Invariant Theory and Symmetry Analysis of Magnetism and Spin-Orbitronics

Aurélien Manchon, Aix-Marseille University, France

Objectives

1. Learn interesting physical mechanisms of major interest in condensed matter and magnetism

2. Learn some key concepts about the representation theory in crystals

3. Under how to build and read the character table of a given crystal

4. Deduce the general forms of key physical observables (Hamiltonian, conductivity tensor, DMI and SOT)

Outline

Lecture 1: A primer on spin-orbitronics
Spin-orbit coupling in crystals, Dzyaloshinskii-Moriya interaction, spin-orbit torques

Lecture 2: Representation Theory applied to crystals
Group of symmetries, reducible and irreducible representations, orthogonality theorem, characters

Lecture 3: Character tables of crystal point groups
Salient features of the character table, invariant functions, decomposition theorem, product group

Lecture 4: Application to the C_{3v} point group
Hamiltonian, conductivity tensor, DMI and SOT

Lecture 5: Your turn, with the C_{4v} point group
Surprise me ☺

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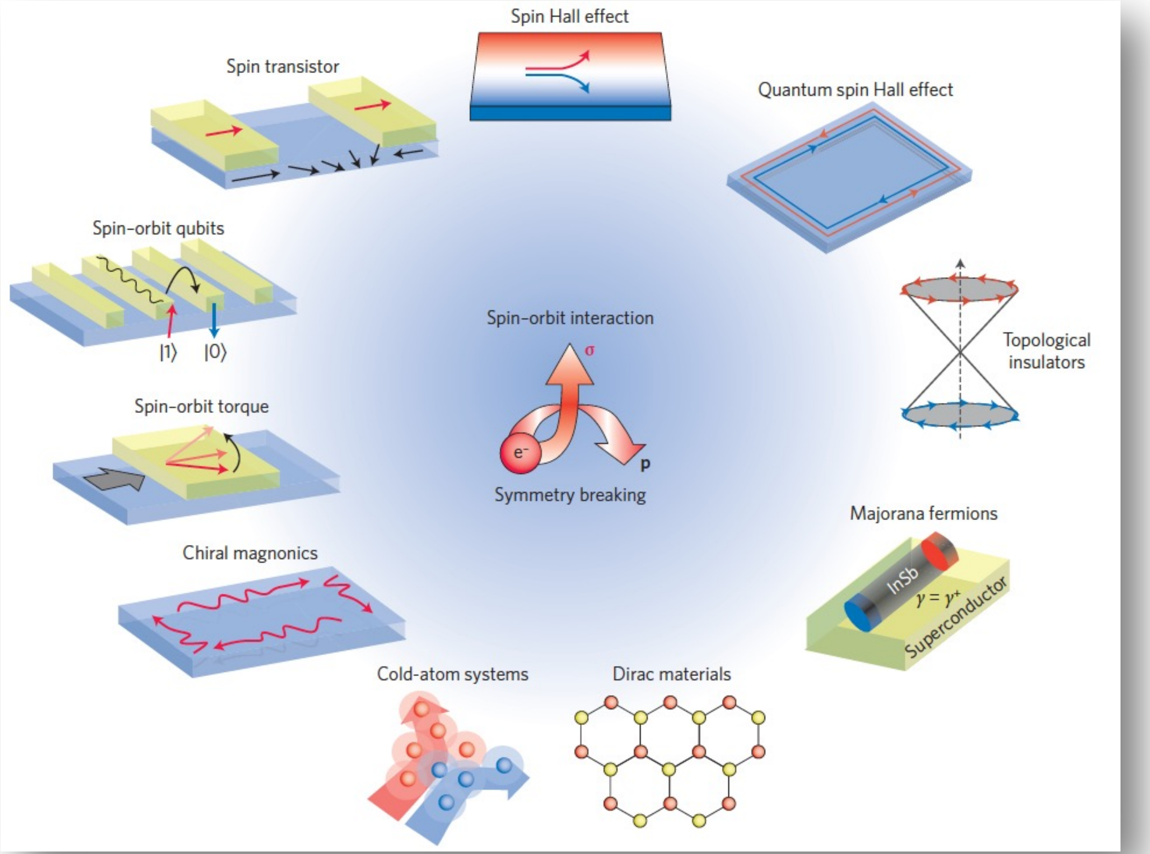
Surprise me ☺

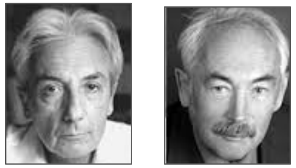
Lecture I

A brief introduction to selected topics in spin-orbitronics



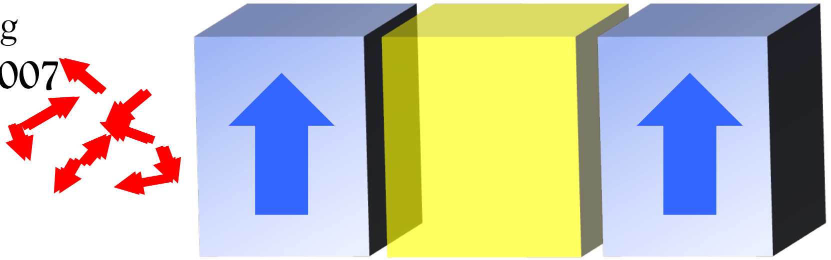
Manchon et al., *New perspectives for Rashba spin-orbit coupling*, Nature Materials **14**, 871 (2015)
Bihlmayer et al. *Rashba-like physics in condensed matter*, Nature Reviews Physics **4**, 642 (2022).

Spintronics: A history of revolutions

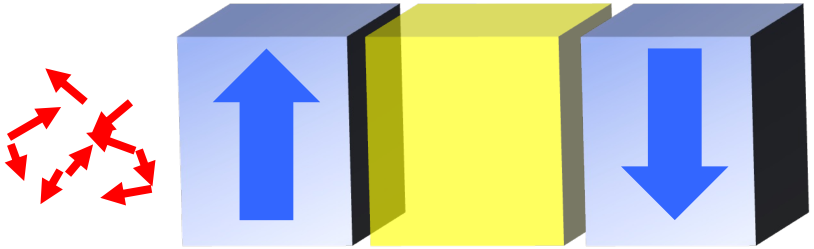


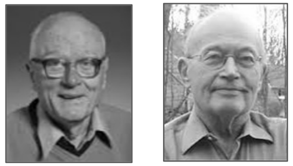
Fert & Grünberg
Nobel Laureates 2007

Giant magnetoresistance



Spin transfer torque

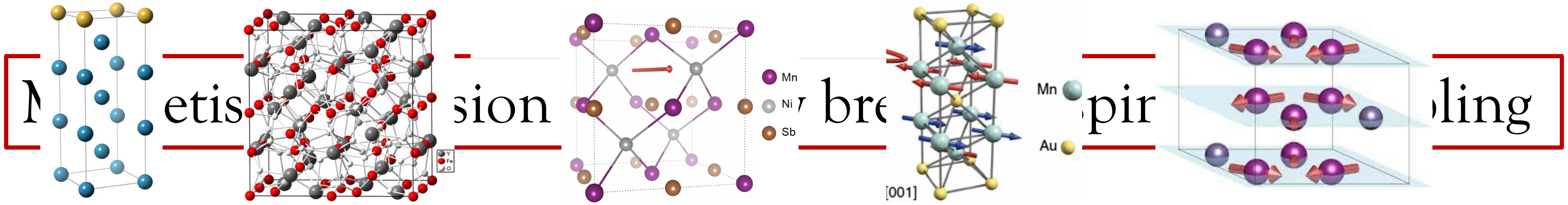




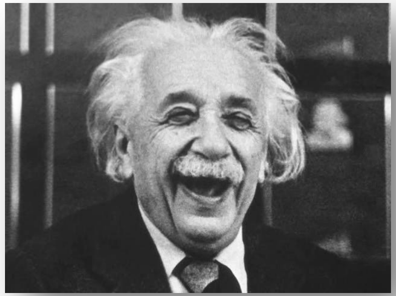
Berger & Slonczewski
Buckley price 2013

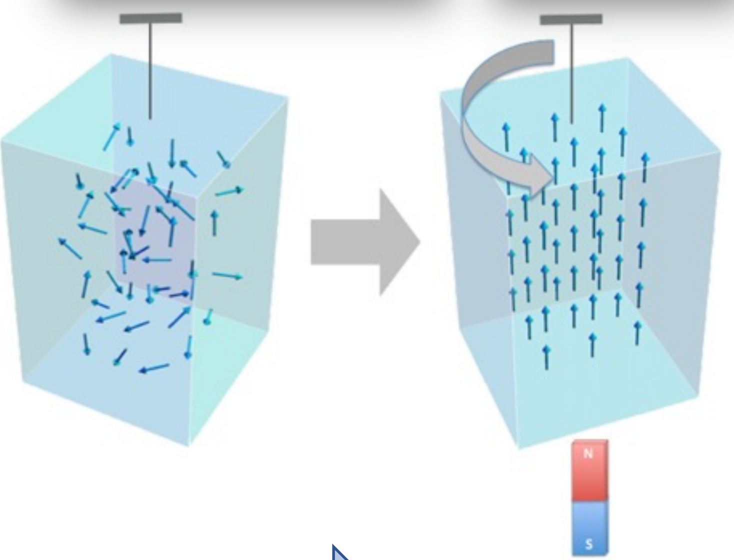
Typically: Co/Cu/Co, CoFeB/MgO/CoFeB

Typically: (Pt, Ta, W etc.)/Magnet



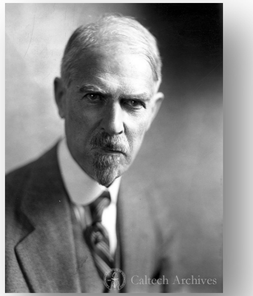
Einstein de Haas effect

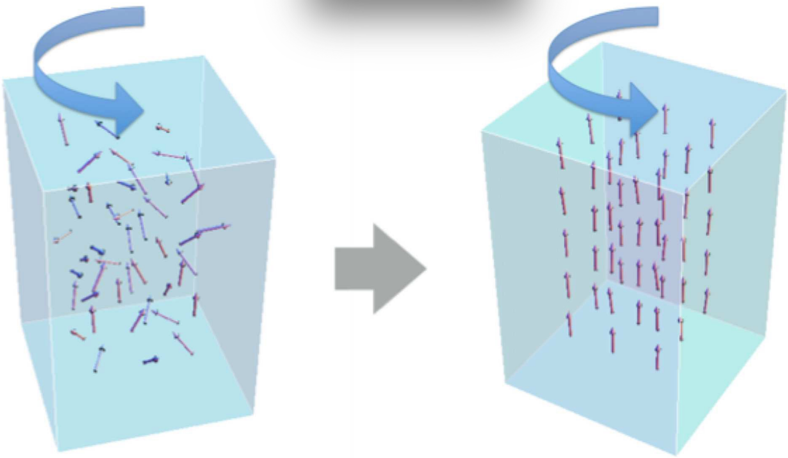




Magnetic field ⇨ Mechanical torque

Barnett effect





Mechanical Torque ⇨ Magnetization

For more information

Matsuo, Mechanical generation of spin current, Frontiers in Physics 3, 54 (2015)

Also Comment by Kovalev, Nature Nanotechnology 3, 710 – 711 (2008).

Angular momentum conservation: spin transfer torque

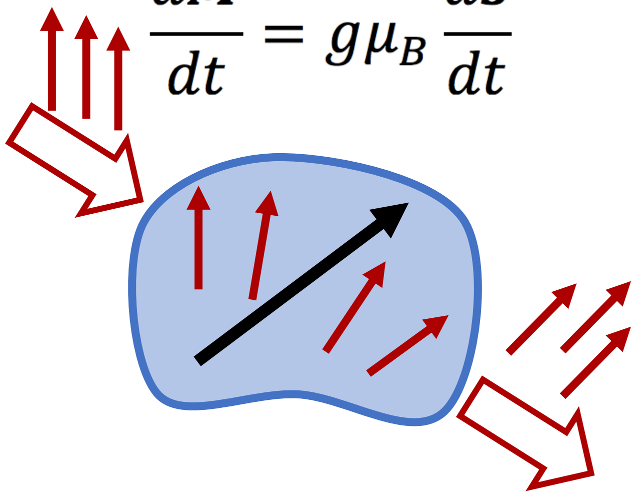
Slonczewski's picture

$$\boldsymbol{M} - g\mu_B \boldsymbol{s} = \text{constant}$$

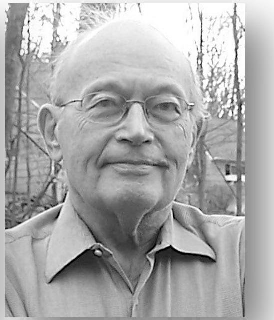
"Local" magnetization

"Conduction" spin

$$\frac{d\boldsymbol{M}}{dt} = g\mu_B \frac{d\boldsymbol{s}}{dt}$$

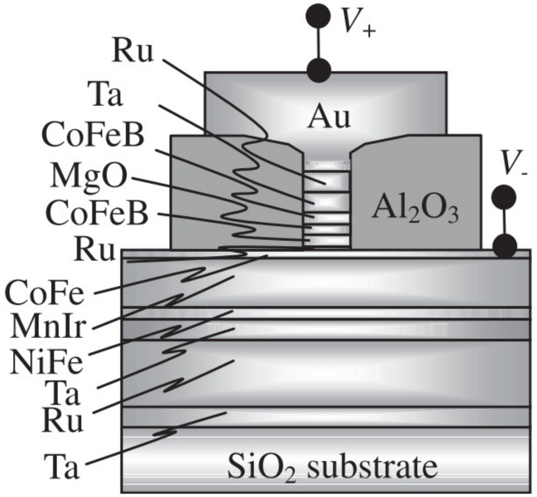


L. Berger



J. Slonczewski

The torque exerted by the conduction spins on the magnetization is given by the balance between incoming and outgoing spin current



$$\frac{d\boldsymbol{M}}{dt} = \boldsymbol{T} = \int d\Omega\, \boldsymbol{m}\times\left[\left(\boldsymbol{J}_s^{in} - \boldsymbol{J}_s^{out}\right)\times\boldsymbol{m}\right]$$

Spin current *transverse* to **M**

J. C. Slonczewski, Journal of Magnetism and Magnetic Materials 159, L1 (1996)
L. Berger, Physical Review B 54, 9353 (1996)

Hayakawa JJAP 44, L587 (2005)

Introducing spin-orbit coupling

Spin-orbit coupling in crystals

$$\hat{\mathcal{H}}_{\text{so}} = -\frac{e\hbar}{2m^2c^2}\hat{\boldsymbol{\sigma}}\cdot(\boldsymbol{\nabla}V\times\hat{\mathbf{p}})$$

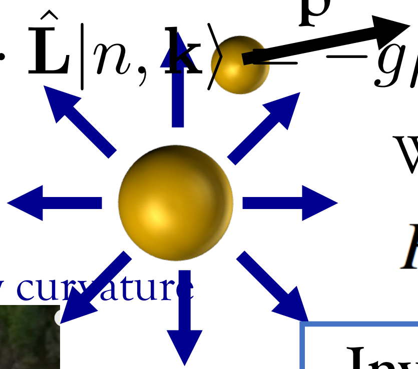
Electron's momentum

Spin Potential gradient

In atoms, $\boldsymbol{\nabla}V \approx \frac{\partial_r V}{r}\mathbf{r}$ ⇒ $\hat{\mathcal{H}}_{\text{so}} = \xi_{\text{so}}\hat{\boldsymbol{\sigma}}\cdot\hat{\mathbf{L}}$

In crystals, the spin-orbit coupling induces a *momentum-dependent effective field*

$$\langle n,\mathbf{k}|\xi_{\text{so}}\hat{\boldsymbol{\sigma}}\cdot\hat{\mathbf{L}}|n,\mathbf{k}\rangle = -g\mu_B\hat{\boldsymbol{\sigma}}\cdot\mathbf{B}_{\mathbf{k}}$$



With inversion symmetry

$$\hat{\mathbf{v}}_s = \partial_{\hbar\mathbf{k}}\varepsilon^s_{\mathbf{k}} + s\boldsymbol{\Omega}_{\mathbf{k}}\times\dot{\mathbf{k}}$$

→Berry curvature

Without inversion symmetry

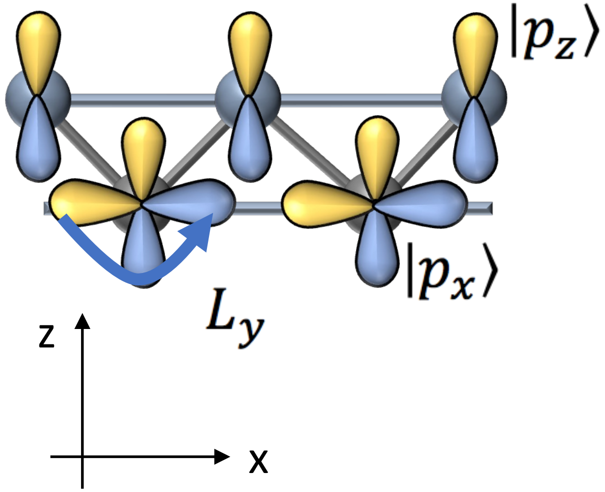
$$H_{\text{R}} \approx -\alpha\hat{\boldsymbol{\sigma}}\cdot(\mathbf{z}\times\mathbf{k})$$

Inv **ect**

Ivch

A toy model for interfacial spin-momentum locking

Consider an atomic chain with p-orbitals



Top p_z · p_z-p_z hopping · p_z-p_x hopping · Bottom p_z · Bottom p_x

$$H = \begin{pmatrix} \varepsilon_k^T & V_{zz} & V_{zx} \\ V_{zz}^* & \varepsilon_k^0 & 0 \\ V_{zx}^* & 0 & \varepsilon_k^0 \end{pmatrix}$$

Slater-Koster parametrization

$$V_{zz} = (V_\sigma + V_\pi)\cos k_x a$$
$$V_{zx} = -i(V_\sigma - V_\pi)\sin k_x a$$

The diagonalization brings three eigenstates. For instance

$$\varepsilon_0(k) = \varepsilon_k^0, |0\rangle = \frac{1}{\sqrt{|V_{zz}|^2 + |V_{zx}|^2}}(-V_{zx}|p_z\rangle + V_{zz}|p_x\rangle)$$

The orbital moment of this state reads

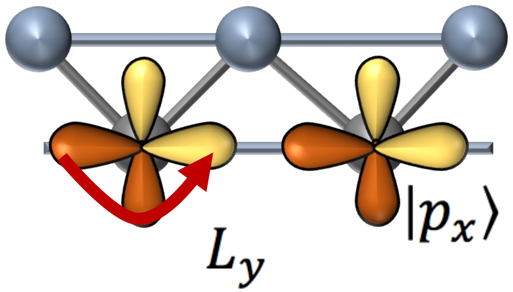
$$\langle 0|\boldsymbol{L}|0\rangle = \frac{}{(V_\sigma + V_\pi}\langle 0|\boldsymbol{L}|0\rangle = \frac{2V_{zx}V_{zz}}{|V_{zz}|^2 + |V_{zx}|^2}\boldsymbol{y}\frac{}{k_x a}\sin 2k_x a\ \boldsymbol{y}$$

Symmetry breaking promotes orbital mixing, and non-vanishing orbital moment

See G. Manchon et al., Physical Review B **101**, 174423 (2020)

The Rashba effect

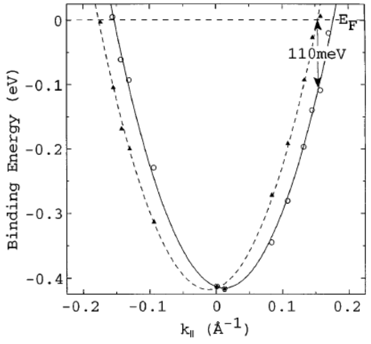
E. Rashba



Orbital Rashba effect $L_y \sim k_x$

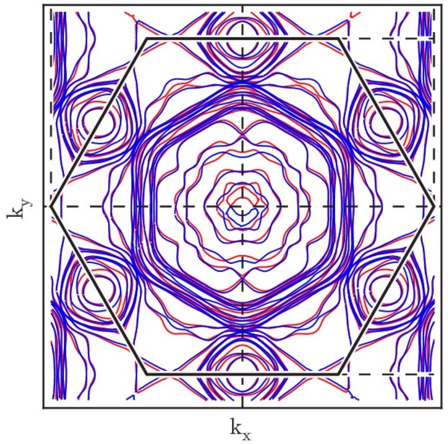
Spin-orbit coupling $\xi_{so}\boldsymbol{L}\cdot\boldsymbol{S}$

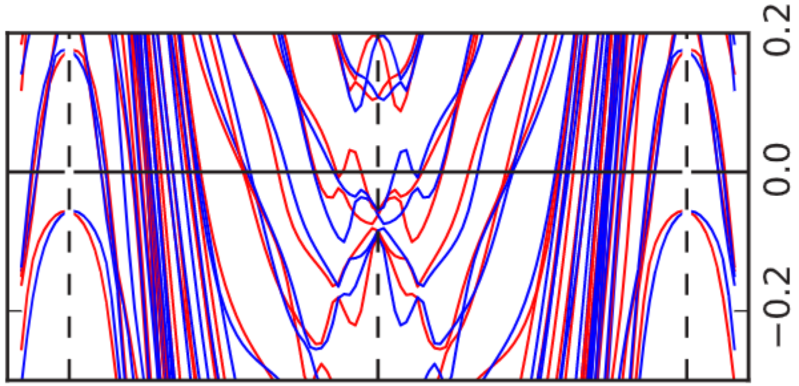
Tadaaa.... $H_R = -\alpha_R \boldsymbol{\sigma}\cdot(\boldsymbol{z}\times\boldsymbol{k})$

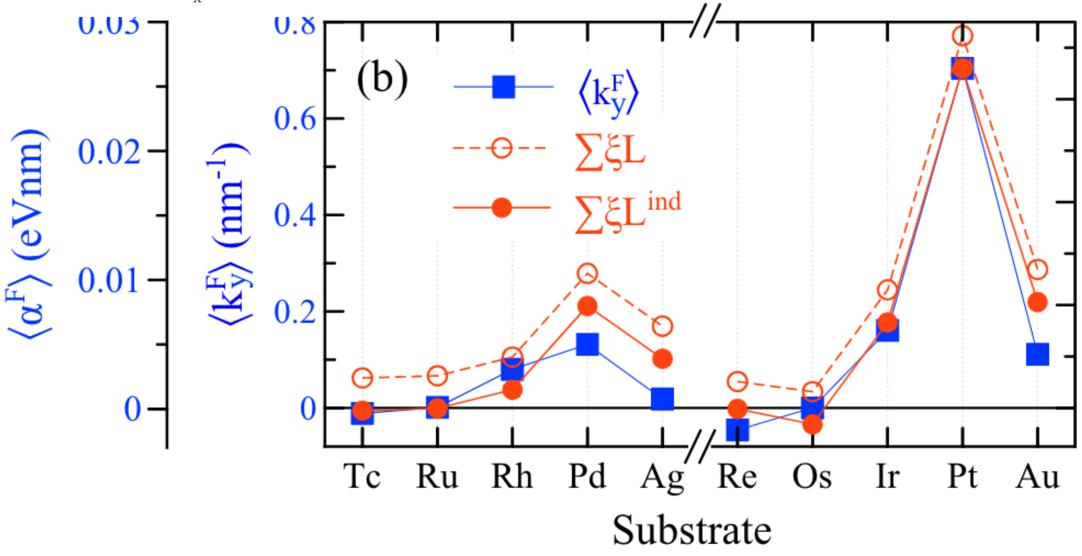


Lashell et al., PRL 77. 3419 (1996)

Transition metal interfaces: (4d,5d)/Co



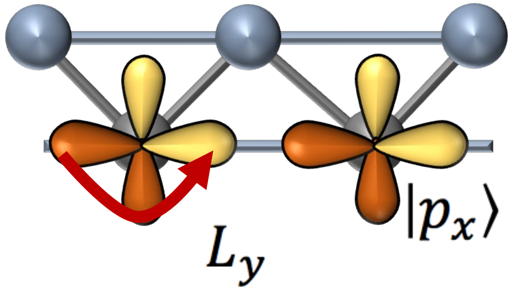




Grytsyuk et al. PRB 93, 174421 (2016)

The Rashba effect

E. Rashba



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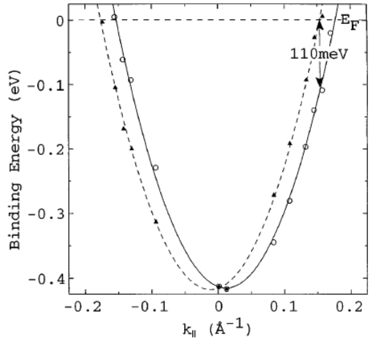
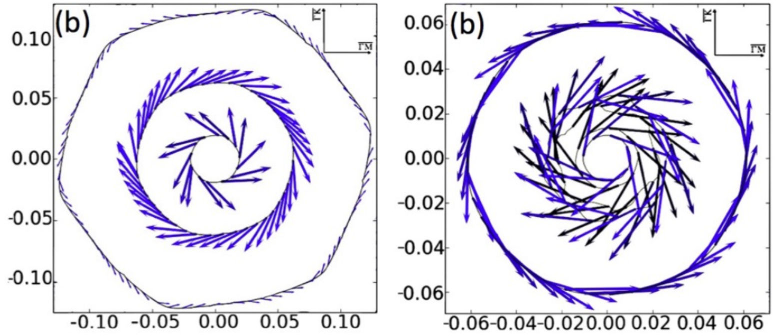
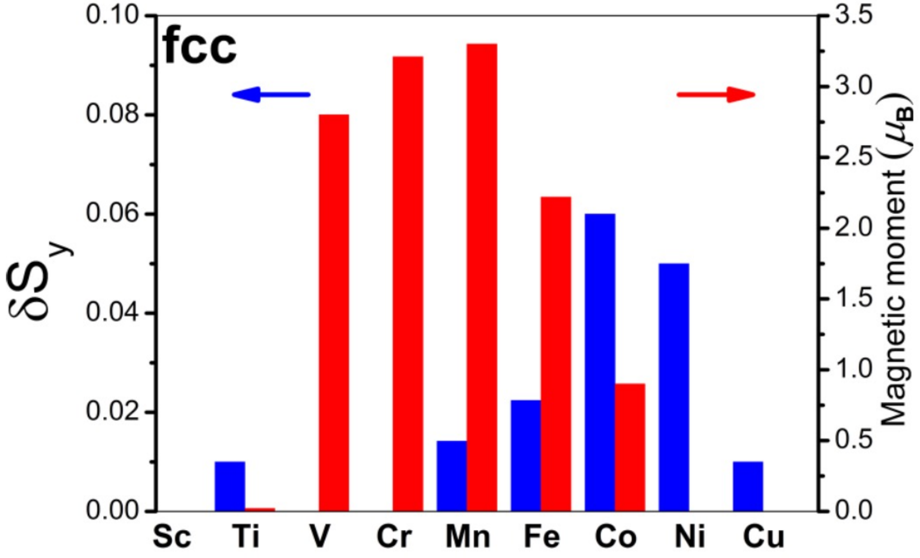


Lashell et al., PRL 77. 3419 (1996)

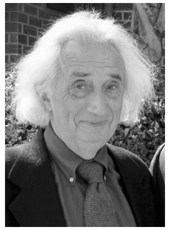
Topological insulator interfaces: Bi_2Se_3/3d



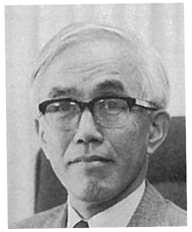


Laref et al. PRB 101, 220410(R) (2020)

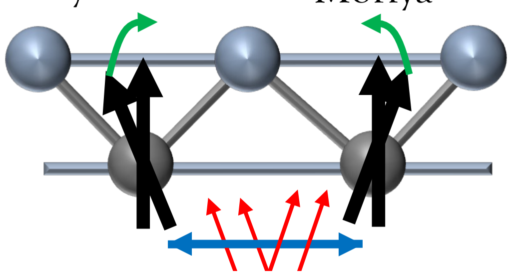
The Dzyaloshinskii-Moriya interaction



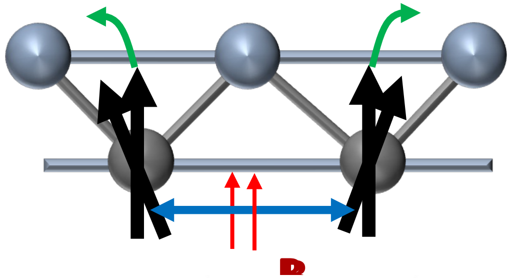
Dzyaloshinskii



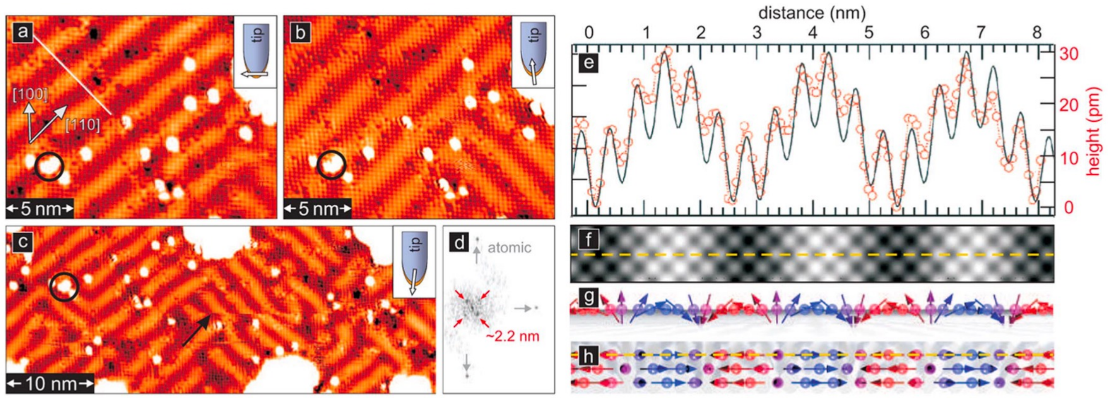
Moriya



$$-J\boldsymbol{S}_1 \cdot \boldsymbol{S}_2$$



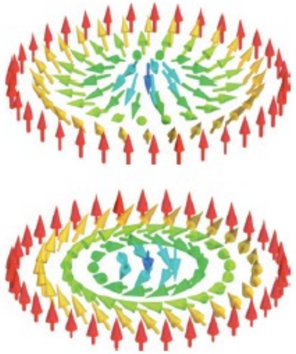
$$-\boldsymbol{D} \cdot (\boldsymbol{S}_1 \times \boldsymbol{S}_2)$$

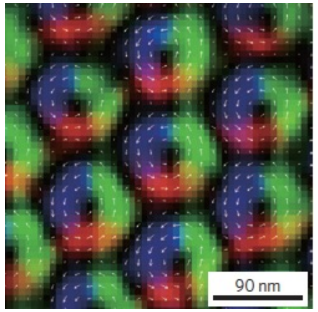


Ferriani, PRL 101, 027201 (2008)

See Manchon et al., PRB 101, 174423 (2020)
Hajr et al., PRB 102, 224427 (2020)

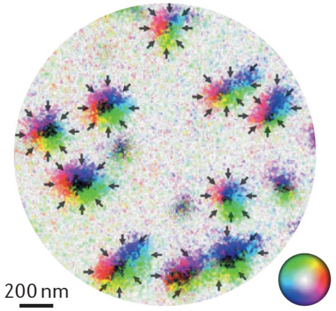
Spin spirals and magnetic skyrmions

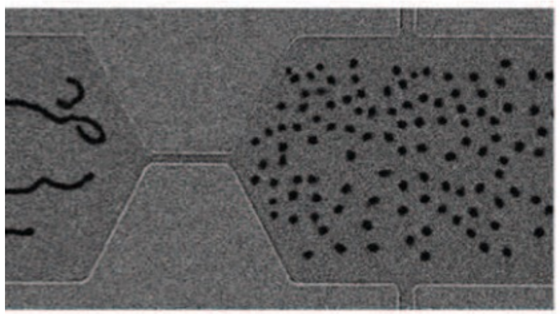




Yu Nature 2010; Nagaosa & Tokura, Nat. Nano 2013

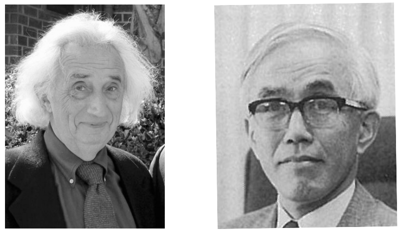
Room temperature skyrmions

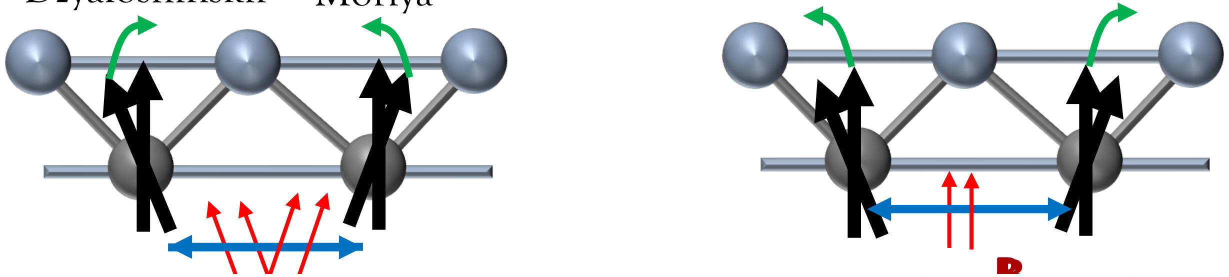




Chen, APL **106** 242404 (2015) Jiang, Science **349** 283 (2015)

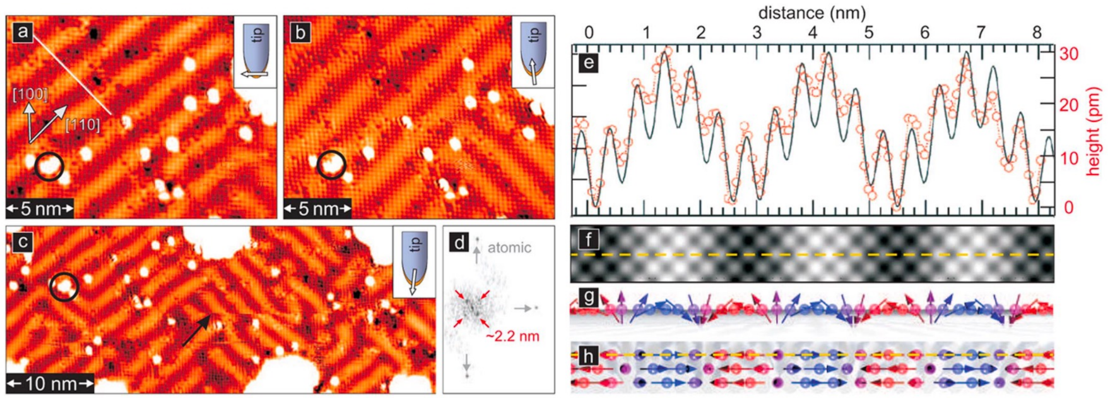
The Dzyaloshinskii-Moriya interaction





$-J\boldsymbol{S_1}\cdot\boldsymbol{S_2}$

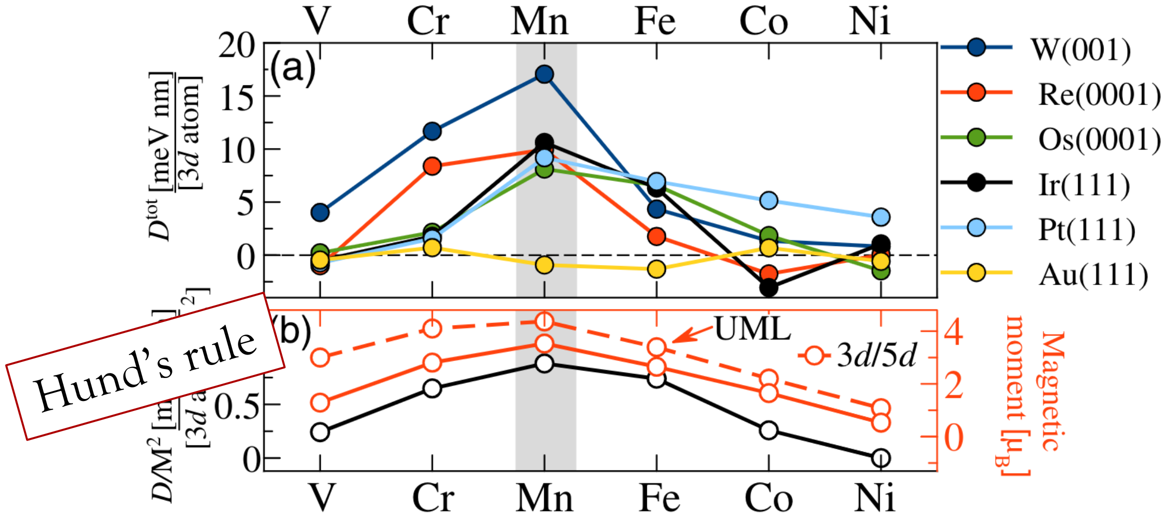
$-\boldsymbol{D}\cdot(\boldsymbol{S_1}\times\boldsymbol{S_2})$



Ferriani, PRL 101, 027201 (2008)

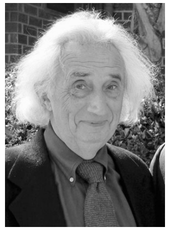
See Manchon et al., PRB 101, 174423 (2020)
Hajr et al., PRB 102, 224427 (2020)

Transition metal interfaces (4d,5d)/3d

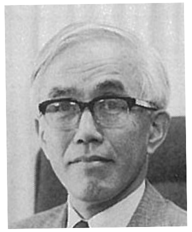


Belabbes et al. PRL 117, 247202 (2016)

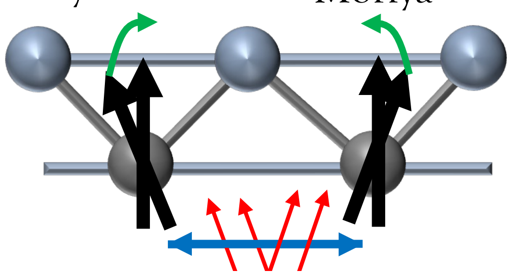
The Dzyaloshinskii-Moriya interaction



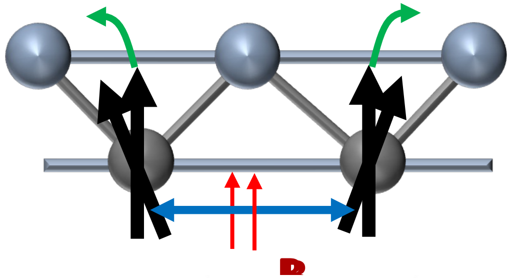
Dzyaloshinskii



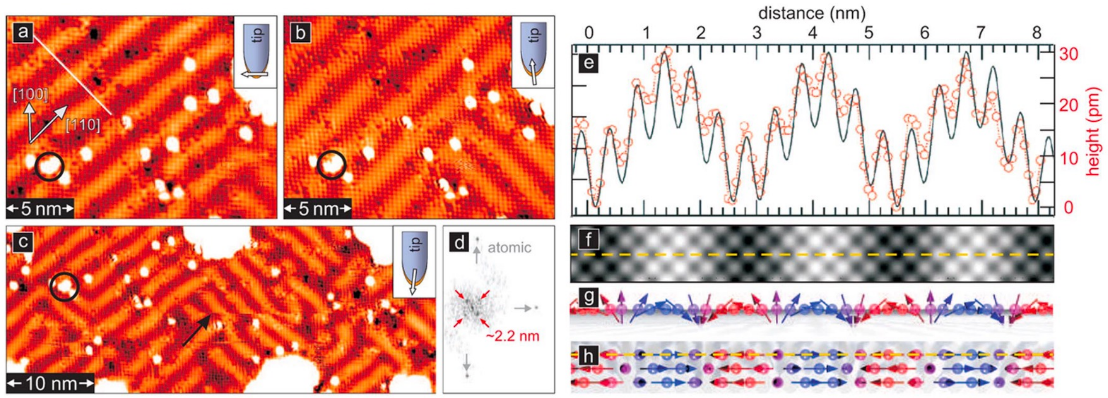
Moriya



$$-J\boldsymbol{S}_1 \cdot \boldsymbol{S}_2$$



$$-\boldsymbol{D} \cdot (\boldsymbol{S}_1 \times \boldsymbol{S}_2)$$



Ferriani, PRL 101, 027201 (2008)

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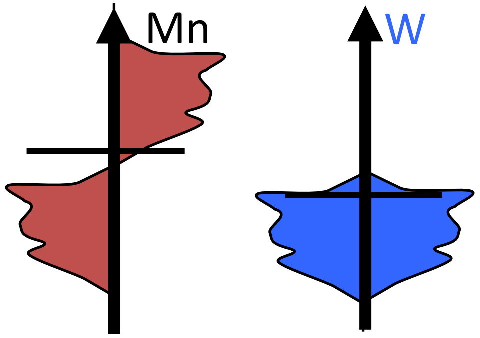
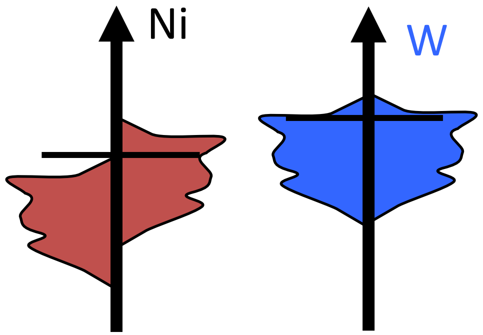


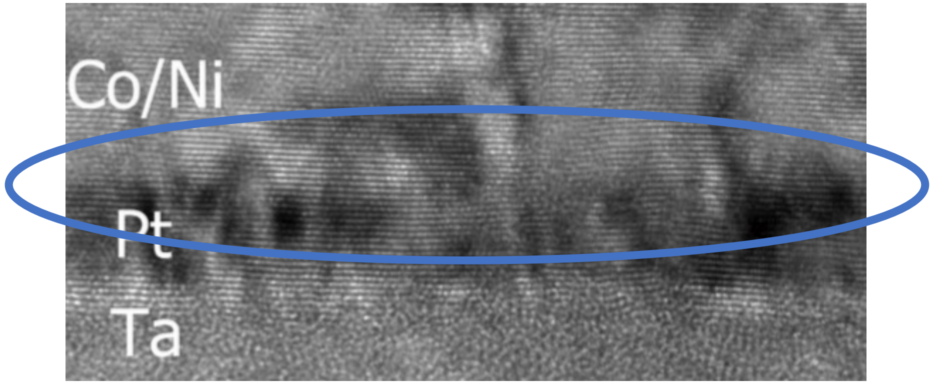
Mn/W
5d>>3d at Fermi level
Large DMI



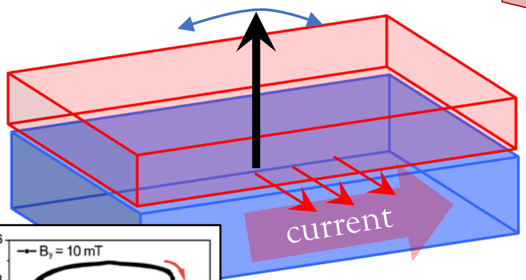
Ni/W
5d~3d at Fermi level
Weak DMI

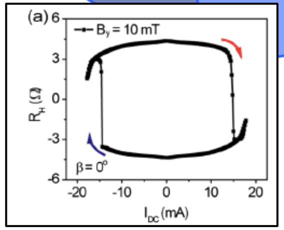
Looking at a magnetic interface...

TEM image taken from Gopman et al. at NIST



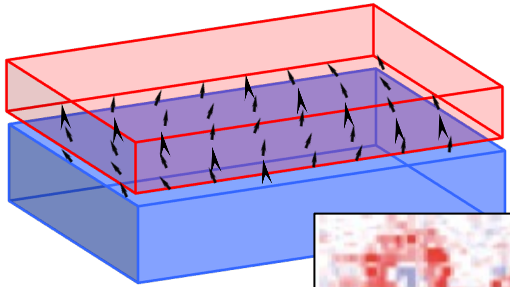
Spin-orbit torques



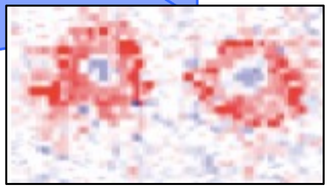


Nature **476**, 189 (2011)
Science **336**, 555 (2012)

Dzyaloshinskii-Moriya



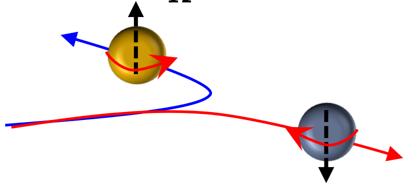
Science **349**, 283 (2015)
Also Woo, Boulle, Chen
Moreau-Luchaire.

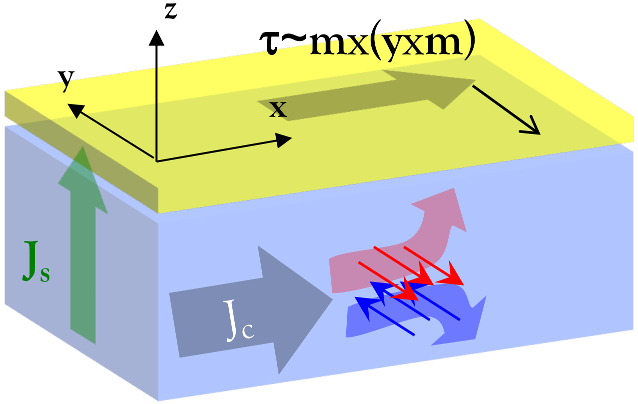


Looking at a magnetic interface…

Spin Hall effect

$$\hat{\mathbf{v}}_s = \partial_{\hbar\mathbf{k}}\varepsilon^s_{\mathbf{k}} + s\hat{\mathbf{\Omega}}_{\mathbf{k}} \times \dot{\mathbf{k}}$$

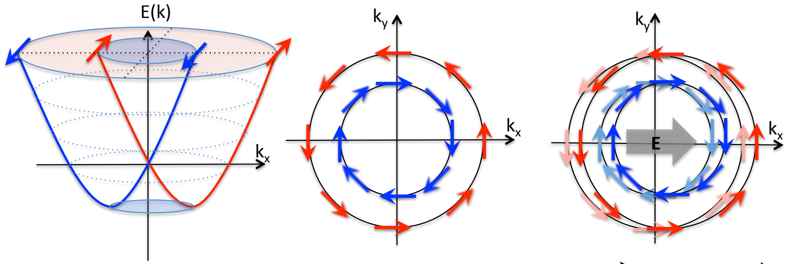




$$\boldsymbol{\tau} = \tau_{\|}\mathbf{m} \times [(\mathbf{z} \times \mathbf{E}) \times \mathbf{m}]$$

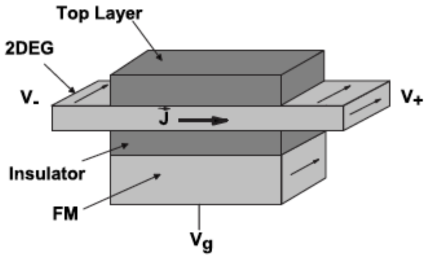
See Haney et al., PRB 87, 174411 (2013)

Inverse spin galvanic (Rashba) effect



$$H_{\mathrm{R}} \approx -\alpha\hat{\boldsymbol{\sigma}} \cdot (\mathbf{z} \times \mathbf{k}) \qquad \vec{S} \propto \vec{z} \times \vec{j}_e$$

Ivchenko, Pikus, P. Zh. Eksp. Teor. Fiz 27, 604 (1978)
Edelstein, Solid State Com. 73, 233 (1990)

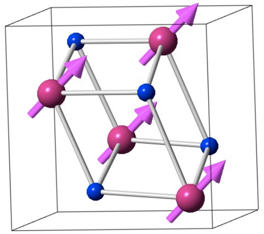


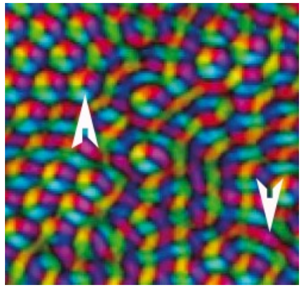
$$\boldsymbol{\tau} = \tau_{\perp}\mathbf{m} \times (\mathbf{z} \times \mathbf{E})$$

Manchon & Zhang, PRB 78, 212405 (2008)

Dzyaloshinskii-Moriya Interaction

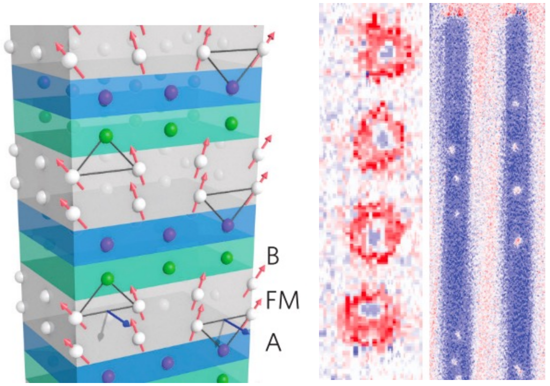
$$W_{3\mathrm{D}} = D_{3\mathrm{D}}\mathbf{m} \cdot (\boldsymbol{\nabla} \times \mathbf{m}).$$





Yu, Nature 465, 901 (2010)

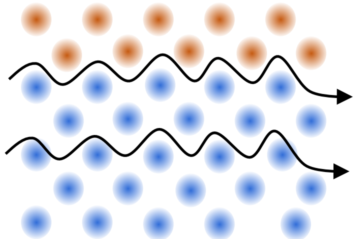
$$W_{2\mathrm{D}} = D_{2\mathrm{D}}\mathbf{m} \cdot [(\mathbf{z} \times \boldsymbol{\nabla}) \times \mathbf{m}].$$



Moreau-Luchaire, Nat. Nano 11, 444 (2016)

The Physics of Spin-Orbit Torques

Inverse spin galvanic or Rashba-Edelstein effect

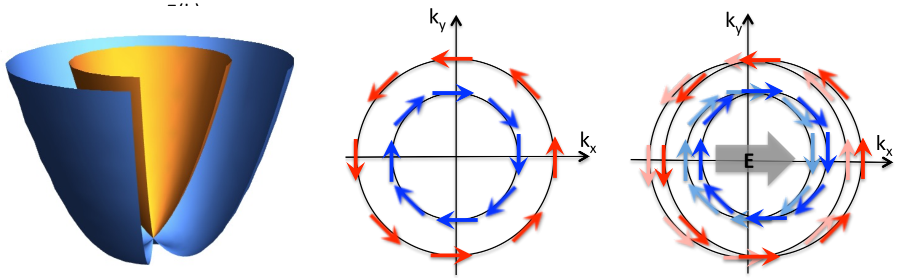


Vas'ko-Rashba Spin-orbit coupling

$$H_R \approx -\alpha \hat{\boldsymbol{\sigma}} \cdot (\mathbf{z} \times \mathbf{k})$$

Bulk spin-orbit coupling

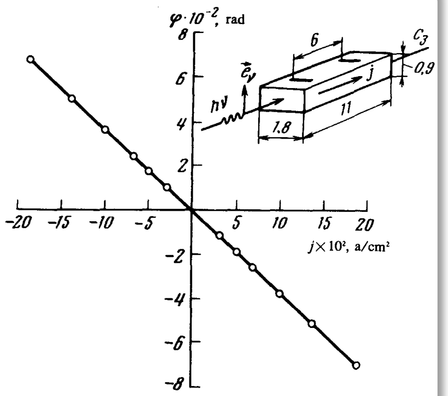
$$\hat{H}_{so} = (\xi/\hbar)\hat{\boldsymbol{\sigma}} \cdot (\nabla V \times \hat{\mathbf{p}})$$



$$\vec{S} \propto \vec{y} \Rightarrow \vec{T} = \Delta\vec{m} \times \vec{S} \propto \vec{y} \times \vec{m}$$

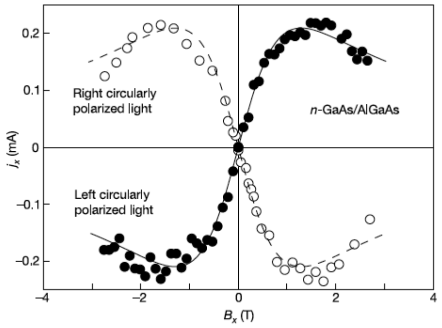
Ivchenko & Pikus, Pis'ma Zh. Eksp. Teor. Fiz 27, 604 (1978)
Edelstein, Solid State Com. 73, 233 (1990)

Tellurium



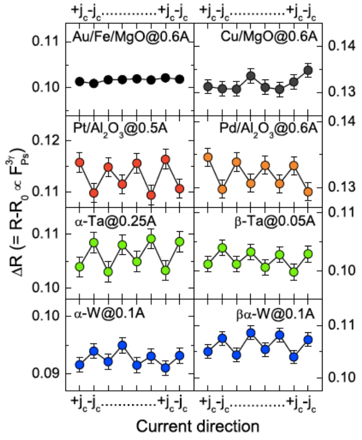
Vorob'ev, JETP Lett. 29, 441 (1979)

GaAs-QW



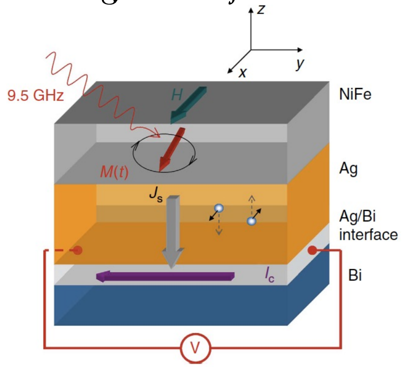
Ganichev, Nature 417, 153 (2002)

TM-surfaces



Zhang, Sci. Rep. 4:4844 (2014)

Ag/Bi surfaces

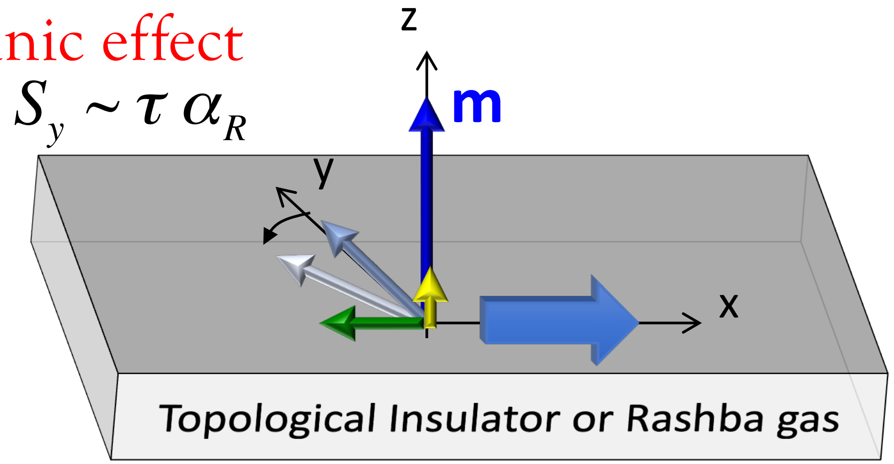


Rojas-Sanchez, Nature Comm. 4:2944 (2013)

The magnetoelectric effect made simple

Inverse spin galvanic effect
Extrinsic

$$S_y \sim \tau\, \alpha_R$$



Magnetoelectric effect
Intrinsic (!)

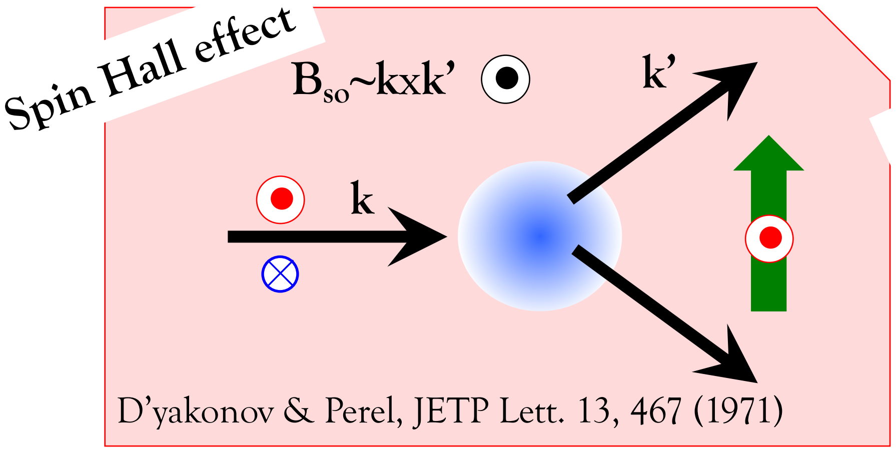
$$S_x \sim \frac{\tau_{sf}}{\tau_\Delta} S_y$$

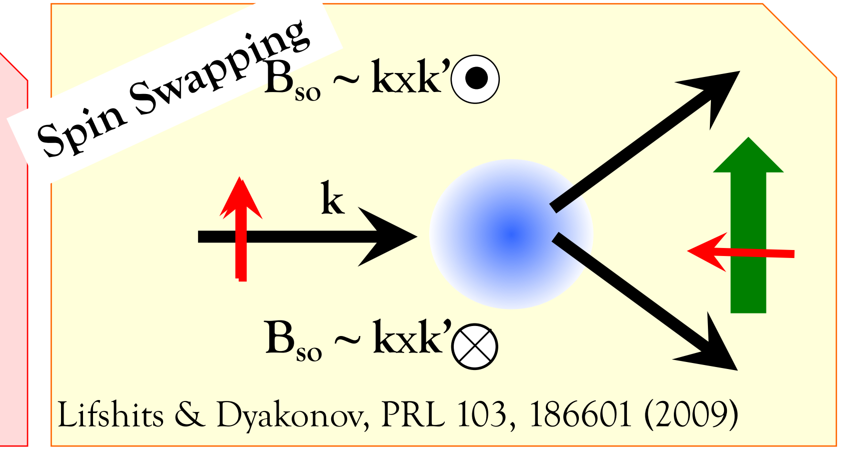
$$\alpha_R k_F >> \Delta, \quad \tau_{sf} = \frac{1}{\alpha_R^2 k_F^2 \tau} \Rightarrow S_x \sim \frac{\Delta}{\alpha_R}$$

$$\Delta >> \alpha_R k_F, \quad \tau_{sf} = \tau_\varphi = \frac{\tau_\Delta^2}{\tau} \Rightarrow S_x \sim \frac{\alpha_R}{\Delta}$$

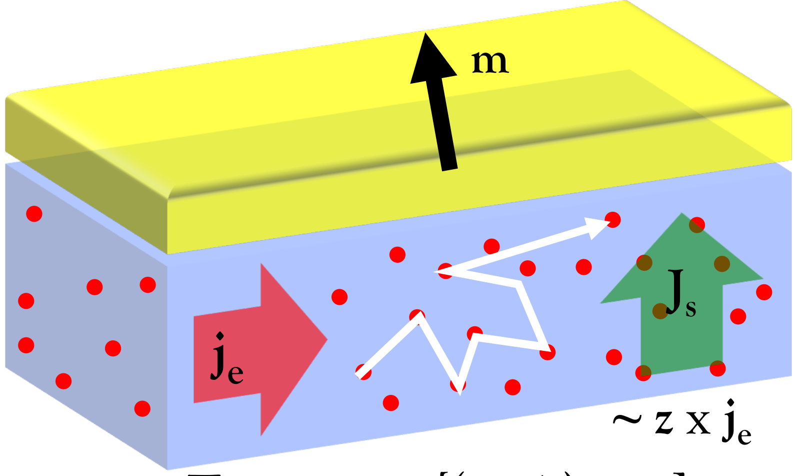
Li et al., PRB **91**, 134402 (2015)

Spin Hall and spin swapping effects



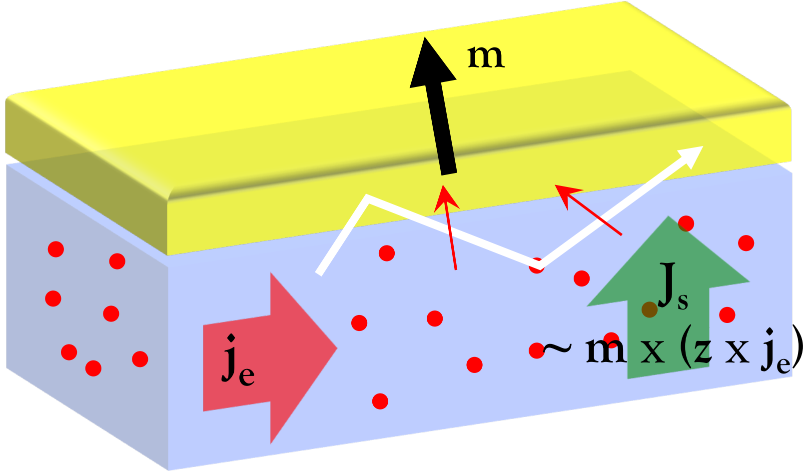


Spin Hall torque



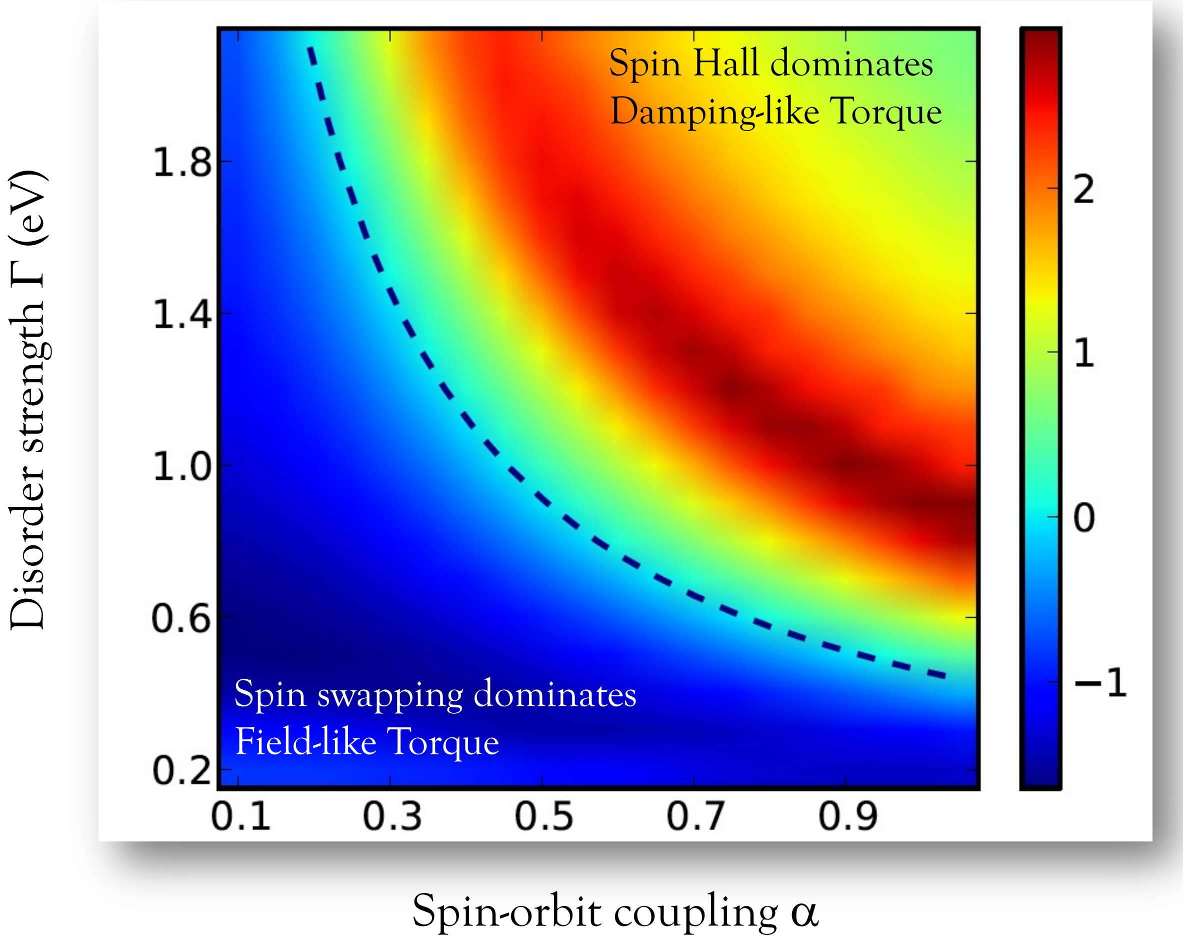
T_{SHE} ~ m x [(z x j_e) x m]

Spin swapping torque



T_{SW} ~ m x (z x j_e)

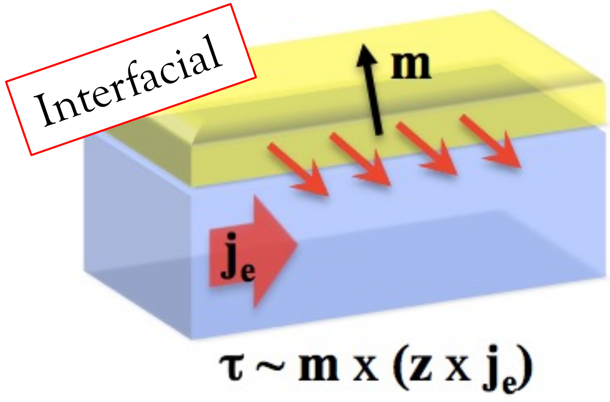
The Ratio Dampinglike/Fieldlike is controlled by disorder



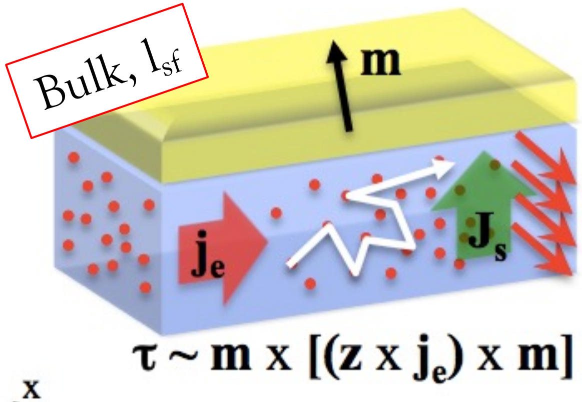
H.B.M. Saidaoui, and A. Manchon, PRL 117, 036601 (2016)
H. B. M. Saidaoui, Y. Otani, and A. Manchon, PRB 92, 024417 (2015)

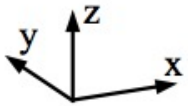
Summary of Microscopic Mechanisms

Inverse spin galvanic effect

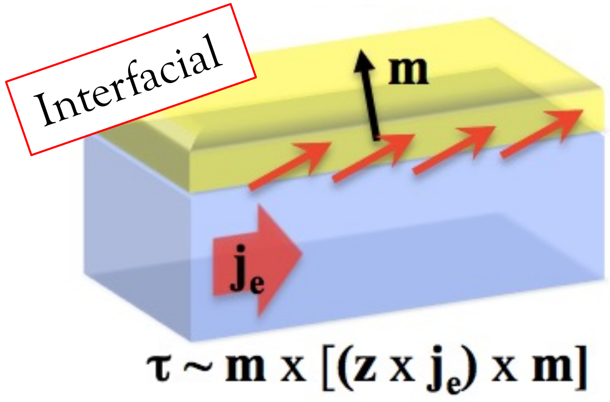


Spin Hall effect

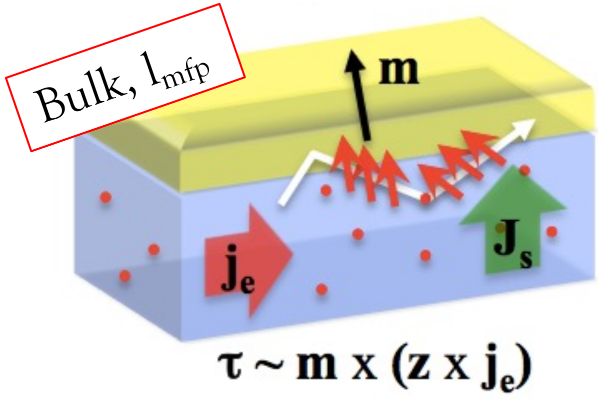




Magnetoelectric effect



Spin swapping effect



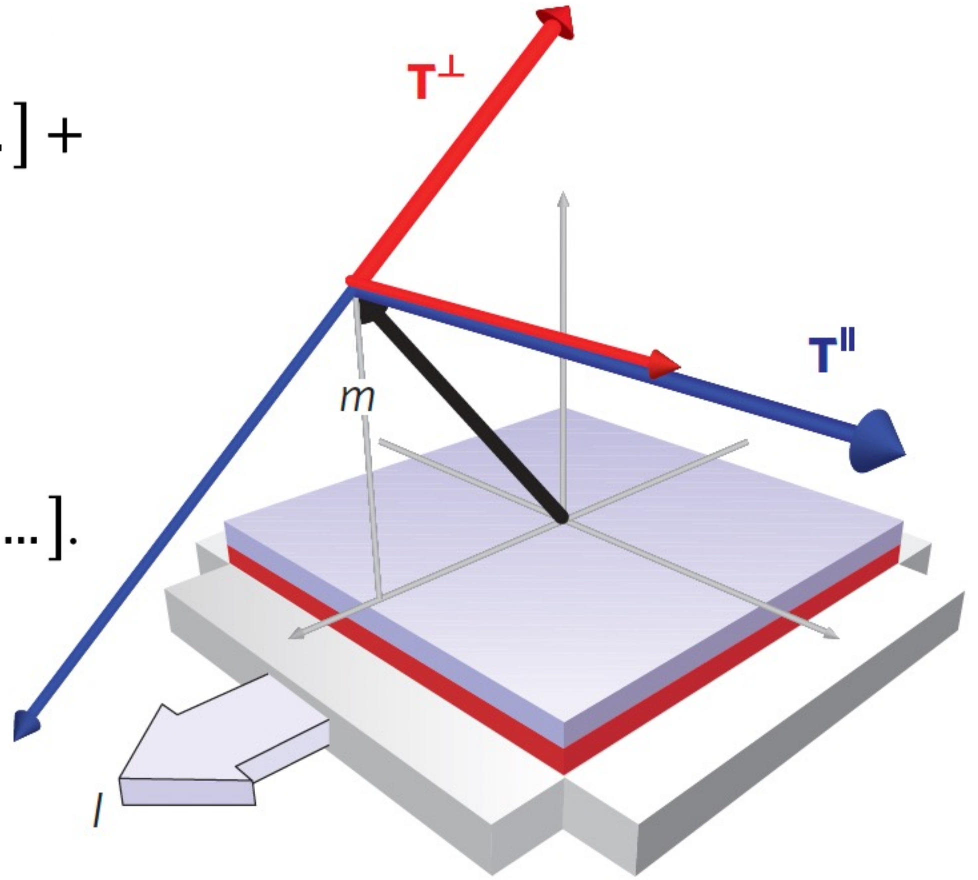
Angular dependence of the spin-orbit torque

$$\boldsymbol{T}^{\parallel} = \boldsymbol{m} \times [(\boldsymbol{e}_z \times \boldsymbol{E}) \times \boldsymbol{m}]\left[A_0^{\varphi} + B_2^{\theta}(\boldsymbol{e}_z \times \boldsymbol{m})^2 + B_4^{\theta}(\boldsymbol{e}_z \times \boldsymbol{m})^4 + \ldots\right] +$$

$$(\boldsymbol{m} \times \boldsymbol{e}_z)(\boldsymbol{m} \cdot \boldsymbol{E})\left[\left(B_2^{\theta} - A_2^{\varphi}\right) + \left(B_4^{\theta} - A_4^{\varphi}\right)(\boldsymbol{e}_z \times \boldsymbol{m})^2 + \ldots\right]$$

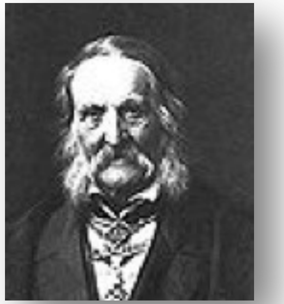
$$\boldsymbol{T}^{\perp} = (\boldsymbol{e}_z \times \boldsymbol{E}) \times \boldsymbol{m}\left[A_0^{\theta} - B_2^{\varphi}(\boldsymbol{e}_z \times \boldsymbol{m})^2 - B_4^{\varphi}(\boldsymbol{e}_z \times \boldsymbol{m})^4 - \ldots\right] +$$

$$\boldsymbol{m} \times [(\boldsymbol{m} \times \boldsymbol{e}_z)(\boldsymbol{m} \cdot \boldsymbol{E})]\left[\left(A_2^{\theta} + B_2^{\varphi}\right) + \left(A_4^{\theta} + B_4^{\varphi}\right)(\boldsymbol{e}_z \times \boldsymbol{m})^2 + \ldots\right].$$



Garello et al., Nature Nanotechnology 8, 587 (2013)
Ortiz Pauyac, Applied Physics Letters 102, 252403 (2013)

Symmetry considerations



Neumann

In 1885 Voigt stated: "***the symmetry of the physical phenomenon is at least as high as the crystallographic symmetry,***" which became a fundamental postulate of crystal physics known as "**Neumann's principle**".

Voigt

$$\chi = \det(R) R \chi R^{-1}$$

Tensor response (Torque, damping etc.) → χ

Symmetry operator → R^{-1}

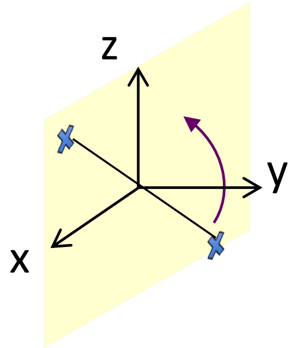
Bravais lattice	Point Group	Centrosymmetric	Non-centrosymmetric	
			Piezoelectric group	Pyroelectric group
Triclinic	$1, \bar{1}$	$\bar{1}$	1	1
Monoclinic	$2, m, 2/m$	$2/m$	$2, m$	$2, m$
Orthorhombic	$222, mm2, mmm$	mmm	$222, mm2$	$mm2$
Tetragonal	$4, \bar{4}, 4/m, 422, 4mm, \bar{4}2m, 4/m\ mm$	$4/m, 4/m\ mm$	$4, \bar{4}, 422, 4mm, \bar{4}2m$	$4, 4mm$
Trigonal	$3, \bar{3}, 32, 3m, \bar{3}m$	$\bar{3}, \bar{3}m$	$3, 32, 3m$	$3, 3m$
Hexagonal	$6, \bar{6}, 6/m, 622, 6mm, \bar{6}m2, 6/m\ mm$	$6/m, 6/m\ mm$	$6, \bar{6}, 622, 6mm, \bar{6}m2$	$6, 6mm$
Cubic	$23, m\bar{3}, 432, 4\bar{3}m, m\bar{3}m$	$m3, m\bar{3}m$	$23, 4\bar{3}m$	–

Ciccarelli et al., Nature Physics 12, 855 (2016); Zelezny et al., Phys. Rev. B 95, 014403 (2017)

Two examples

$$\chi = \det(R) R \chi R^{-1}$$

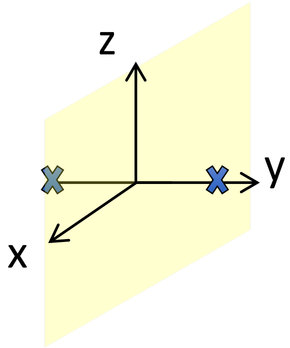
2-fold rotation symmetry



(x,y,z) -> (-x,y,-z)

2	$\begin{pmatrix} x_{11} & 0 & x_{13} \\ 0 & x_{22} & 0 \\ x_{31} & 0 & x_{33} \end{pmatrix}$

Mirror symmetry

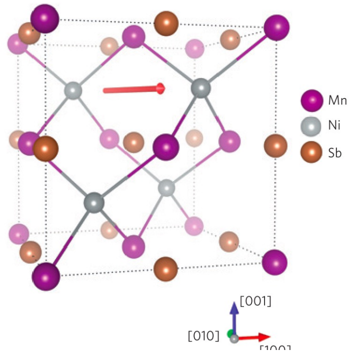


(x,y,z) -> (x,-y,z)

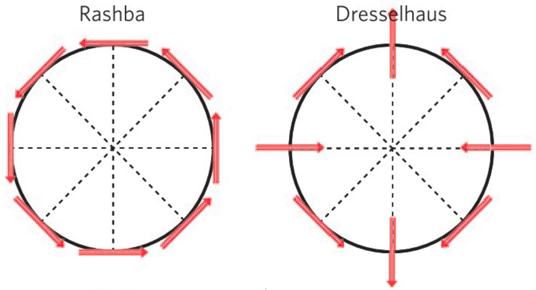
m	$\begin{pmatrix} 0 & x_{12} & 0 \\ x_{21} & 0 & x_{23} \\ 0 & x_{32} & 0 \end{pmatrix}$

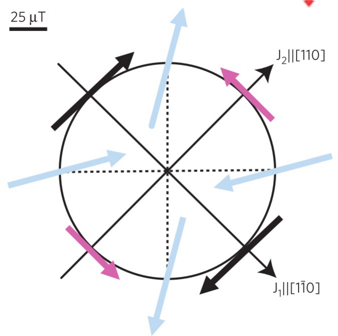
Ciccarelli et al., Nature Physics 12, 855 (2016)
See also D. MacNeill et al., Nature Physics 13, 300 (2017)

Bulk MnNiSb: Rashba + Dresselhaus



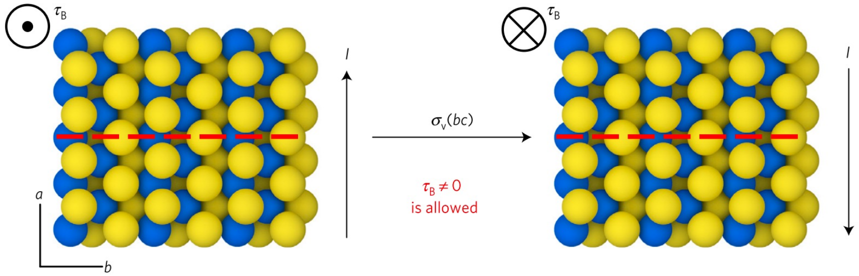
$$-42m \quad \begin{pmatrix} x_{11} & 0 & 0 \\ 0 & -x_{11} & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

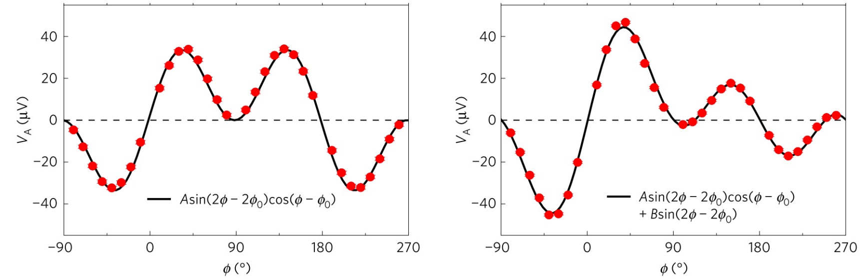


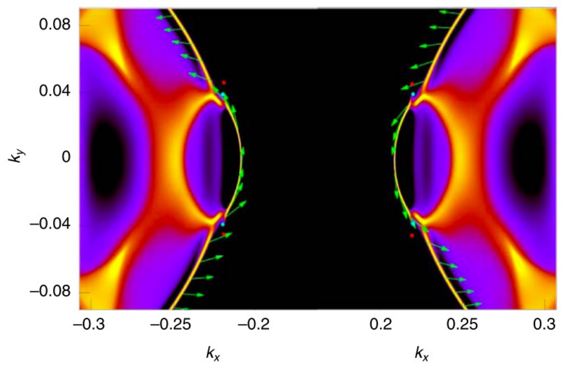


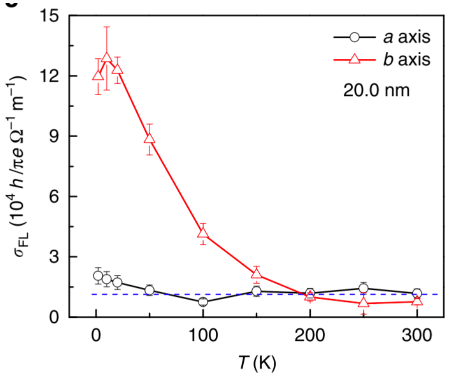
Ciccarelli et al., Nature Physics 12, 855 (2016)

WTe_2/Py: Perpendicular DL+anisotropic FL







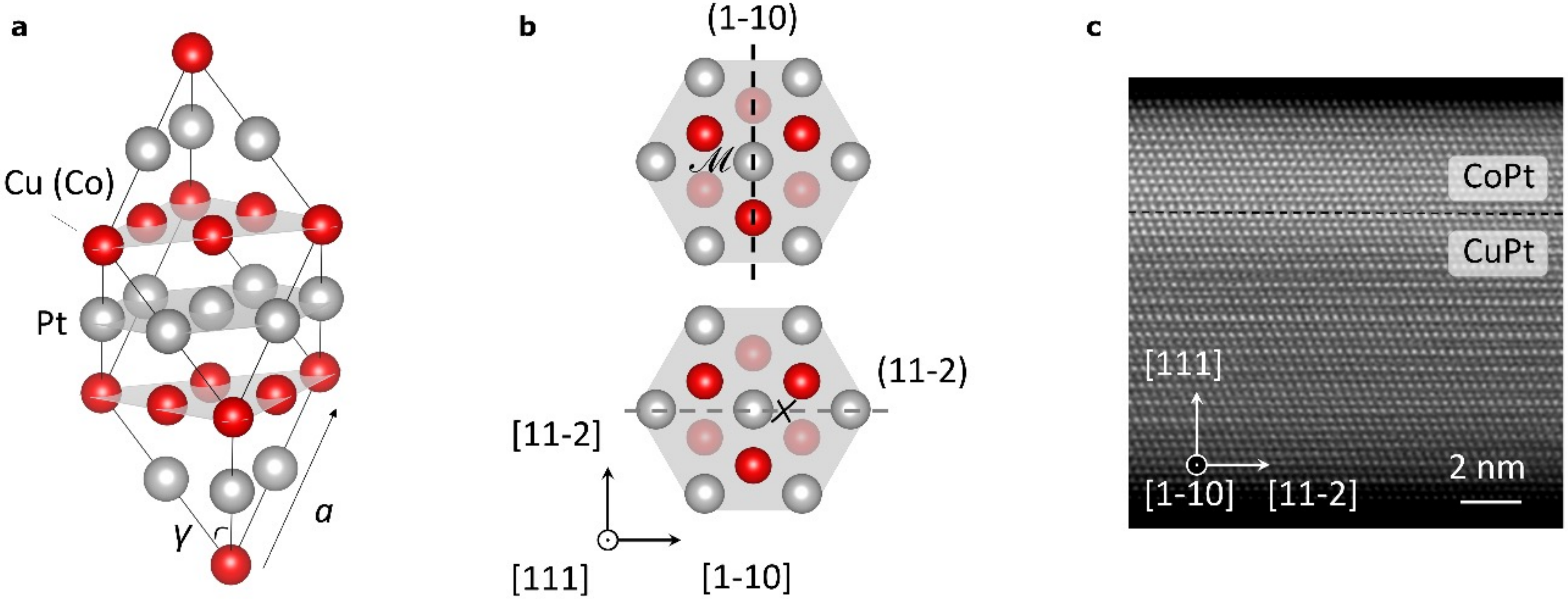


MacNeill et al., Nature Physics 13, 300 (2017)
Peng Li et al., Nature Communications 9, 3990 (2018)

Crystal system	Point group	$\chi^{(0)}$	$\chi^{(1)}$
triclinic	1	$\begin{pmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ x_{31} & x_{32} & x_{33} \end{pmatrix}$	$\begin{pmatrix} \hat{n}_x x_{111} + \hat{n}_y x_{112} + \hat{n}_z x_{113} & \hat{n}_x x_{121} + \hat{n}_y x_{122} + \hat{n}_z x_{123} & \hat{n}_x x_{131} + \hat{n}_y x_{132} + \hat{n}_z x_{133} \\ \hat{n}_x x_{211} + \hat{n}_y x_{212} + \hat{n}_z x_{213} & \hat{n}_x x_{221} + \hat{n}_y x_{222} + \hat{n}_z x_{223} & \hat{n}_x x_{231} + \hat{n}_y x_{232} + \hat{n}_z x_{233} \\ \hat{n}_x x_{311} + \hat{n}_y x_{312} + \hat{n}_z x_{313} & \hat{n}_x x_{321} + \hat{n}_y x_{322} + \hat{n}_z x_{323} & \hat{n}_x x_{331} + \hat{n}_y x_{332} + \hat{n}_z x_{333} \end{pmatrix}$
monoclinic	2	$\begin{pmatrix} x_{11} & 0 & x_{13} \\ 0 & x_{22} & 0 \\ x_{31} & 0 & x_{33} \end{pmatrix}$	$\begin{pmatrix} \hat{n}_y x_1 & \hat{n}_x x_{13} + \hat{n}_z x_{12} & \hat{n}_y x_3 \\ \hat{n}_x x_5 + \hat{n}_z x_6 & \hat{n}_y x_{11} & \hat{n}_x x_4 + \hat{n}_z x_7 \\ \hat{n}_y x_{10} & \hat{n}_x x_8 + \hat{n}_z x_9 & \hat{n}_y x_2 \end{pmatrix}$
	m	$\begin{pmatrix} 0 & x_{12} & 0 \\ x_{21} & 0 & x_{23} \\ 0 & x_{32} & 0 \end{pmatrix}$	$\begin{pmatrix} \hat{n}_x x_{12} + \hat{n}_z x_9 & \hat{n}_y x_{14} & \hat{n}_x x_{13} + \hat{n}_z x_8 \\ \hat{n}_y x_3 & \hat{n}_x x_{11} + \hat{n}_z x_{10} & \hat{n}_y x_4 \\ \hat{n}_x x_7 + \hat{n}_z x_6 & \hat{n}_y x_5 & \hat{n}_x x_1 + \hat{n}_z x_2 \end{pmatrix}$
orthorhombic	222	$\begin{pmatrix} x_{11} & 0 & 0 \\ 0 & x_{22} & 0 \\ 0 & 0 & x_{33} \end{pmatrix}$	$\begin{pmatrix} 0 & \hat{n}_z x_5 & \hat{n}_y x_4 \\ \hat{n}_z x_1 & 0 & \hat{n}_x x_6 \\ \hat{n}_y x_3 & \hat{n}_x x_2 & 0 \end{pmatrix}$
	mm2	$\begin{pmatrix} 0 & x_{12} & 0 \\ x_{21} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} \hat{n}_z x_4 & 0 & \hat{n}_x x_6 \\ 0 & \hat{n}_z x_5 & \hat{n}_y x_7 \\ \hat{n}_x x_3 & \hat{n}_y x_2 & \hat{n}_z x_1 \end{pmatrix}$
tetragonal	4	$\begin{pmatrix} x_{11} & -x_{21} & 0 \\ x_{21} & x_{11} & 0 \\ 0 & 0 & x_{33} \end{pmatrix}$	$\begin{pmatrix} \hat{n}_z x_6 & -\hat{n}_z x_2 & \hat{n}_x x_5 - \hat{n}_y x_7 \\ \hat{n}_z x_2 & \hat{n}_z x_6 & \hat{n}_x x_7 + \hat{n}_y x_5 \\ \hat{n}_x x_4 - \hat{n}_y x_3 & \hat{n}_x x_3 + \hat{n}_y x_4 & \hat{n}_z x_1 \end{pmatrix}$
	-4	$\begin{pmatrix} x_{11} & x_{21} & 0 \\ x_{21} & -x_{11} & 0 \\ 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} \hat{n}_z x_5 & \hat{n}_z x_1 & \hat{n}_x x_4 + \hat{n}_y x_6 \\ \hat{n}_z x_1 & -\hat{n}_z x_5 & \hat{n}_x x_6 - \hat{n}_y x_4 \\ \hat{n}_x x_3 + \hat{n}_y x_2 & \hat{n}_x x_2 - \hat{n}_y x_3 & 0 \end{pmatrix}$
	422	$\begin{pmatrix} x_{11} & 0 & 0 \\ 0 & x_{11} & 0 \\ 0 & 0 & x_{33} \end{pmatrix}$	$\begin{pmatrix} 0 & -\hat{n}_z x_3 & -\hat{n}_y x_2 \\ \hat{n}_z x_3 & 0 & \hat{n}_x x_2 \\ -\hat{n}_y x_1 & \hat{n}_x x_1 & 0 \end{pmatrix}$
	4mm	$\begin{pmatrix} 0 & -x_{21} & 0 \\ x_{21} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} \hat{n}_z x_4 & 0 & \hat{n}_x x_1 \\ 0 & \hat{n}_z x_4 & \hat{n}_y x_1 \\ \hat{n}_x x_3 & \hat{n}_y x_3 & \hat{n}_z x_2 \end{pmatrix}$
	-42m	$\begin{pmatrix} x_{11} & 0 & 0 \\ 0 & -x_{11} & 0 \\ 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & \hat{n}_z x_3 & \hat{n}_y x_2 \\ \hat{n}_z x_3 & 0 & \hat{n}_x x_2 \\ \hat{n}_y x_1 & \hat{n}_x x_1 & 0 \end{pmatrix}$
	-4m2	$\begin{pmatrix} 0 & x_{21} & 0 \\ x_{21} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} \hat{n}_z x_3 & 0 & \hat{n}_x x_1 \\ 0 & -\hat{n}_z x_3 & -\hat{n}_y x_1 \\ \hat{n}_x x_2 & -\hat{n}_y x_2 & 0 \end{pmatrix}$

Zelezny et al., Phys. Rev. B 95, 014403 (2017)

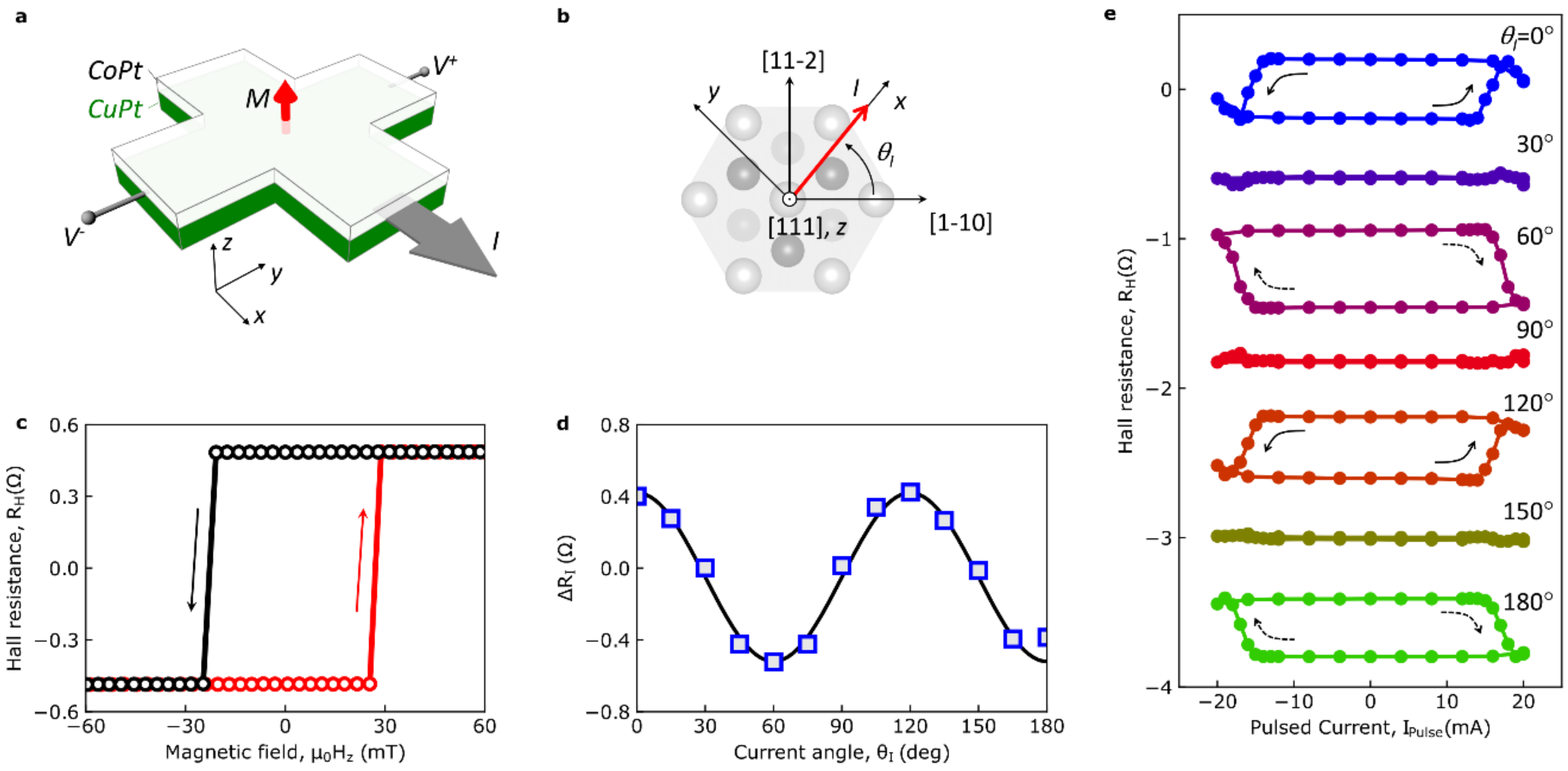
Eve more intriguing: field-free switching with 3-fold symmetry



Collaboration with
Jingsheng Chen @ NUS

Liu et al. Nature Nanotechnology 16, 277 (2021)

Eve more intriguing: field-free switching with 3-fold symmetry



Collaboration with
Jingsheng Chen @ NUS

Liu et al. Nature Nanotechnology 16, 277 (2021)

The Physics of Dzyaloshinskii-Moriya interaction

Key ideas behind DMI

Assume a general magnetic energy $W = \sum_{ij} \boldsymbol{S}_i \bullet \underline{\underline{\boldsymbol{\Lambda}}}_{ij} \bullet \boldsymbol{S}_j$

$$W = \underbrace{\sum_{ij} J_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j}_{\text{Symmetric exchange}} + \sum_{i,j} \underbrace{\boldsymbol{D}_{ij} \cdot (\boldsymbol{S}_i \times \boldsymbol{S}_j)}_{\text{Antiymmetric exchange}} + \sum_i \underbrace{\boldsymbol{S}_i \bullet \underline{\underline{\boldsymbol{K}}}_i \bullet \boldsymbol{S}_i}_{\text{Magnetocrystalline anisotropy + dipolar interaction}}$$

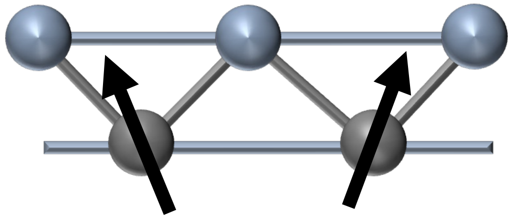
Symmetric exchange Antiymmetric exchange Magnetocrystalline anisotropy
+ dipolar interaction

Micromagnetic picture $W = \sum_{ij} J_{ij} \partial_i \boldsymbol{m} \cdot \partial_j \boldsymbol{m} + D_{ijk} m_i \, \partial_j m_k + K_i m_i^2 + \cdots$

$$\sum_{ijk} D_{ijk} m_i \, \partial_j m_k = \sum_{ijk} \underbrace{D^A_{ijk}(m_i \, \partial_j m_k - m_k \, \partial_j m_i)}_{\text{Lifshitz invariant}} + D^S_{ijk}(m_i \, \partial_j m_k + m_k \, \partial_j m_i)$$

Lifshitz invariant

Key ideas behind DMI



$$W \propto \mathrm{Tr}[(\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{S}_A) G_{A \to B} (\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{S}_B) G_{B \to A}]$$

$$G_{A \to B} \approx G_0 + G_0 H_{so} G_0$$

$$W_0 \propto \mathrm{Tr}[(\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{S}_A) G_0 (\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{S}_B) G_0] \equiv \boldsymbol{S}_A \cdot \boldsymbol{S}_B$$

$$W_1 \propto \mathrm{Tr}[(\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{S}_A)(\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{B}_{\mathbf{eff}})(\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{S}_B)] \equiv \boldsymbol{B}_{\boldsymbol{eff}} \cdot (\boldsymbol{S}_A \times \boldsymbol{S}_B)$$

Various mechanims have been proposed:
Superexchange in weak ferromagnets (Moriya 1960), RKKY in dilute alloys (Fert 1990), « Rashba » effect in metals (Kim 2013) etc.

Moriya's rules

1. When a center of inversion is located at C,

$$\mathbf{D}=0.$$

2. When a mirror plane perpendicular to AB passes through C,

$$\mathbf{D} \parallel \text{mirror plane or } \mathbf{D} \perp AB.$$

3. When there is a mirror plane including A and B,

$$\mathbf{D} \perp \text{mirror plane.}$$

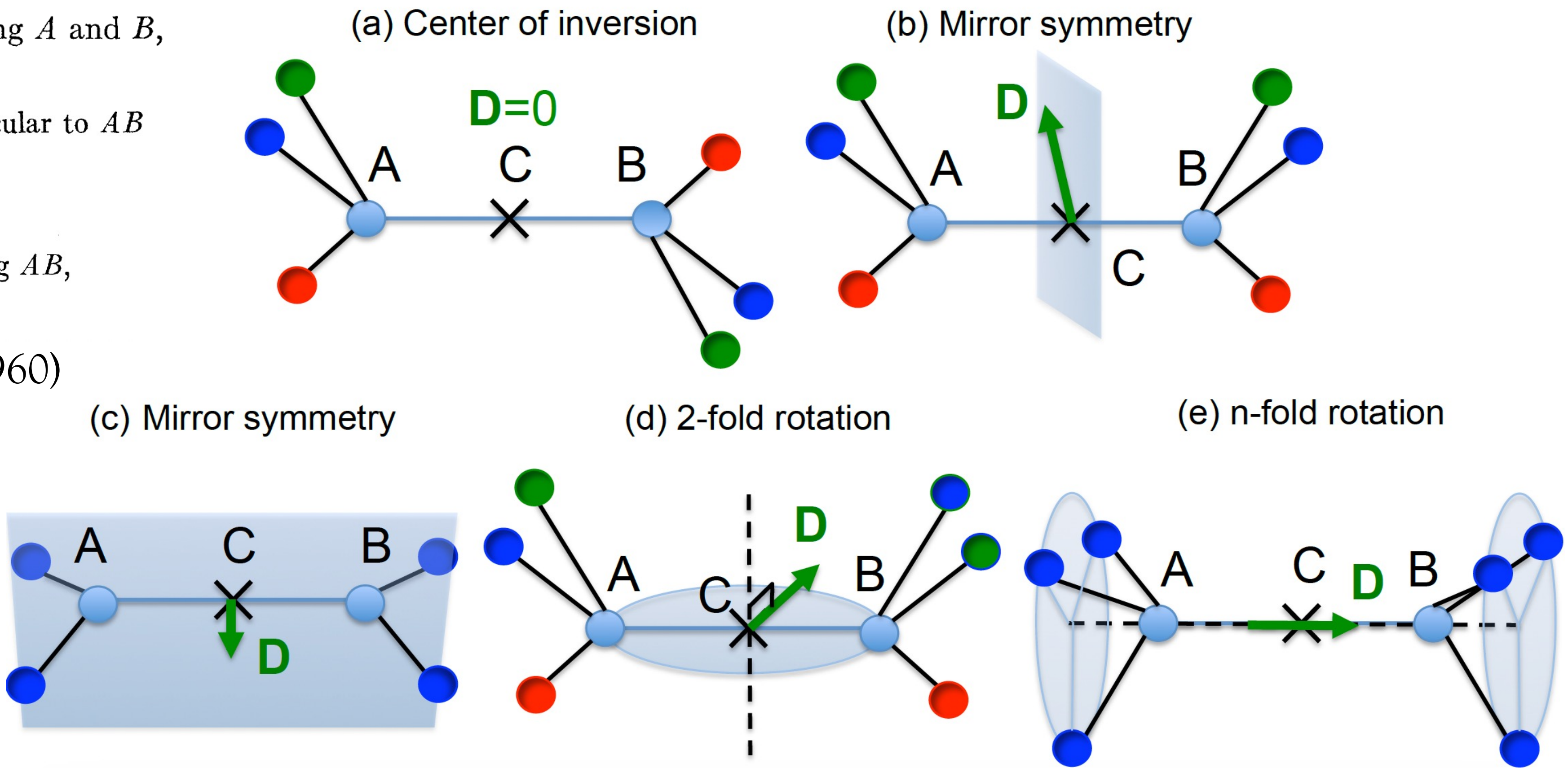
4. When a two-fold rotation axis perpendicular to AB passes through C,

$$\mathbf{D} \perp \text{two-fold axis.}$$

5. When there is an n-fold axis ($n \geq 2$) along AB,

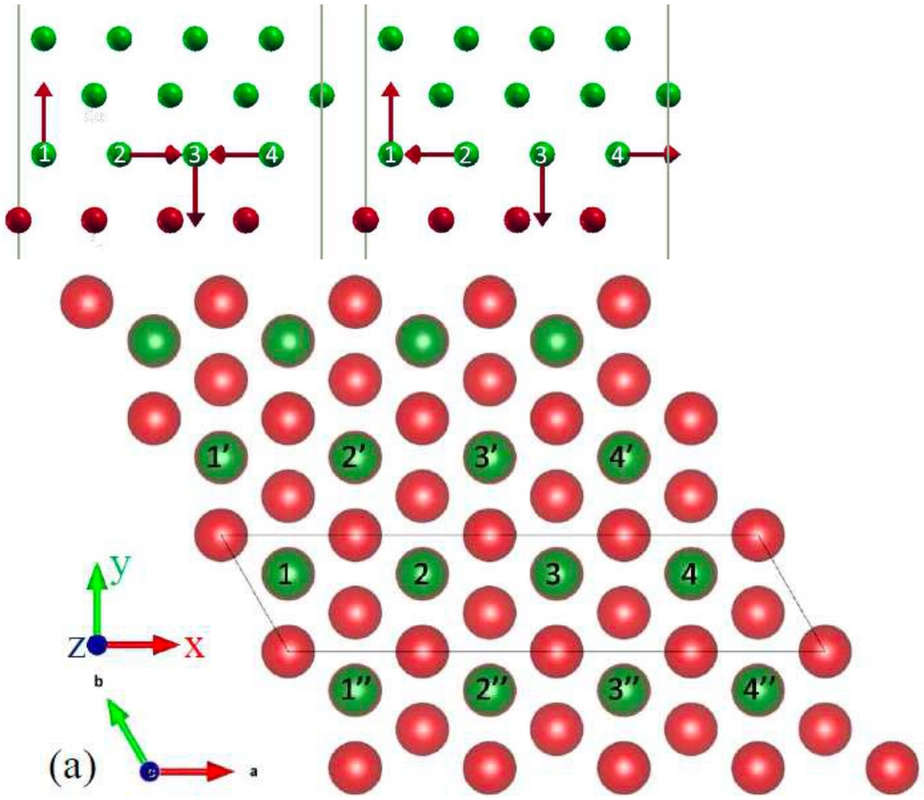
$$\mathbf{D} \parallel AB.$$

Moriya Physical Review 101, 91 (1960)



Computing DMI: DFT+ Force Theorem

Build a spin spiral in large supercells by employing the Force Theorem (energy penalty cost) and compute the different in energy between two opposite chiralities



Yang et al., PRL 115, 267210 (2015)

Advantages:

No assumption on the spin-orbit coupling strength

Fast and relatively easy to compute

Limitations:

Impractical to model long wavelength systems (walls and skyrmions)

Rather inadapted to metals (long-range interactions)

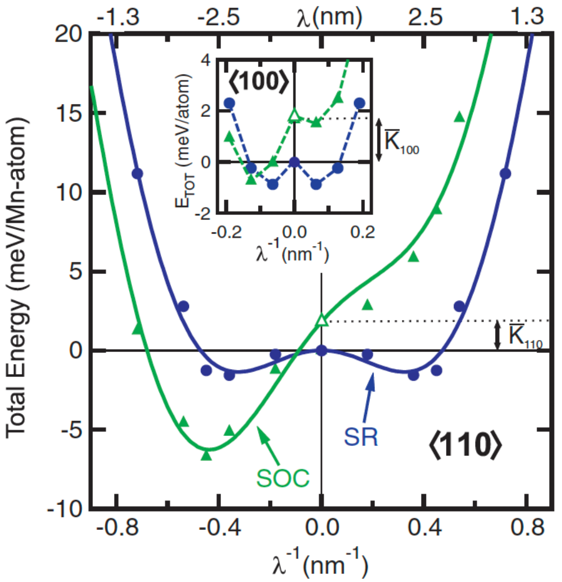
The penalty cost needed to impose the spin spiral might overcome the DMI energy and deteriore the accuracy

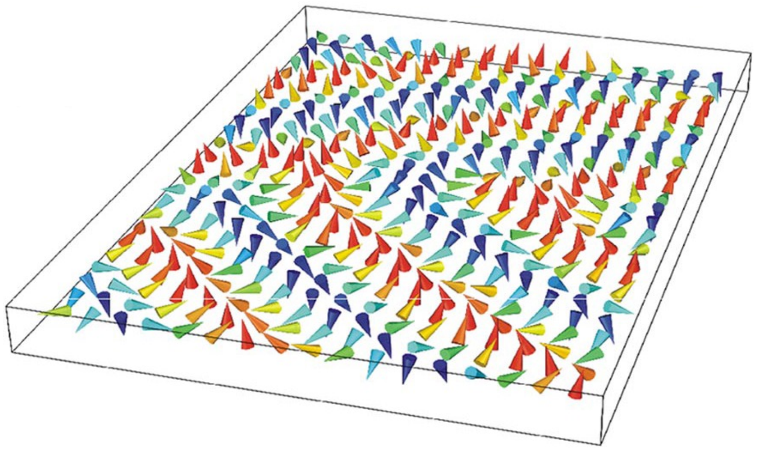
Computing DMI: Generalized Bloch theorem

Build a spin spiral in momentum space and compute the total energy up to the first order in spin-orbit coupling as a function of the spiral wave length

$$\Psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{R}_n} \begin{pmatrix} e^{-i\frac{\vec{q}\cdot\vec{r}}{2}} u_{\downarrow}(\vec{r}) \\ e^{-i\frac{\vec{q}\cdot\vec{r}}{2}} u_{\downarrow}(\vec{r}) \end{pmatrix}$$

Only valid in the absence of spin-orbit coupling
see Heide Physica B 404, 2678 (2009)





Ferriani, PRL 101, 027201 (2008)

Advantages:

Full range of wave length is available
The q=0 slode provides DMI
Beyond nearest-neighbor approximation

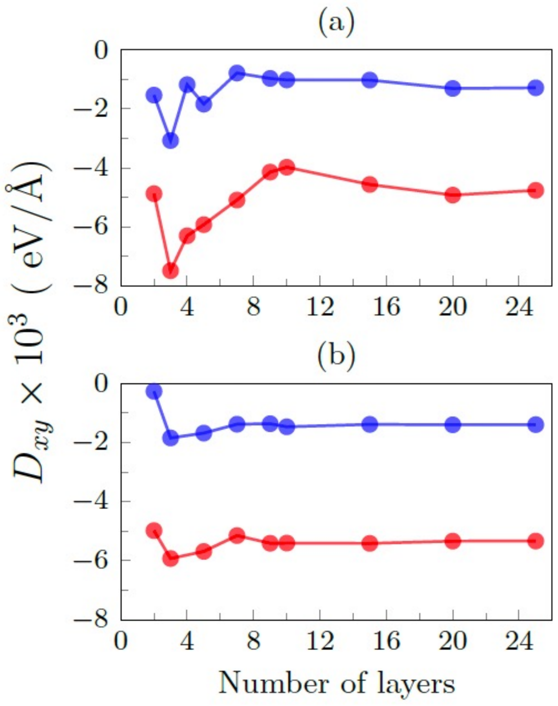
Limitations:

Limited to first order perturbation in spin-orbit coupling (intermediate Z)
Pretty heavy calculation

Computing DMI: Linear response theory

Compute the total energy to the first order in magnetization gradient

$$D_{ij} = \hbar \mathrm{Re} \int \frac{d\varepsilon}{2\pi} (\varepsilon - \mu) f(\varepsilon) \times \mathrm{Tr}\left[\mathcal{T}_i \left(\partial_\varepsilon \hat{G}_0^R \hat{v}_j \hat{G}_0^R - \hat{G}_0^R \hat{v}_j \partial_\varepsilon \hat{G}_0^R\right)\right]$$



		D_{yx} (meV Å/u.c.)
Co/Pt(111)	$\hat{\mathbf{n}} = \hat{\mathbf{e}}_z$	11.3
O/Co/Pt(111)	$\hat{\mathbf{n}} = \hat{\mathbf{e}}_z$	15.0
Al/Co/Pt(111)	$\hat{\mathbf{n}} = \hat{\mathbf{e}}_z$	20.7
	$\hat{\mathbf{n}} = \hat{\mathbf{e}}_x$	6.8

Advantages:

Green's function formula, well suited to multiband systems
Valid for any spin-orbit coupling strength
Doesn't require a dedicated DFT code
Beyond nearest-neighbor interaction

Limitations:

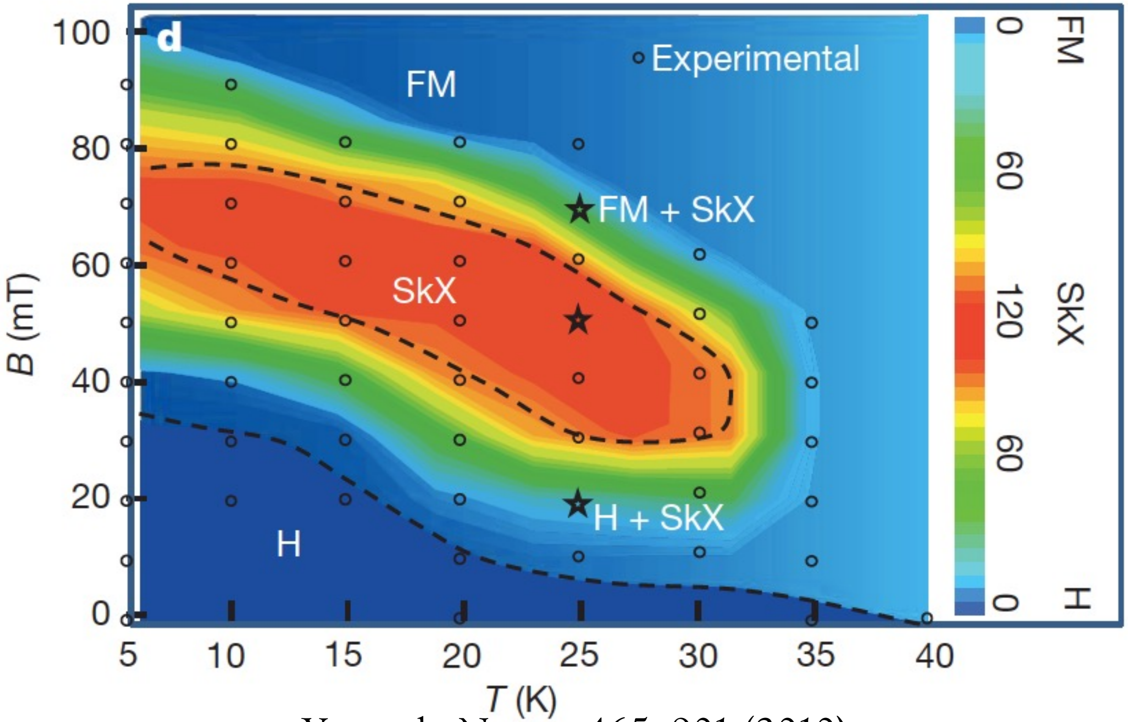
First order gradient only, beyond that it becomes very cumbersome

Freimuth et al. J. Phys. Cond. Matter 26, 104202 (2014)
Hajr Physical Review B 102, 224427 (2020)

Magnetic skyrmions in perpendicular magnets

Spin spirals and skyrmion crystal in $Fe_{0.5}Co_{0.5}Si$

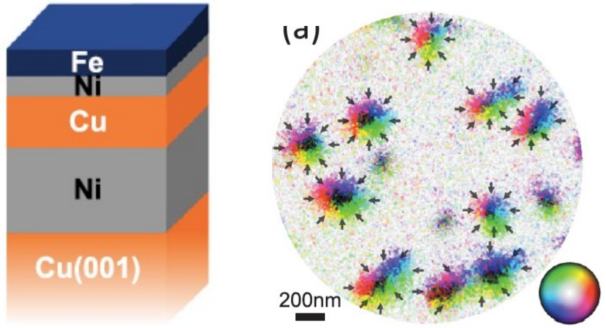
$$W_{DMI} = D\boldsymbol{m} \cdot (\boldsymbol{\nabla} \times \boldsymbol{m})$$



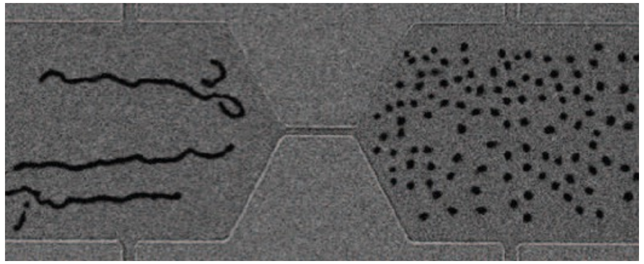
Yu et al., Nature 465, 901 (2010)
Mühlbauer et al., Science 323, 915 (2009)
Heinze et al., Nature Physics 7, 713 (2011)

Metastable skyrmions in multilayers

$$W_{DMI} = D\boldsymbol{m} \cdot [(\boldsymbol{z} \times \boldsymbol{\nabla}) \times \boldsymbol{m}]$$



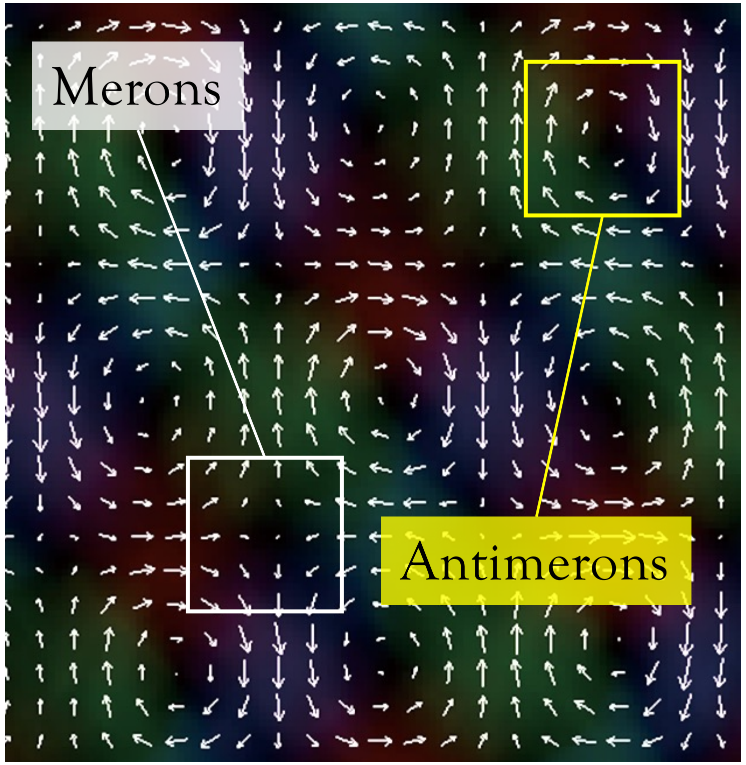
Chen et al., Applied Physics Letters 106, 242404 (2015)



Jiang et al., Science 349, 283 (2015)
Moreau-Luchaire et al., Nature Nano. 11, 444 (2016)
Boulle et al., Nature Nano. 11, 449 (2016)
Woo et al., Nature Materials 15, 501 (2016)
Pollard Nat. Comm. 8, 14761 (2017)

Magnetic merons and bimerons in easy-plane magnets

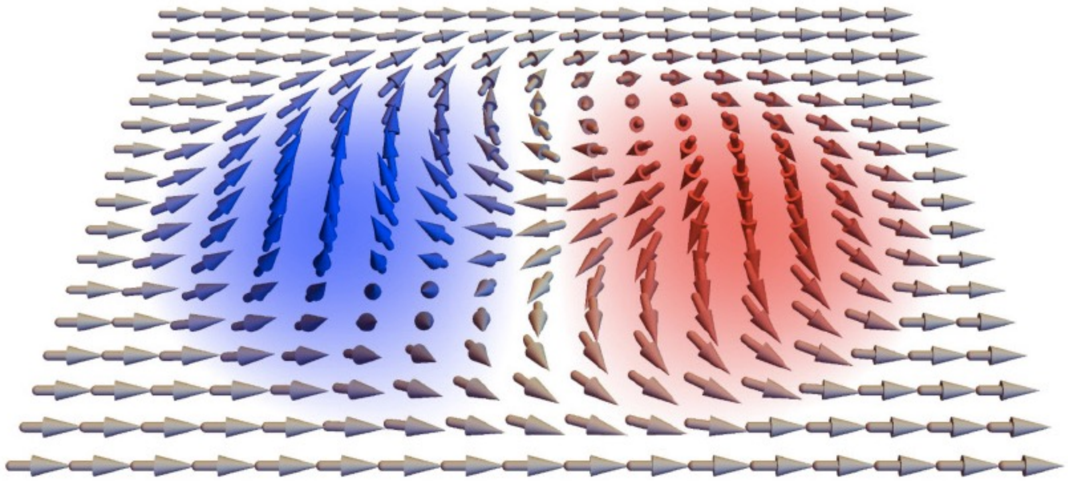
Meron lattices in $Co_8Zn_9Mn_3$



Yu et al., Nature 564, 95 (2018)

Bimerons in frustrated planar magnets

$$W_M = D(m_z\partial_x m_x - m_x\partial_x m_z + m_x\partial_y m_y - m_y\partial_y m_x)$$



Gobel et al., Physical Review B 99, 060407(R) (2019)

A major inconvenience of microscopic theory is that it does not provide a general form of the observable as a function of the system's variable (electric field, magnetization, gradients etc.)

The plan

Express the physical observable in terms of combinations of **E**, **m** that are allowed by the crystal structure

1. Choose a point group (extension to magnetic and spin group not covered)

2. Analyze the character table and determine its invariant functions

O	E	$8C_3$	$6C'_2$	$6C_4$	$3C_2 = (C_4)^2$	linear functions, rotations	quadratic functions	cubic functions
A_1	+1	+1	+1	+1	+1	-	$x^2+y^2+z^2$	-
A_2	+1	+1	-1	-1	+1	-	-	xyz
E	+2	-1	0	0	+2	-	$(x^2-y^2, 2z^2-x^2-y^2)$	-
T_1	+3	0	-1	+1	-1	(x, y, z) (R_x, R_y, R_z)	-	(x^3, y^3, z^3) $[x(z^2+y^2), y(z^2+x^2), z(x^2+y^2)]$
T_2	+3	0	+1	-1	-1	-	(xy, xz, yz)	$[x(z^2-y^2), y(z^2-x^2), z(x^2-y^2)]$

3. Determine the observable to the desired order in "small" variables

Outline

Lecture 1: A primer on spin-orbitronics

Spin-orbit coupling in crystals, Dzyaloshinskii-Moriya interaction, spin-orbit torques

Lecture 2: Representation Theory applied to crystals

Group of symmetries, reducible and irreducible representations, orthogonality theorem, characters

Lecture 3: Character tables of crystal point groups

Salient features of the character table, invariant functions, decomposition theorem, product group

Lecture 4: Application to the C_{3v} point group

Hamiltonian, conductivity tensor, DMI and SOT

Lecture 5: Your turn, with the C_{4v} point group

Surprise me ☺