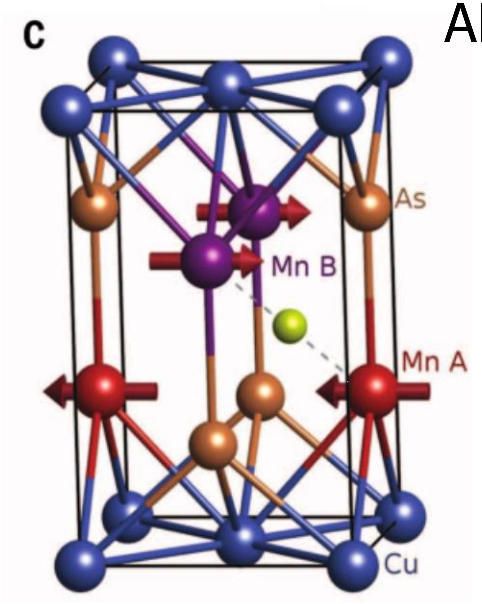


$$\delta S_y = \chi^S_{yx} E_x$$

Edelstein effect

E_x

AFM CuMnAs



Landau-Lifshitz-Gilbert dynamics of spin moment:

$$\dot{\boldsymbol{S}}_i = -\frac{\gamma}{\mu_s}\boldsymbol{S}_i \times \boldsymbol{H}_i^{\mathrm{eff}} + \alpha \boldsymbol{S}_i \times \dot{\boldsymbol{S}}_i + \frac{\gamma}{\mu_s}\boldsymbol{T}_i^{\mathrm{SOT}}$$

$$\boldsymbol{T}_i^{\mathrm{SOT}} = -\boldsymbol{S}_i \times \boldsymbol{H}_i^{\mathrm{SOT}}$$

$$\boldsymbol{T}_i^{\mathrm{SOT}} \propto \boldsymbol{S}_i \times \delta \boldsymbol{S}_i$$

(needs also SHE)

Contains contributions, both field-like and damping-like, due to induced δS moments

Staggered torques:

$$dM_{A,B}/dt \sim M_{A,B} \times \delta S_{A,B}$$

Anti-damping-like torque

$$dM_{A,B}/dt \sim M_{A,B} \times (M_{A,B} \times \delta S_{A,B})$$

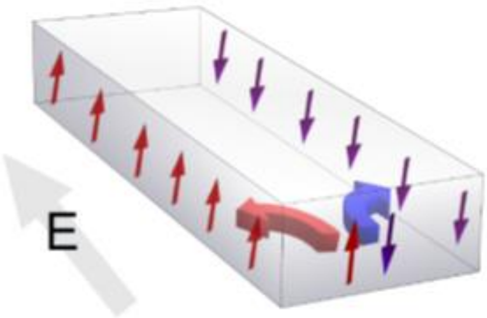
$$\boxed{\delta S_A = -\delta S_B}$$

Wadley et al, Science **351**, 587 (2016)

Review on spin-orbit torque: Manchon et al, Rev. Mod. Phys. **91**, 035004 (2019)

More general: theory description of *charge-to-spin conversion*

Spin Hall effect



Transport

$$J_y^{S_z} = \sigma_{yx}^{S_z} \cdot E_x$$

Spin Conductivity Tensor

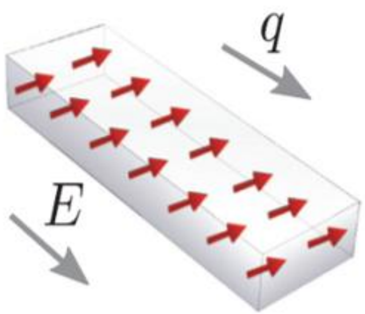
Dyakonov & Perel, JETP Lett. **13**, 467 (1971)

Hirsch, Phys.Rev.Lett. **83**, 1834 (1999)

Infinite bulk 3D crystal

http://zfmezo.home.amu.edu.pl/research.php

Rashba-Edelstein effect



Local

$$\delta S_y = \chi_{yx} \cdot E_x$$

Spin Susceptibility Tensor

Edelstein, Solid State Commun. **73**, 233 (1990)

Originally: Rashba SOC + 2D symm.

Bychkov & Rashba, JETP Lett. **39**, 78 (1984)

Methodology - Electronic structure calculations & linear-response theory

Rashba-Edelstein effect (requires inv. symmetry breaking)

$$\delta S_i = \chi^S_{ij} E_j$$

$$\delta L_i = \chi^L_{ij} E_j$$

Spin magneto-electric susceptibility

Orbital magneto-electric susceptibility

<u>DFT + linear response theory</u>

$A = \hat{L} \; or \; \hat{S}$

$$\chi^A_{ij} = -\frac{ie}{m_e}\int_\Omega \frac{dk}{\Omega}\sum_{n\neq m}\frac{f_{nk}-f_{mk}}{\hbar\omega_{nmk}}\frac{A^i_{mnk}\,p^j_{nmk}}{-\omega_{nmk}+i\tau^{-1}_{\text{inter}}}$$

Interband (Fermi sea)

$$-\frac{ie}{m_e}\int_\Omega \frac{dk}{\Omega}\sum_{n}\frac{\partial f_{nk}}{\partial\epsilon}\frac{A^i_{nnk}\,p^j_{nnk}}{i\tau^{-1}_{\text{intra}}}$$

Intraband (Fermi Surface)

$$\hbar\omega_{nm\boldsymbol{k}} = \epsilon_{n\boldsymbol{k}} - \epsilon_{m\boldsymbol{k}}$$

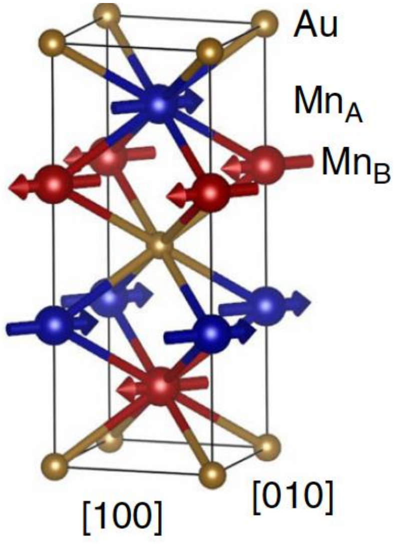
Kohn-Sham band energies

$$\delta M = \mu_B \delta(\boldsymbol{L} + 2\boldsymbol{S})$$

Salemi et al, Nat. Commun. **10**, 5381 (2019)

Ab initio calculations: Dominant *orbital* Rashba-Edelstein effect (OREE)

AFM Mn_2Au

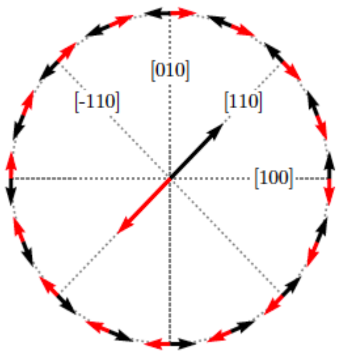


OREE

$$M_i^{ind} = \chi_{ij} \cdot E_j$$

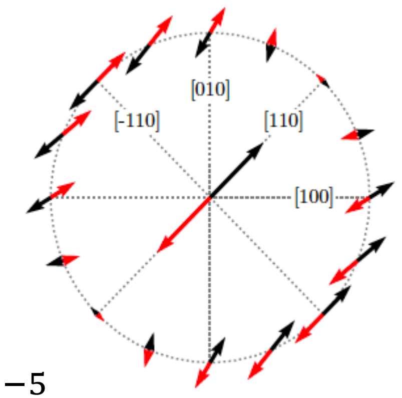
SREE

$M \parallel [110]$



Mn1

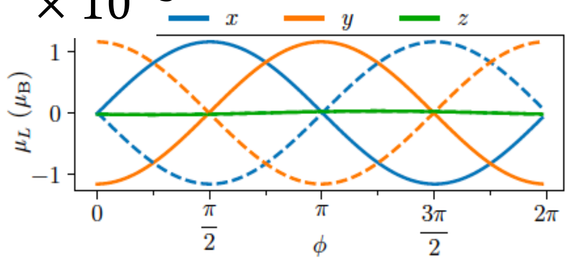
Mn2



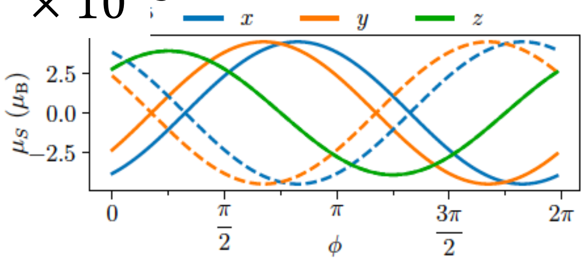
$$\delta L_i = \chi_{ij}^L E_j$$

$$\delta S_i = \chi_{ij}^S E_j$$

μ_L $\times 10^{-3}$



μ_S $\times 10^{-5}$



$E = 10^7$ V/m

- Dominant staggered induced *orbital* polarization in-plane (40 x larger than spin)
- Induced orbital polarization - not due to SOC (but spin Rashba-Edelstein effect is)
- Induced orb.polarization of Rashba-type, induced spin polarization mixed Rashba-Dresselhaus type

Salemi et al, Nat. Commun. **10**, 5381 (2019)

Spin and orbital currents – linear-response theory calculations

Spin Hall effect $\boldsymbol{J}^{S_i} = \boldsymbol{\sigma}^{S_i}\boldsymbol{E}$

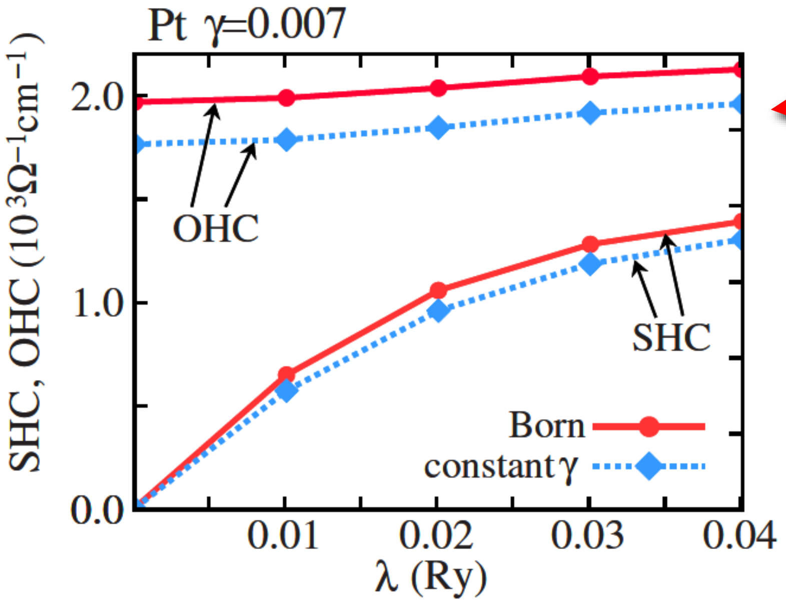
Orbital Hall effect $\boldsymbol{J}^{L_i} = \boldsymbol{\sigma}^{L_i}\boldsymbol{E}$

$$A = \hat{\boldsymbol{J}}^{S_i} = \frac{1}{2}\{S_i\boldsymbol{v} + \boldsymbol{v}S_i\}$$

Spin/orbital current operator

Include scattering effects in an average through lifetimes $\tau_{intra}, \tau_{inter}$

SHE of Pt: Guo et al, PRL **100**, 096401 (2008)



OHE & SHE: Tanaka et al, PRB **77**, 165117 (2008)

$$H_{SOC} = \lambda(\boldsymbol{L}\cdot\boldsymbol{S})$$

OHE non-zero without SOC,
SHE vanishes without SOC !

Orbital Hall effect in inversion symmetric crystals?

Inv. symmetric systems $\boldsymbol{L}(\boldsymbol{k}) = \boldsymbol{L}(-\boldsymbol{k})$

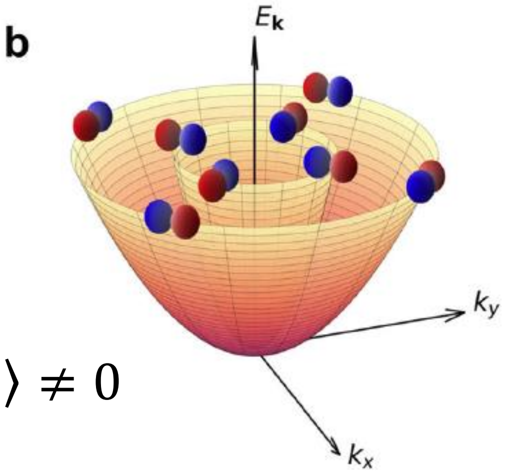
Time-reversal symmetry: $\boldsymbol{L}(\boldsymbol{k}) = -\boldsymbol{L}(-\boldsymbol{k})$

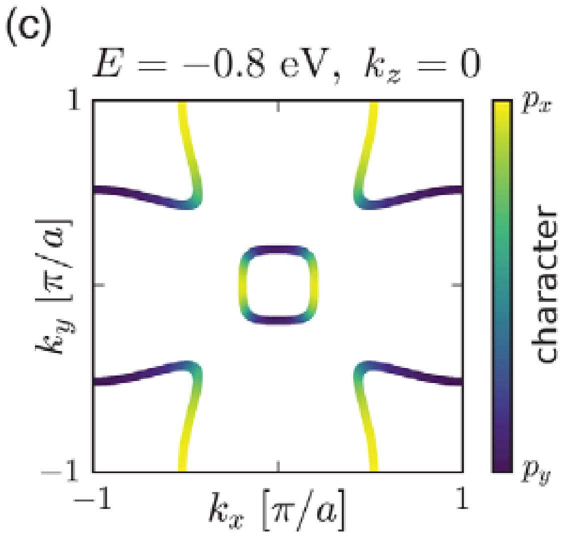
OAM vanishes at each k-point, but orbital texture present

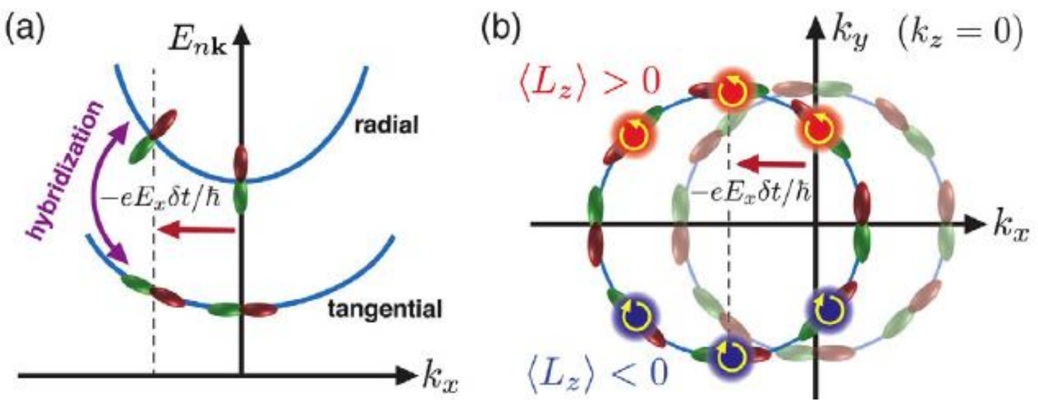
Perturbation due to electric field =>

$$|u'_{nk}\rangle = |u_{nk}\rangle - |e|E_x \tau v_{nn'k} \frac{|u_{n'k}\rangle}{\varepsilon_{nk} - \varepsilon_{n'k}} \Longrightarrow \langle u'_{nk}|L_z|u'_{nk}\rangle \neq 0$$

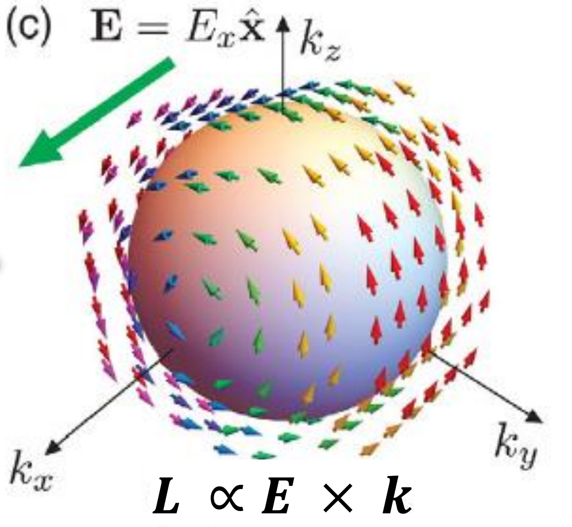
Orbital texture in k-space







$\Longrightarrow$



$\Longrightarrow$ $\langle L_z v_y\rangle \neq 0$

$\Downarrow$

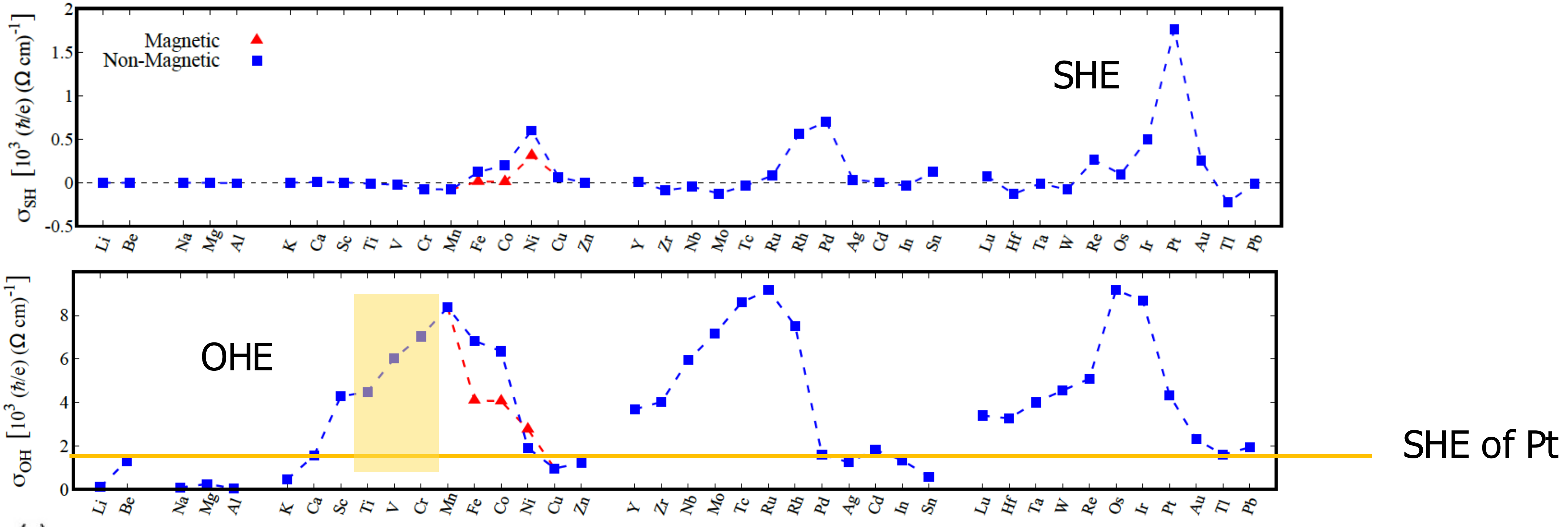
Nonzero OHE

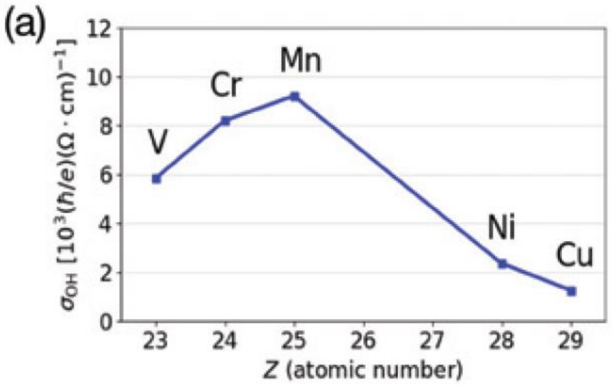
$J \perp \delta L \perp E$

Shift due to electric field enables hybridization =>
Rashba type OAM texture – total induced $\langle L\rangle = 0$

Go, Jo, Kim & Lee, PRL **121**, 086602 (2018)

Ab initio calculations of spin and orbital Hall effects in metal series





Salemi & Oppeneer, Phys.Rev.Mat. **6**, 095001 (2022)

- Large effects for light 3d metals – NOT due to SOC !
- Cheap, light metals for future orbitronics?

Jo, Go & Lee, PRB **98**, 214405 (2018)

Summarizing – two related cases leading to spin-orbit torques

Inv. symm. broken, time-rev. preserved

Orbital Rashba effect, OAM texture $\langle L \rangle_{E_F} = 0$

SOC

Rashba effect

E field

OAM accum.
$\langle \delta L \rangle_{E_F} \propto E$

spin accum.
$\langle \delta S \rangle_{E_F} \propto E$

Orbital Edelstein
$\delta L \perp E$

Spin Edelstein
$\delta S \perp E$

Inv. symmetry and time-rev. preserved

Orbital texture $L(k) = 0, \langle L \rangle_{E_F} = 0$

E field

Orbital Rashba effect, OAM texture, no OAM accum. $\langle L \rangle_{E_F} = 0$ $\langle \delta L \rangle_{E_F} = 0$

SOC

Non-zero orbital current
$\langle L_z v_x \rangle \propto E$

Non-zero spin current
$\langle S_z v_x \rangle \propto E$

Orbital Hall effect
$J \perp \delta L \perp E$

Spin Hall effect
$J \perp \delta S \perp E$

Spin/orbital transport developments & Outlook

Spin polarized currents
Spin transfer torque (STT)
→
Spin currents
Spin-orbit torque (SOT)
→
Orbital currents
??

Altermagnets

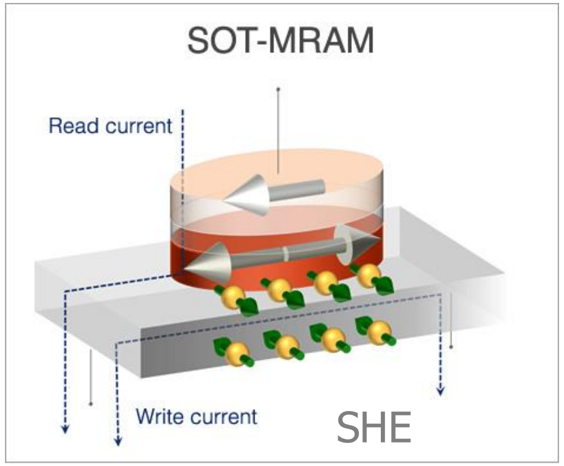
Slonczewski, 1996

STT-MRAM

Everspin, Samsung, IBM

market-ready product
after ~20 years

Hirsch 1999 (SHE)
Miron et al, 2011



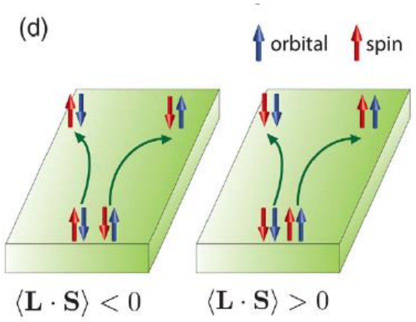
TSMC, Antaios

Technology being
developed for market

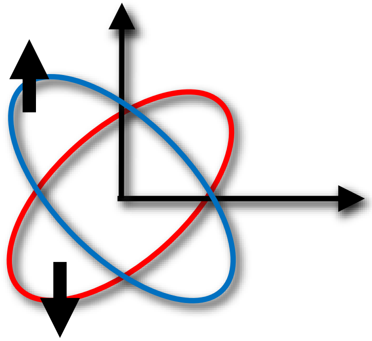
Observation SHE Pt:
Stamm et al, 2017

Go et al, ~2018 (OHE)

Orbital torque?



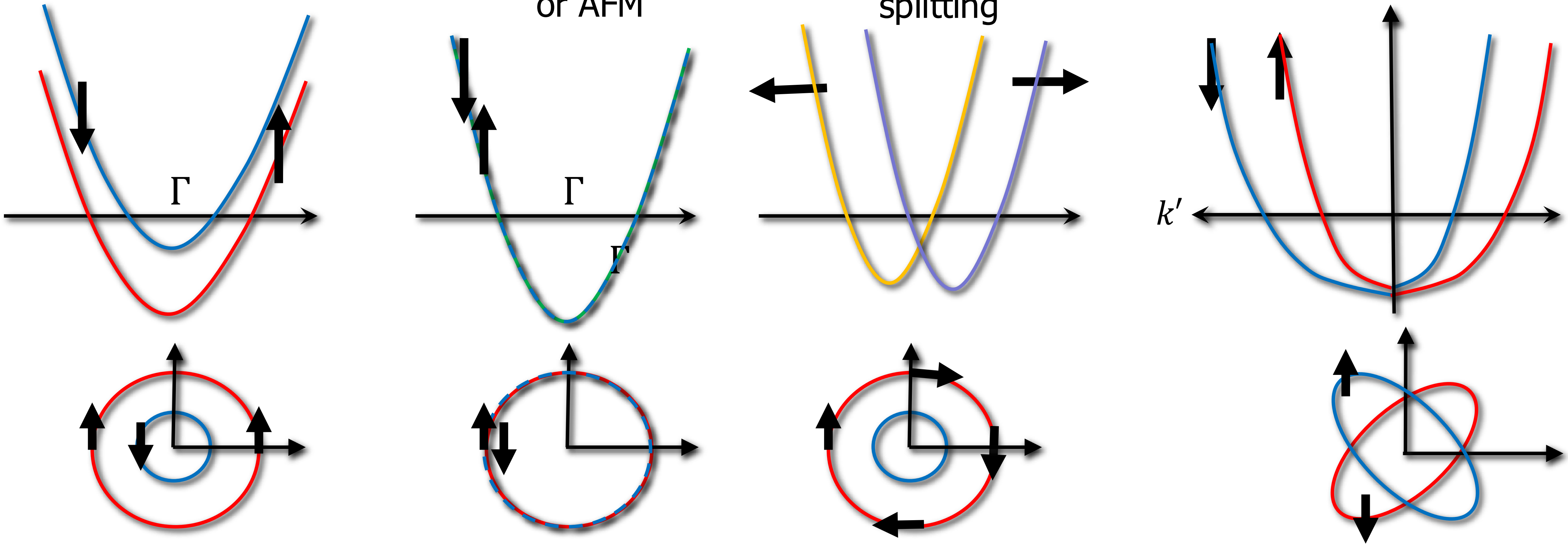
Or *k* dependent
spin splitting?



Current fundamental research topics

Other recent developments in *k*-dependent spin splitting

Ferromagnet | Nonmagnetic metal, or AFM | Rel. Rashba spin splitting | Non-rel. spin splitting AFM



Ferromagnet: $\mathcal{T}$ broken

$\varepsilon_n(-\boldsymbol{k},-\sigma) \neq \varepsilon_n(\boldsymbol{k},\sigma)$

Nonmagnetic metal, or AFM: $\mathcal{PT}$ symmetry preserved

$\varepsilon_n(\boldsymbol{k},-\sigma) = \varepsilon_n(\boldsymbol{k},\sigma)$

Rel. Rashba spin splitting: $\mathcal{T}$ pres., $\mathcal{P}$ broken

$\varepsilon_n(-\boldsymbol{k},\sigma) \neq \varepsilon_n(\boldsymbol{k},\sigma)$

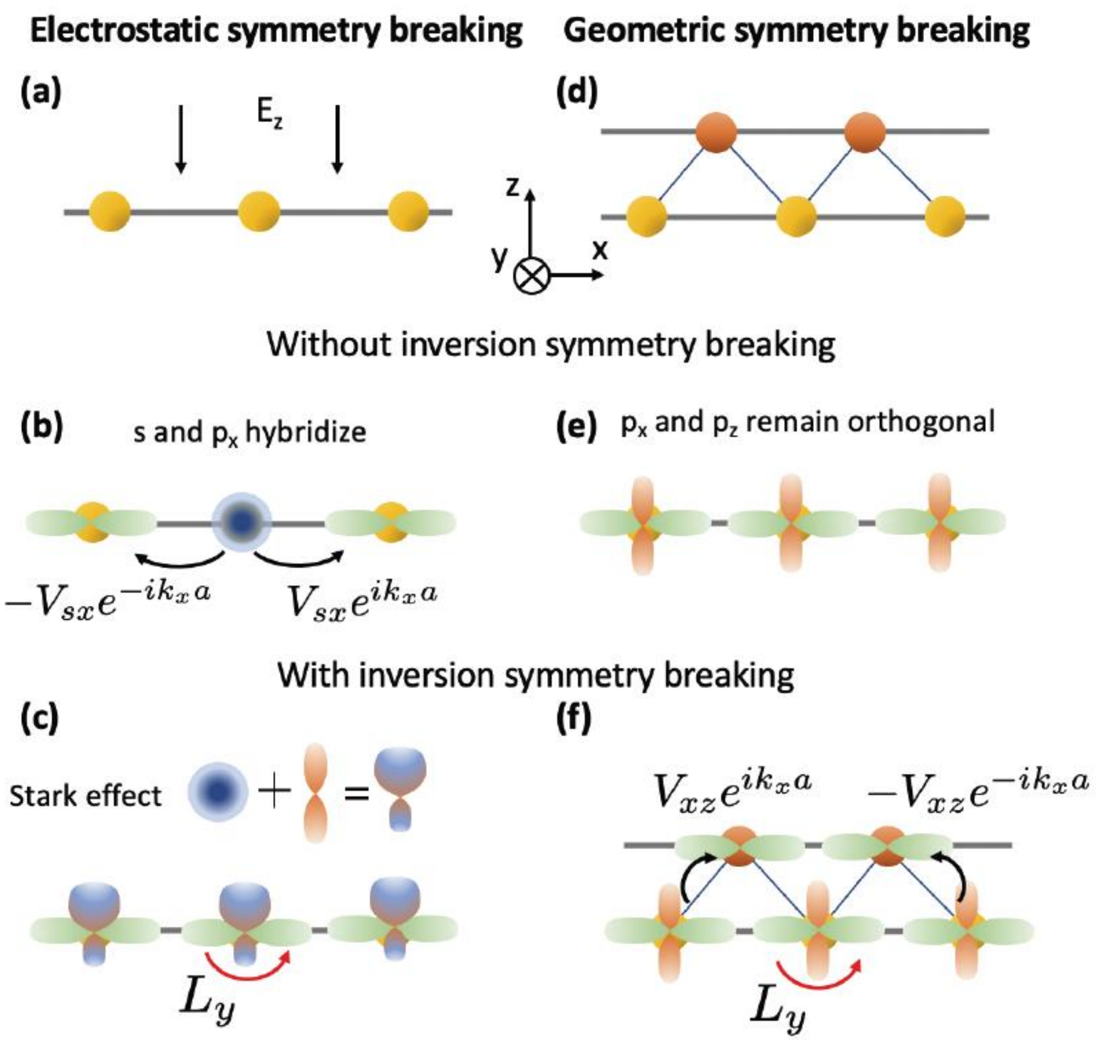
$\varepsilon_n(-\boldsymbol{k},-\sigma) = \varepsilon_n(\boldsymbol{k},\sigma)$

Non-rel. spin splitting AFM: $\mathcal{P}$ pres., $\mathcal{T}$ broken

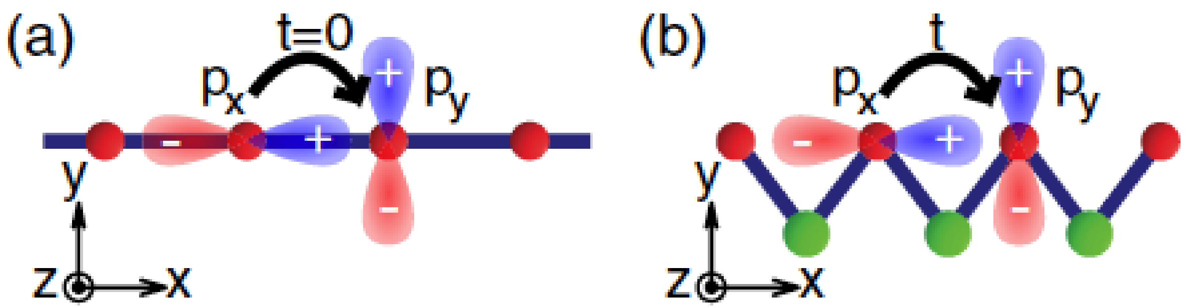
$\varepsilon_n(-\boldsymbol{k},\sigma) = \varepsilon_n(\boldsymbol{k},\sigma)$

$\varepsilon_n(-\boldsymbol{k},-\sigma) \neq \varepsilon_n(\boldsymbol{k},\sigma)$

Reserve slides



Hybridization is forbidden when there is z axis symmetry, allowed when there is no z symmetry



Gives hybridization of p_x and p_z orbitals

$$\langle p_z|H|p_x\rangle = -2iV_{xz}\sin k_xa$$

Bihlmayer et al, Nature Rev. Phys. **4**, 642 (2022)

E.g. Collinear AFMs with $\mathcal{P}$ preserved, but $\mathcal{T}$ broken

Low-energy Hamiltonian:

$$\mathcal{H}(\boldsymbol{k}, \boldsymbol{\sigma}) = \frac{\hbar^2 k^2}{2m^*} \sigma_0 + \eta\, \mathcal{M}^{\ell}(\boldsymbol{k})\, \sigma_{\boldsymbol{z}}$$

d-wave altermagnet:

$$\mathcal{M}^{\ell=d}(k) = M_1\left(k_x^2 - k_y^2\right) + M_2 k_x k_y$$

And can combine with e.g. Rashba spin-orbit coupling