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DRIVING
THE EXASCALE
TRANSITION

Spin-Orbit Coupling Effects

and their modeling with the FLEUR code

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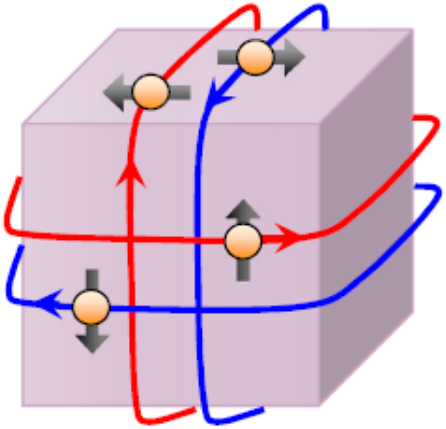
Overview

- basics
  - the Dirac equation
  - Pauli equation and spin-orbit coupling
- relativistic effects in non-magnetic solids
  - bulk: Rashba and Dresselhaus effect
  - topological insulators
- magnetic systems
  - Dzyaloshinskii-Moriya interaction
  - magnetic anisotropy



images: Wikipedia/OeNB

Schrödinger type DFT Hamiltonian

classical Hamiltonian

$$E = \frac{1}{2m} p^2 + V(\vec{r})$$

$$E \rightarrow i\hbar \frac{\partial}{\partial t} \qquad \vec{p} \rightarrow -i\hbar \vec{\nabla}$$

$$i\hbar \frac{\partial}{\partial t} \Psi(\vec{r},t) = \left[-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}) \right] \Psi(\vec{r},t)$$

quantum mechanical Hamiltionian
and interpretation of wavefunction

spin enters (ad-hoc) as quantum number

image: OeNB

continuity equation

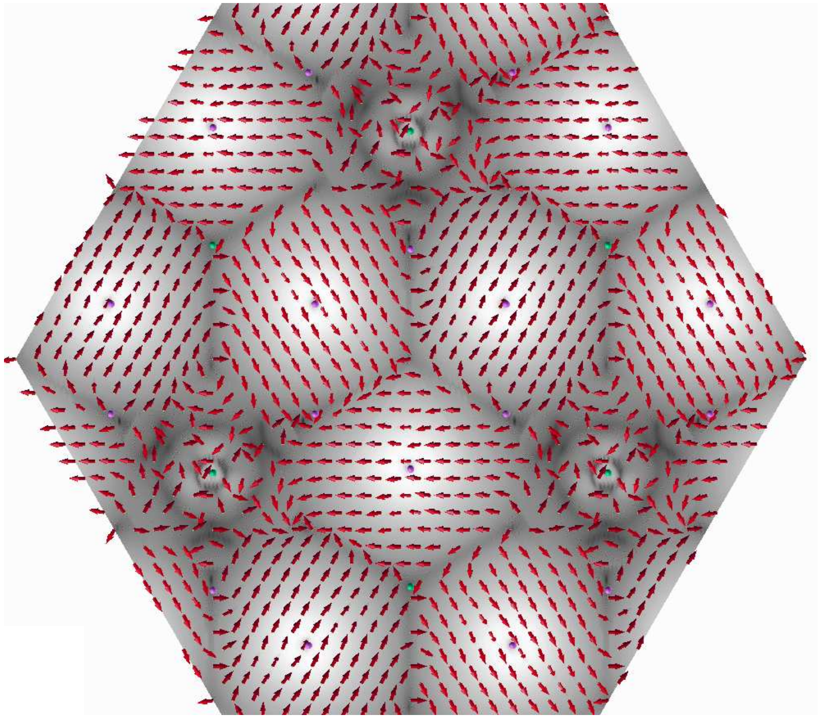
$$\frac{\partial}{\partial t} \rho(\vec{r},t) + \vec{\nabla} \cdot \vec{j}(\vec{r},t) = 0$$

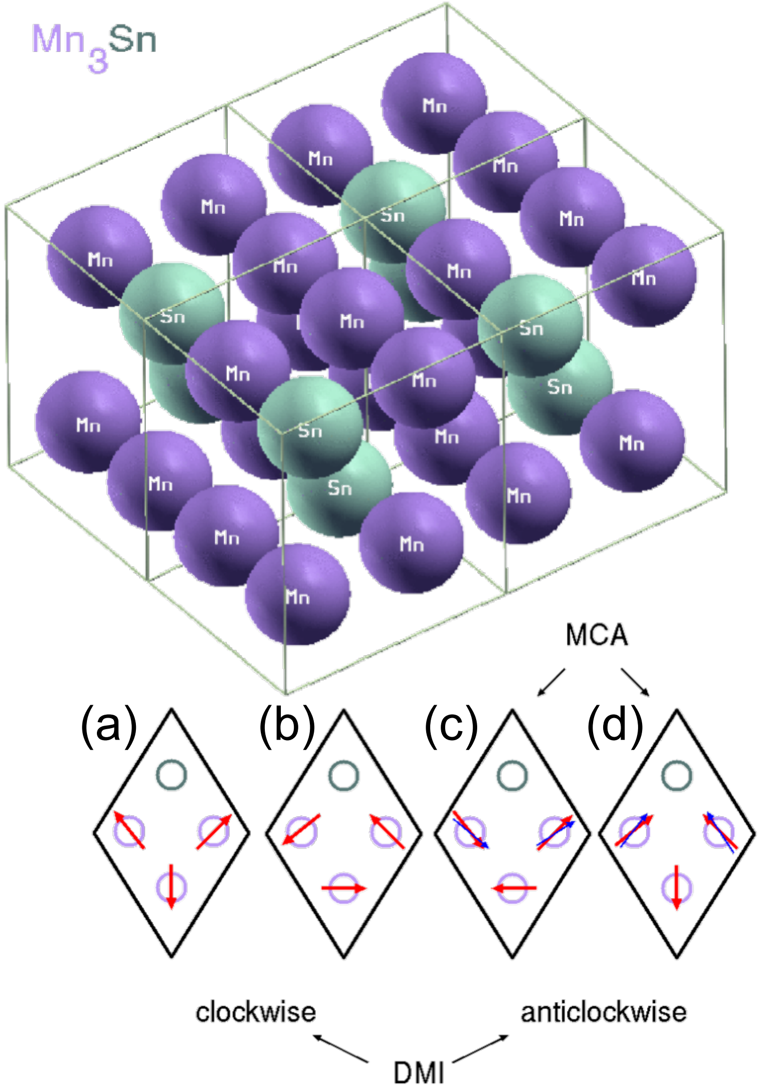
$$\rho(\vec{r},t) = \Psi^*(\vec{r},t)\, \Psi(\vec{r},t)$$

$$\vec{j}(\vec{r},t) = \frac{\hbar}{2im} \left[\Psi^* \vec{\nabla} \Psi - \Psi \vec{\nabla} \Psi^* \right]$$

Non-collinear DFT calculation

120^o Néel state obtained from Schrödinger-type Hamiltonian:





These configurations are indistighuishable without SOC!

Relativistic extension by P.A.M.Dirac

classical Hamiltonian

$$E^2 = m^2c^4 + p^2c^2$$

$$E \rightarrow i\hbar\frac{\partial}{\partial t} \qquad \vec{p} \rightarrow -i\hbar\vec{\nabla}$$

Dirac's Ansatz:

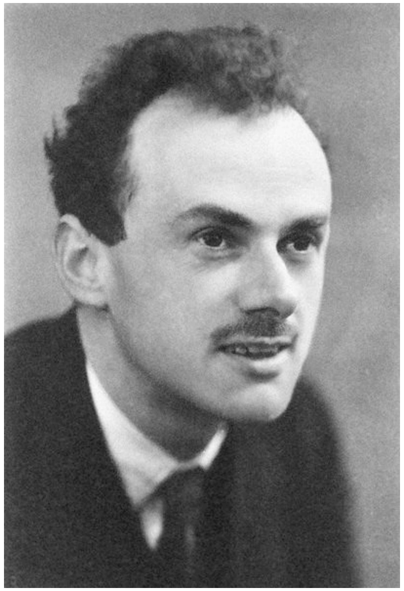


image: Wikipedia

$$i\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t) = \left(\beta mc^2 - \hbar c\vec{\alpha}\cdot\vec{\nabla}\right)\Psi(\vec{r},t)$$

$$E^2 = \left(\beta mc^2 + c\vec{\alpha}\cdot\vec{p}\right)^2 = \beta^2m^2c^4 + c^2\left(\vec{\alpha}\cdot\vec{p}\right)^2 + mc^3\left(\beta\vec{\alpha}\cdot\vec{p} + \vec{\alpha}\cdot\vec{p}\beta\right)$$

$$\beta^2 = 1 \qquad \{\alpha_i,\alpha_j\} = 2\delta_{ij} \qquad \{\beta,\alpha_i\} = 0$$

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2D- and 3D- Dirac equation

2D solution with Pauli spin matrices:

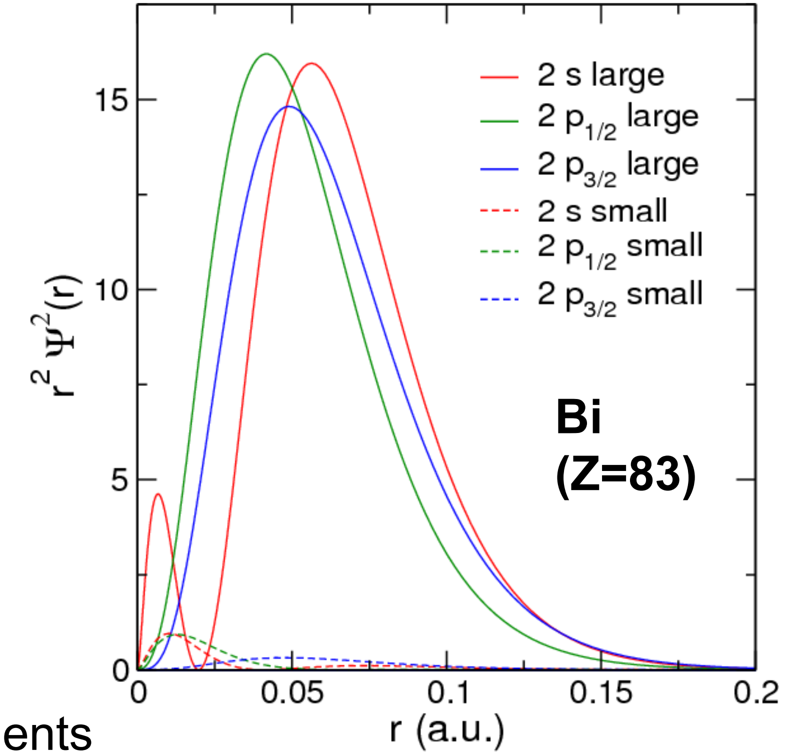
$$\alpha_1 = \sigma_x \quad \alpha_2 = \sigma_y \quad \beta = \sigma_z \qquad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\hat{H} = c\vec{\sigma} \cdot \vec{p} + mc^2\sigma_z$$

3D solution with 4x4 mat.: $\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}$

$$\hat{H} = \beta mc^2 - \hbar c\vec{\alpha} \cdot \vec{p} \qquad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

bi-spinor wavefunction: $\Psi = \begin{pmatrix} \psi \\ \chi \end{pmatrix}$



In the FLEUR code we consider both components in the construction of the density.

3D- Dirac equation

Dirac equation with scalar (V) and vector potential (A):

$$\hat{H}\Psi = i\hbar\frac{\partial}{\partial t}\Psi = E'\Psi; \quad \hat{H} = -eV(\vec{r}) + \beta mc^2 + \vec{\alpha}\cdot\left(c\vec{p} + e\vec{A}(\vec{r})\right)$$

bi-spinor wavefunction: $\Psi = \begin{pmatrix}\psi \\ \chi\end{pmatrix}$

$$\left(E' - mc^2 + eV(\vec{r})\right)\psi = \vec{\sigma}\cdot\left(c\vec{p} + e\vec{A}(\vec{r})\right)\chi$$

$$\left(E' + mc^2 + eV(\vec{r})\right)\chi = \vec{\sigma}\cdot\left(c\vec{p} + e\vec{A}(\vec{r})\right)\psi$$

non-relativistic limit:

$$E' + mc^2 \approx 2mc^2 >> eV(\vec{r}) \qquad E = E' - mc^2$$

$$\left(E + eV(\vec{r}) - \frac{1}{2m}\cdot\left(\vec{p} + \frac{e}{c}\vec{A}(\vec{r})\right)^2\right)\psi = 0$$

Schrödinger and Pauli equation

Usually, we ignore the vector potential in the Schrödinger equation:

$$\left(E + eV(\vec{r}) - \frac{1}{2m} \cdot \left(\vec{p} + \frac{e}{c} \cancel{\vec{A}(\vec{r})} \right)^2 \right) \psi = 0 \qquad \text{but:} \qquad \psi = \begin{pmatrix} \psi^{\uparrow} \\ \psi^{\downarrow} \end{pmatrix}$$

approximation to Dirac equation keeping terms up to 1/c^2:

mass-velocity term

$$\Bigg(E + eV(\vec{r}) - \frac{1}{2m} \cdot \left(\vec{p} + \frac{e}{c} \vec{A}(\vec{r}) \right)^2 + \frac{1}{2mc^2} \left(E + eV(\vec{r}) \right)^2 +$$

$$i \frac{e\hbar}{(2mc)^2} \vec{E}(\vec{r}) \cdot \vec{p} - \frac{e\hbar}{(2mc)^2} \vec{\sigma} \cdot \left(\vec{E}(\vec{r}) \times \vec{p} \right) - \frac{e\hbar}{2mc} \vec{\sigma} \cdot \vec{B}(\vec{r}) \Bigg) \psi = 0$$

direct implementation in DFT Hamiltonian possible (approximate (E+eV)^2 term), SOC & magnetic field term couple the two spin channels

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scalar relativistic calculations:

block-diagonal equation in spin:

$$\left(E + eV(\vec{r}) - \frac{\vec{p}^{\,2}}{2m} - \frac{e\hbar}{2mc} B_z(\vec{r}) \boldsymbol{\sigma}_z + \right.$$

$$\left. \frac{1}{2mc^2} \left(E + eV(\vec{r}) \right)^2 + i \frac{e\hbar}{(2mc)^2} \vec{E}(\vec{r}) \cdot \vec{p} \right) \psi = 0$$

with spin-dependent wave-function: $\psi = \begin{pmatrix} \psi^{\uparrow} \\ \psi^{\downarrow} \end{pmatrix}$

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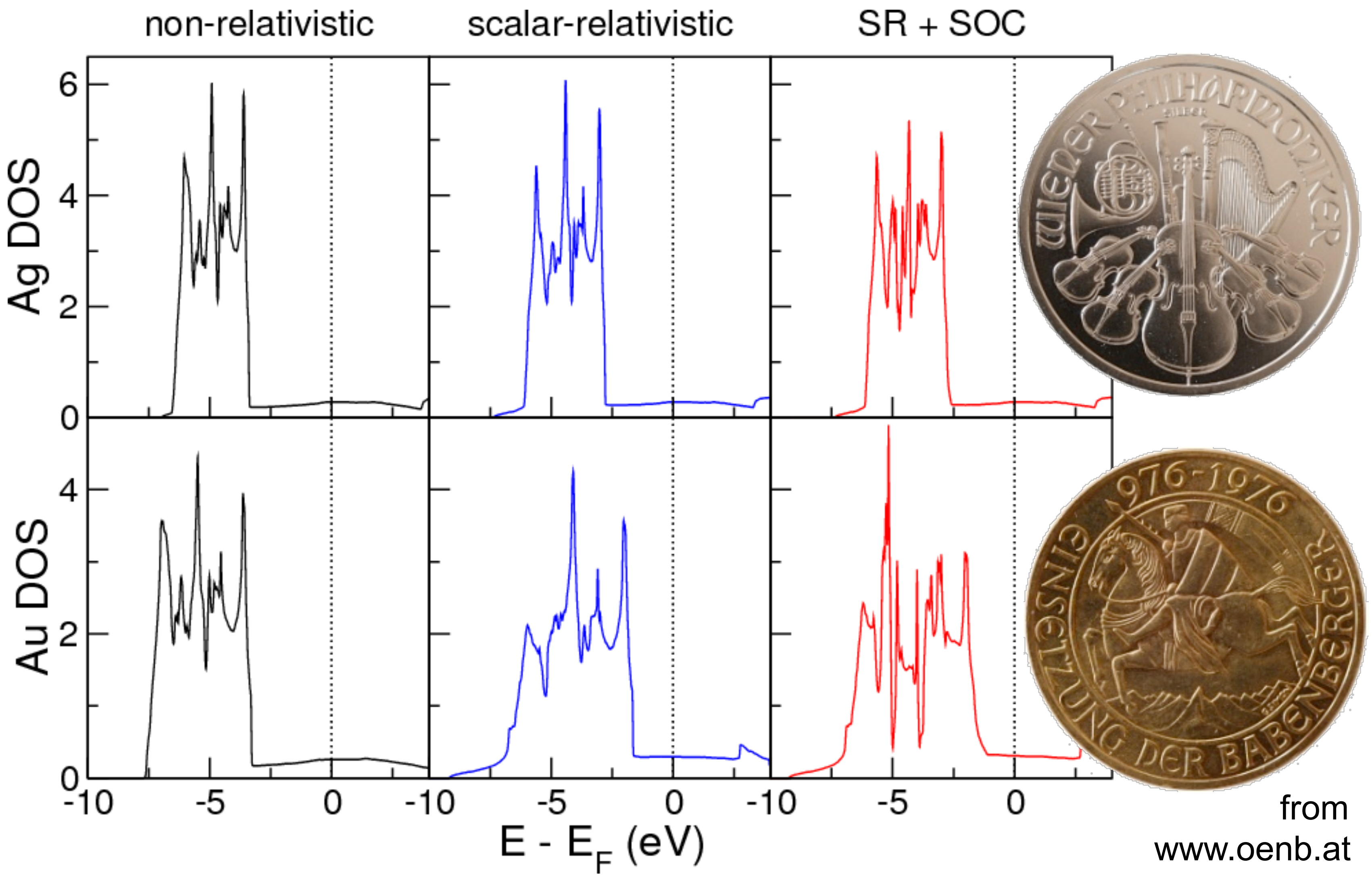
relativistic effects in Ag and Au

density of states (DOS):



from
www.oenb.at

Spin-orbit coupling

interaction with an (internal) magnetic field:

$$\frac{e\hbar}{(2mc)^2}\vec{\sigma}\cdot\left(\vec{E}(\vec{r})\times\vec{p}\right)=\frac{\mu_B}{2mc}\vec{\sigma}\cdot\left(\vec{E}(\vec{r})\times\vec{p}\right)=\frac{\mu_B}{\underset{\uparrow}{2}}\vec{\sigma}\cdot\underbrace{\left(\frac{1}{c}\vec{E}(\vec{r})\times\vec{v}\right)}_{\vec{B}_0(\vec{r})}$$

similar to: $\frac{e\hbar}{2mc}\vec{\sigma}\cdot\vec{B}(\vec{r})=\mu_B\vec{\sigma}\cdot\vec{B}(\vec{r})$ with Thomas factor

in a central potential (atom):

$$\frac{\mu_B}{2mc}\vec{\sigma}\cdot\left(\vec{E}(\vec{r})\times\vec{p}\right)=\frac{\mu_B}{2mc}\vec{\sigma}\cdot\left(\vec{\nabla}V(\vec{r})\times\vec{p}\right)=\underbrace{\frac{\mu_B}{2mcr}\frac{dV(r)}{dr}}_{\xi}\vec{\sigma}\cdot\left(\vec{r}\times\vec{p}\right)=\xi\vec{\sigma}\cdot\vec{L}$$

note that the spin and the orbital momentum (L) couple antiparallel!

Spin-orbit coupling effects in non-magnetic solids

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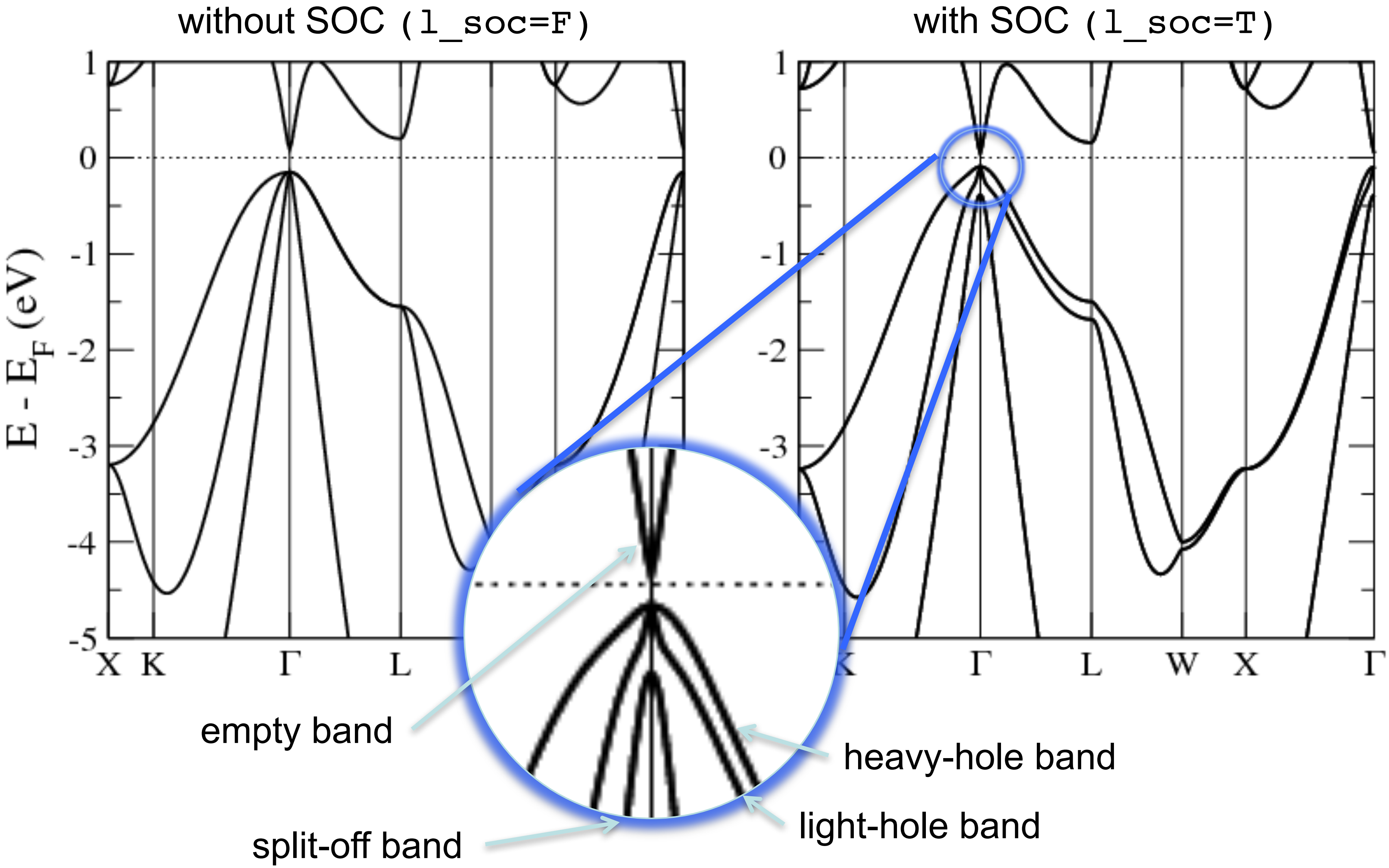
A typical semiconductor: Ge



Some symmetry considerations:

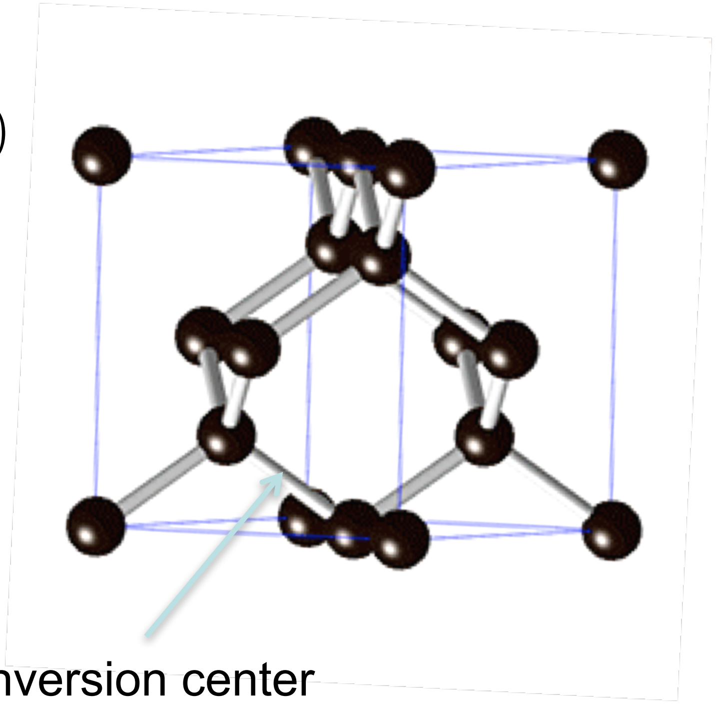
Ge, Γ-point:

- three *p*-orbitals, one split-off by SOC (atomic behavior)
- all bands are doubly (spin) degenerate (Kramers pairs)

Time reversal (TR) symmetry: $\epsilon(\vec{k},\uparrow) = \epsilon(-\vec{k},\downarrow)$

Inversion (I) symmetry: $\epsilon(\vec{k}) = \epsilon(-\vec{k})$

TR + I symmetry: $\epsilon(\vec{k},\uparrow) = \epsilon(\vec{k},\downarrow)$

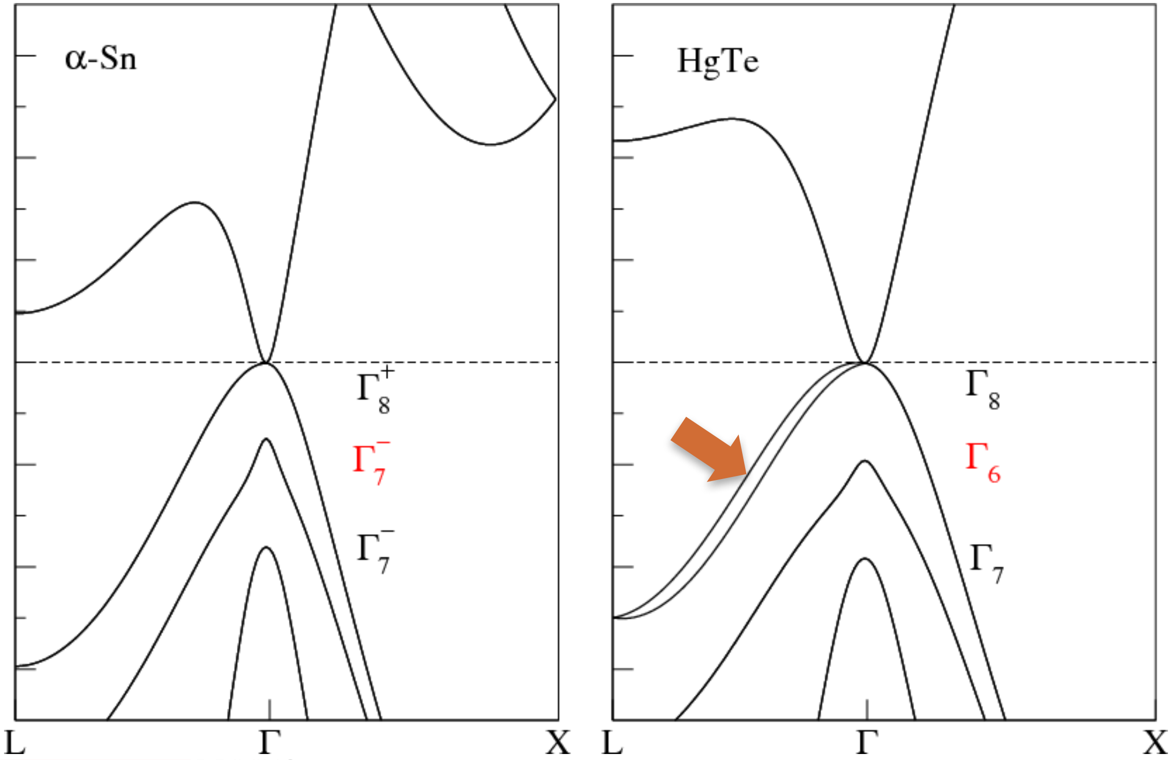


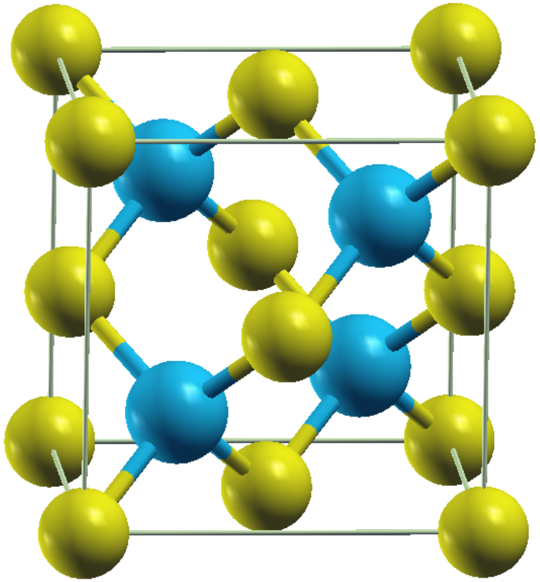
Broken I symmetry: Dresselhaus effect

in presence of SOC: $\epsilon(\vec{k},\uparrow) \neq \epsilon(\vec{k},\downarrow)$ i.e. *k*-dependent spin splitting (here: α k^3)

Dresselhaus Hamiltonian (*k•p*-theory, e.g. in (111) direction):

$$\hat{H}_D = \alpha_D\left[\sigma_x p_x\left(p_y^2 - p_z^2\right) + \sigma_y p_y\left(p_z^2 - p_x^2\right) + \sigma_z p_z\left(p_x^2 - p_y^2\right)\right]$$





zincblende structure

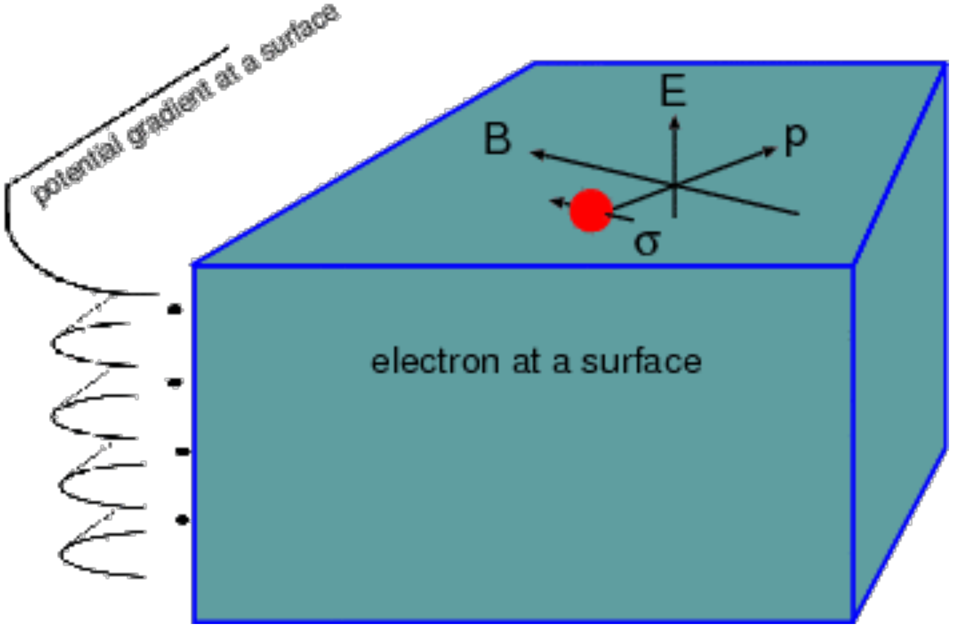
Broken I symmetry at a crystal surface

Free electron gas in electric field:

$$\left[-\frac{1}{2}\nabla^2-\frac{\mu_B}{2mc}\vec{\sigma}\cdot\left(\vec{p}\times\vec{E}(\vec{r})\right)\right]\psi_i=\varepsilon_i\psi_i$$

Suppose $\vec{E}=E\vec{e}_z$ and momentum confined in (*x*,*y*) plane:

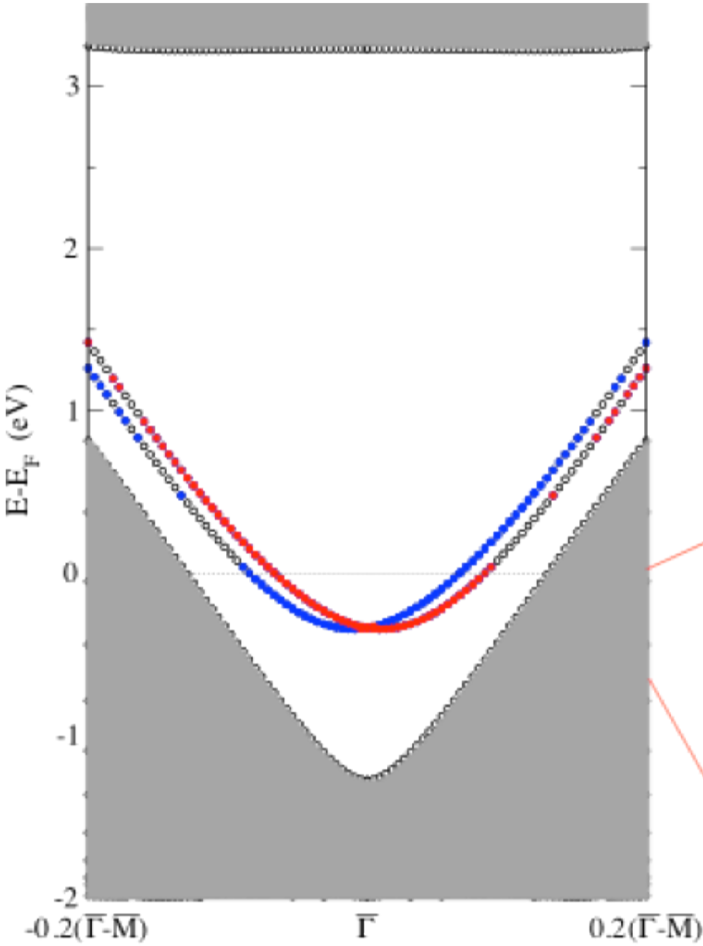
$$\left[-\frac{1}{2}\nabla^2+\alpha_R\vec{\sigma}\cdot\left(\vec{k}_{||}\times\vec{e}_z\right)\right]\psi_i=\varepsilon_i\psi_i$$



this describes electrons at a surface or an interface (e.g. doped layer between two semiconductors)

Example: coinage metal surfaces

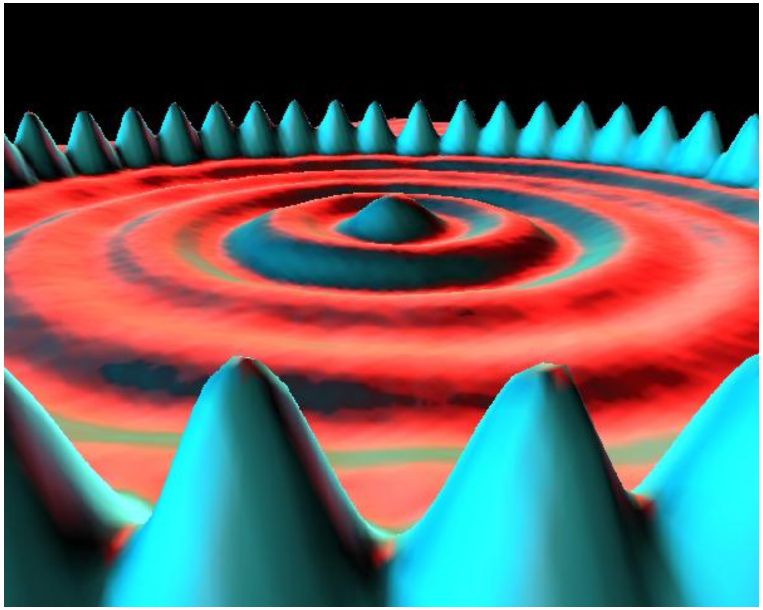
(111) surface states



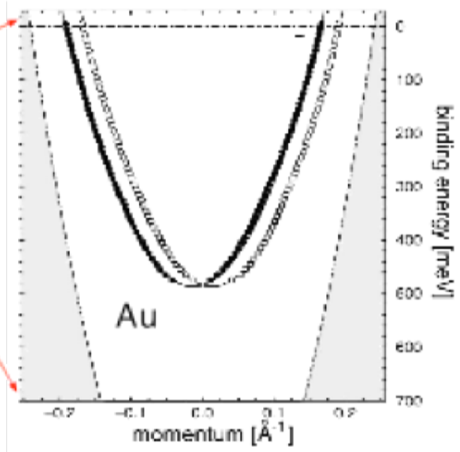
Z(Cu) = 29

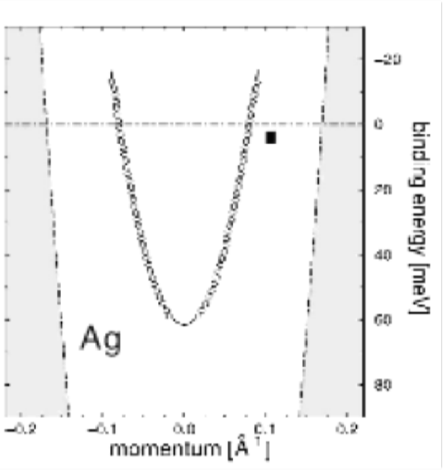
Z(Ag) = 47

Z(Au) = 79



from www.almaden.ibm.cpm





DFT calculations and SP-ARPES agree very well [experiment: Reinert et al., PRB **63**, 115415 (2001)]

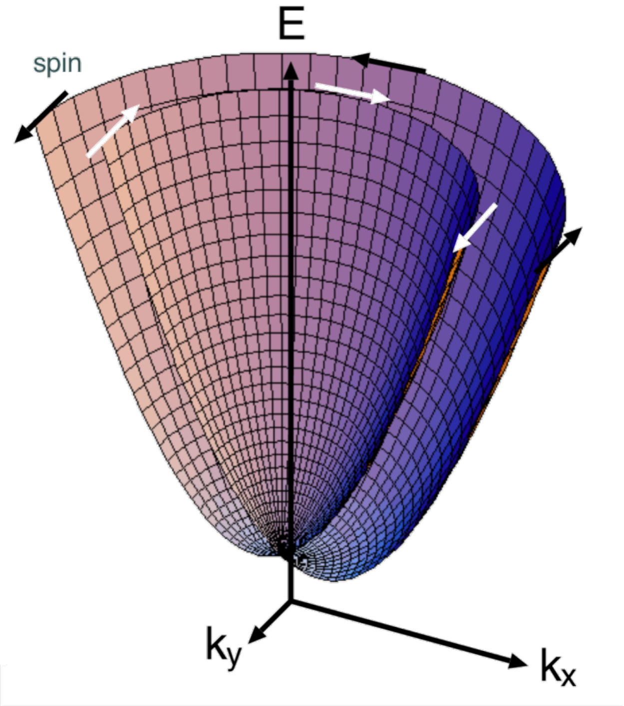
Spin orientation in the Rashba effect

Spin orientation of: $\psi_{\pm\vec{k}_\parallel} = \frac{e^{i\vec{k}_\parallel \cdot \vec{r}_\parallel}}{2\pi} \frac{1}{\sqrt{2}} \begin{pmatrix} i e^{-i\varphi/2} \\ \pm e^{i\varphi/2} \end{pmatrix}$

$$\vec{n}_\pm(\vec{k}_\parallel) = \left\langle \psi_{\pm\vec{k}_\parallel} \middle| \vec{\sigma} \middle| \psi_{\pm\vec{k}_\parallel} \right\rangle = \begin{pmatrix} \sin\varphi \\ -\cos\varphi \\ 0 \end{pmatrix}$$

with energies $\varepsilon_\pm = \frac{k_\parallel^2}{2m} \pm \alpha_R k_\parallel$

i.e. the spin is always perpendicular to the propagation direction (spin-momentum locking)!



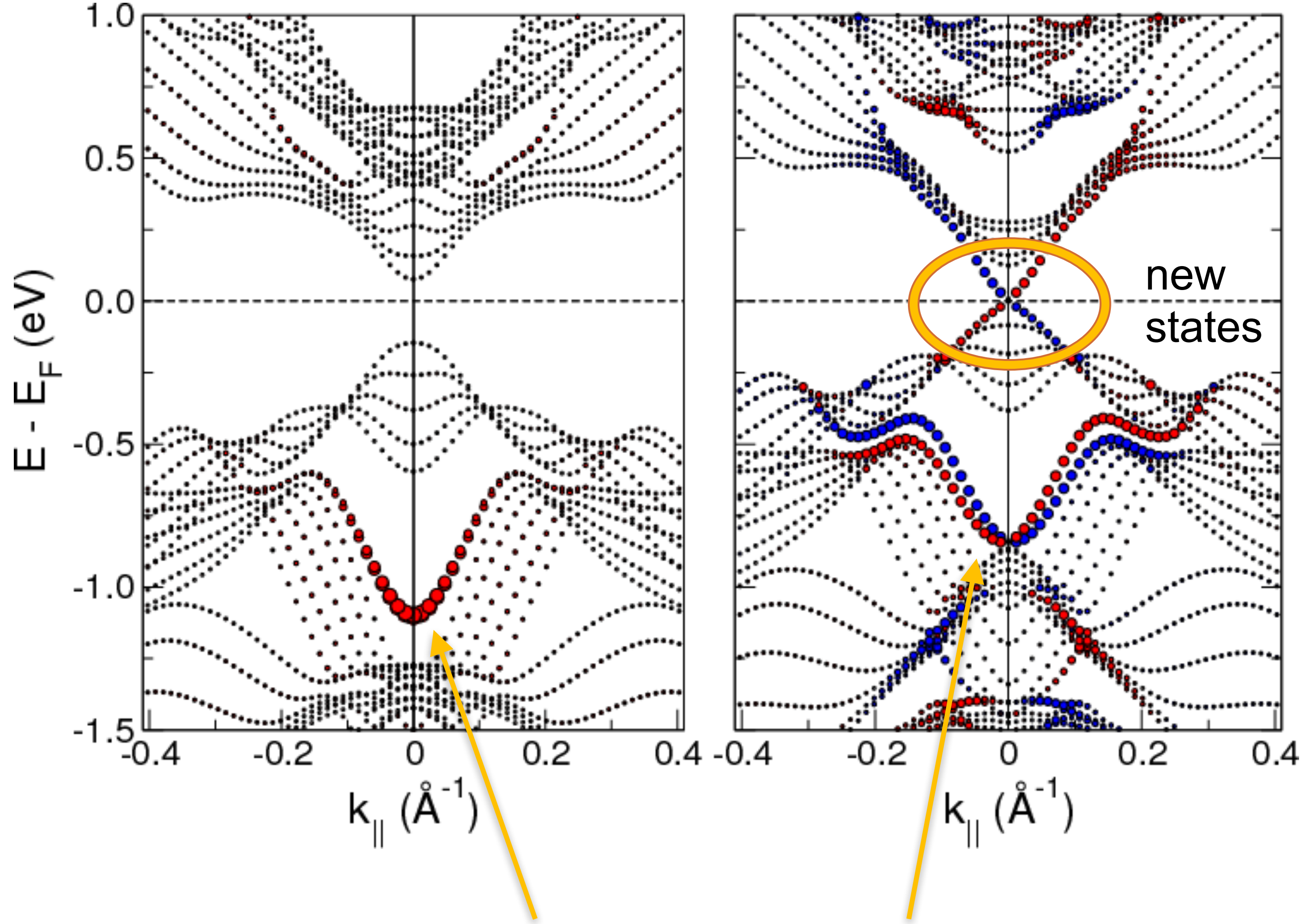
good comparison between calculated and measured α_R

spin-dependent splittings require careful k-point sampling (±k) !

Sb_2Te_3 (0001) surface

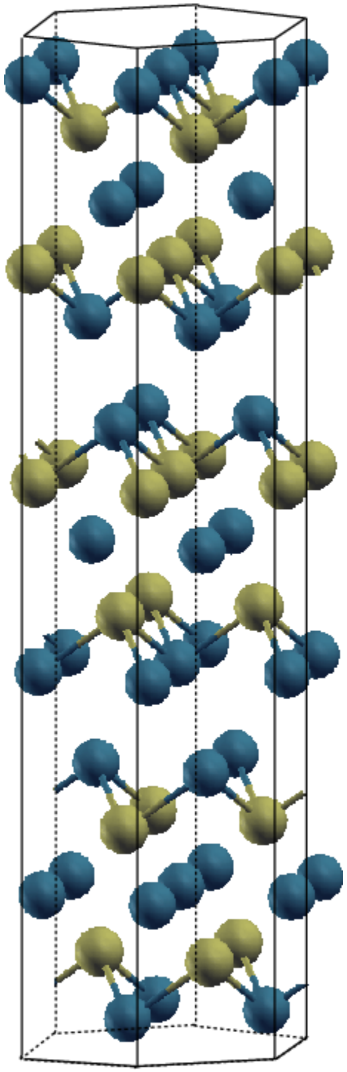
surface without SOC

and with SOC:



new states

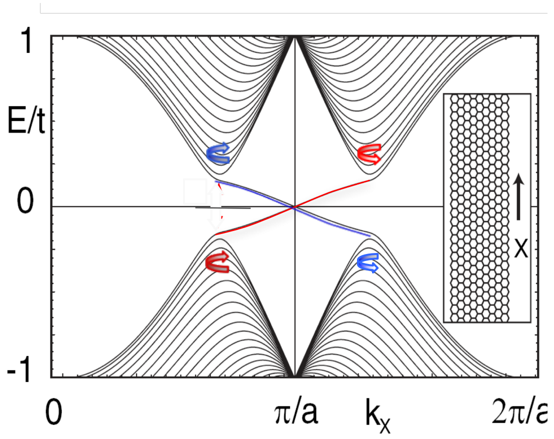
surface state with Rashba splitting



The quantum spin Hall effect (QSHE)

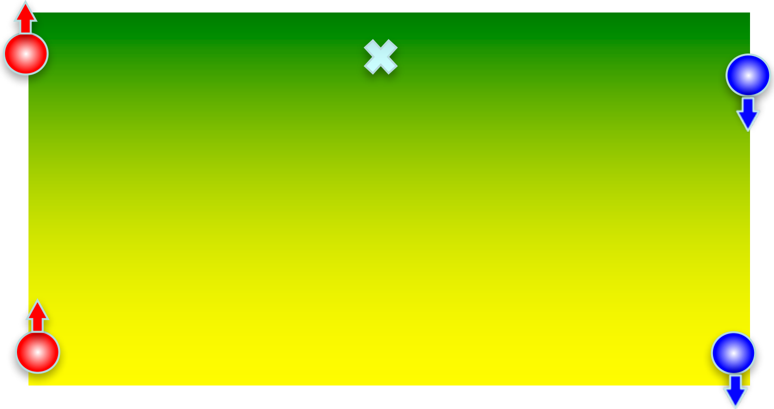
properties:

- valence- and conduction band connected by edge states
- spin-polarization of states is Rashba-like
- one conduction channel per spin in the gap
- topologically protected edge transport



topologically protected edge-state

Kane & Mele, PRL **95,** 226801 (2005)

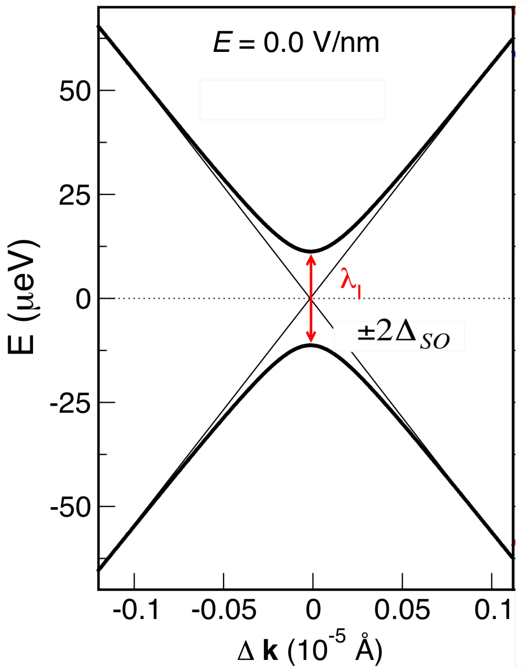


Band inversion in graphene (25μeV)

Bandstructure around K (K’): $\hat{H} = \upsilon_F\left(s_x\tau_z p_x + s_y p_y\right) + \Delta_{SO}\sigma_z\tau_z s_z$

$$\hat{H}_K = \begin{pmatrix} +\Delta_{SO} & \upsilon_F\left(p_x - ip_y\right) \\ \upsilon_F\left(p_x + ip_y\right) & -\Delta_{SO} \end{pmatrix}$$

$$\hat{H}_{K'} = \begin{pmatrix} -\Delta_{SO} & -\upsilon_F\left(p_x + ip_y\right) \\ -\upsilon_F\left(p_x - ip_y\right) & +\Delta_{SO} \end{pmatrix}$$



mass inversion between K and K’:

spin split edge state connecting K and K’

DFT calculation with SOC

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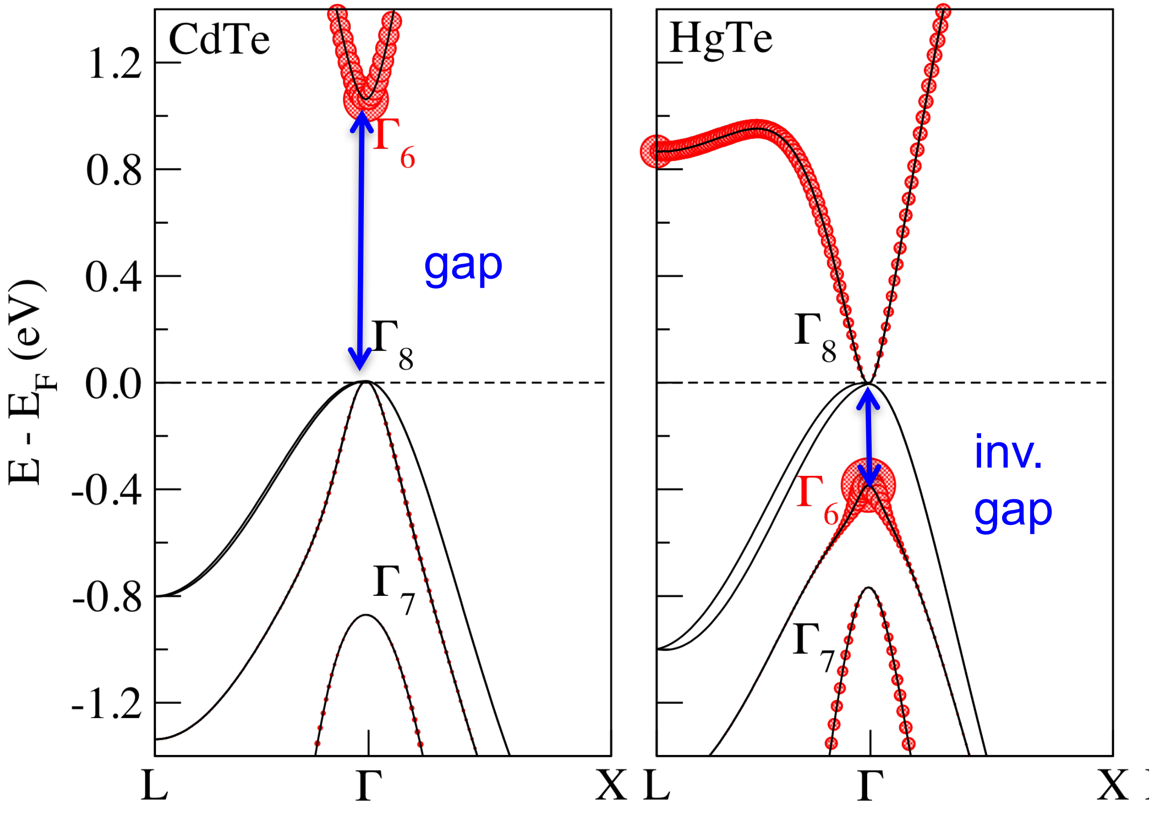
Band inversion II-VI semiconductors

focus on Γ_6 and Γ_8:



responsible for band-inversion: Darwin-term of Pauli-equation

Spin-orbit effects in magnetic systems

Magnetic interactions

Interactions between two spins: $\vec{S}_i \underline{J}_{ij} \vec{S}_j$

on-site		inter-site		
$\vec{S}_i I_{ii} \vec{S}_i$	$\vec{S}_i \underline{J}_{ii} \vec{S}_i$	$\vec{S}_i J_{ij} \vec{S}_j$	$\vec{S}_i \underline{J}^S_{ij} \vec{S}_j$	$\vec{S}_i \underline{J}^A_{ij} \vec{S}_j$
scalar	traceless sym.	scalar	traceless sym.	antisymmetric
Stoner magnet.	magnetic anisotropy	Heisenberg interaction	(pseudo)-dipolar interaction	Dzyaloshinskii Moriya int.

non-relativistic effects

$$\underline{J}^A_{ij} \propto \left(\frac{\Delta g}{g}\right) J \quad ; \quad \underline{J}^S_{ij} \propto \left(\frac{\Delta g}{g}\right)^2 J$$

[T. Moriya, Phys. Rev. **120**, 91 (1960)]

$$\underline{J}^A_{ij} = \begin{pmatrix} 0 & D_z & -D_y \\ -D_z & 0 & D_x \\ D_y & -D_x & 0 \end{pmatrix}$$

leads to $\vec{D} \cdot \left(\vec{S}_i \times \vec{S}_j\right)$

Ansiotropic exchange

ferromagnets: exchange >> Rashba splitting

here: exchange interaction ≈ spin-orbit strength, e.g. two magnetic adatoms (S_A,S_B) on a heavy substrate with conduction electron σ:

$$E \propto \left(\vec{S}_A \cdot \vec{\sigma}\right) \mathcal{G}_{A \to B} \left(\vec{S}_B \cdot \vec{\sigma}\right) \mathcal{G}_{B \to A} \quad ; \quad \mathcal{G}_{A \to B} \approx \mathcal{G}_0 + \mathcal{G}_0 H_{SOC} \mathcal{G}_0$$

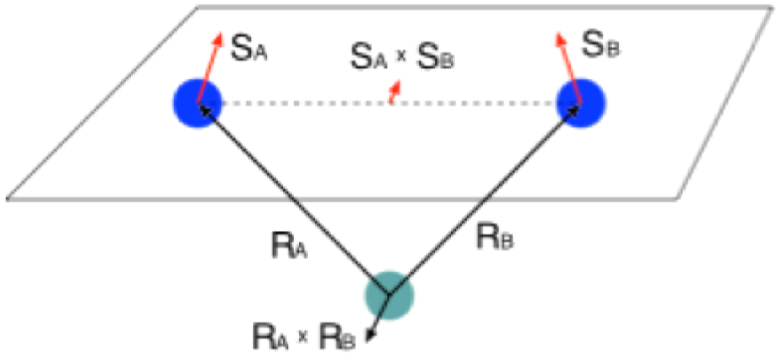
$$H_{SOC} = 0: \quad E \propto \mathrm{Tr}_\sigma \left(\vec{S}_A \cdot \vec{\sigma}\right) \mathcal{G}_0 \left(\vec{S}_B \cdot \vec{\sigma}\right) \mathcal{G}_0 = \frac{1}{2} J_{AB} \vec{S}_A \cdot \vec{S}_B$$

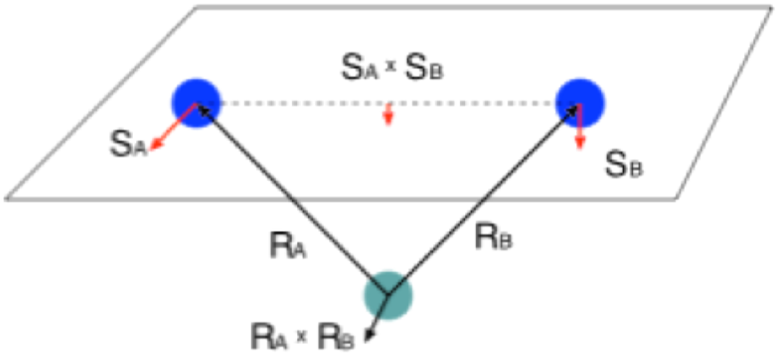
$$H_{SOC} = \vec{B}_{eff} \cdot \vec{\sigma}: \quad E_{DM} \propto \mathrm{Tr}_\sigma \left(\vec{S}_A \cdot \vec{\sigma}\right)\left(\vec{B}_{eff} \cdot \vec{\sigma}\right)\left(\vec{S}_B \cdot \vec{\sigma}\right) \propto \vec{B}_{eff} \cdot \left(\vec{S}_A \times \vec{S}_B\right)$$

D. A. Smith, J. Magn. Magn. Mater. **1,** 214 (1976)

Ansiotropic exchange:

E.g. 2 magnetic adatoms (Fe) on a heavy substrate (W)



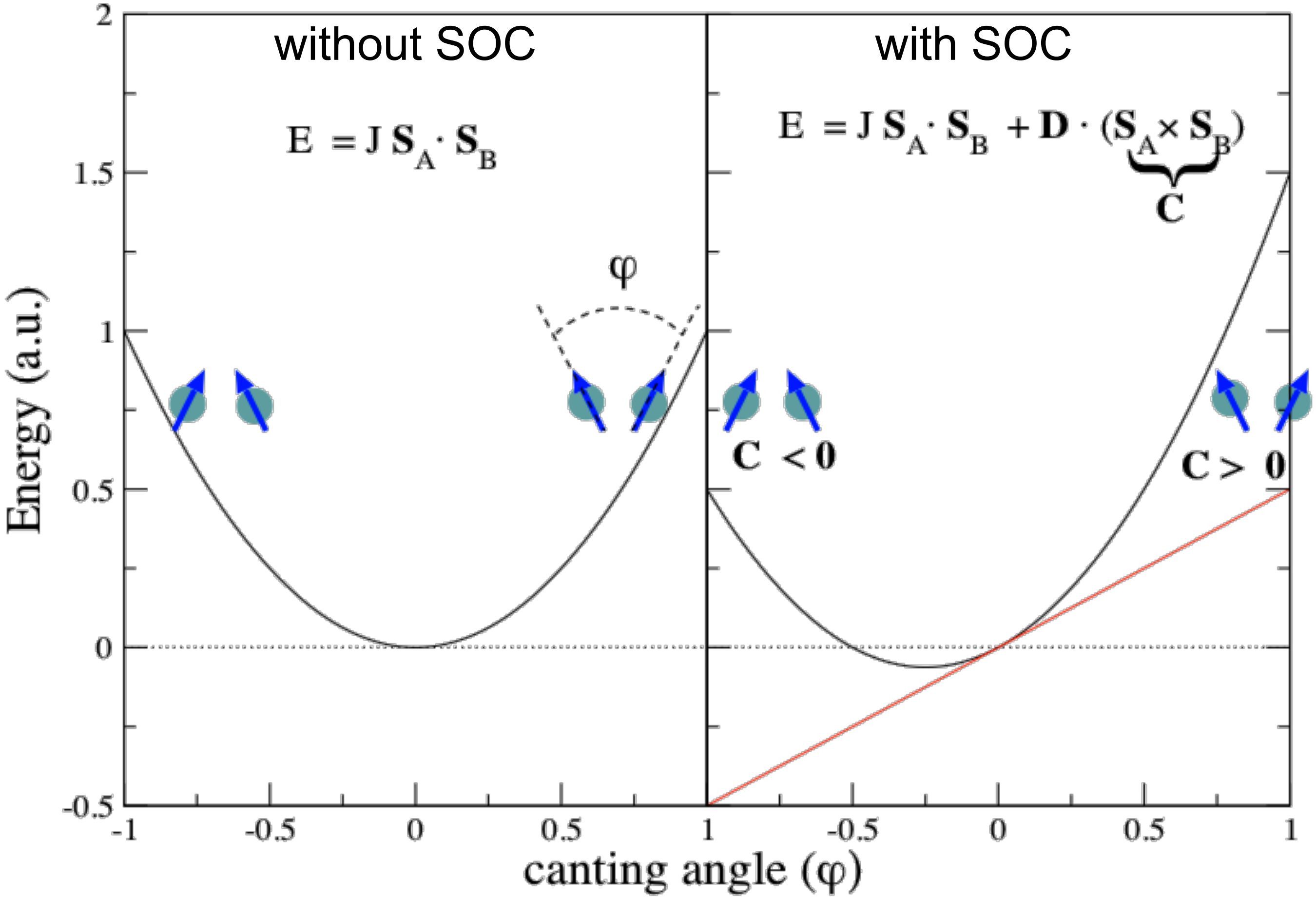


$$H_{DM} = -V(\xi)\frac{\left(\hat{\vec{R}}_A \cdot \hat{\vec{R}}_B\right)\sin\left[k_F\left(R_A + R_B + R_{AB}\right) + \eta\right]}{R_A R_B R_{AB}}\left(\hat{\vec{R}}_A \times \hat{\vec{R}}_B\right)\cdot\left(\vec{S}_A \times \vec{S}_B\right)$$

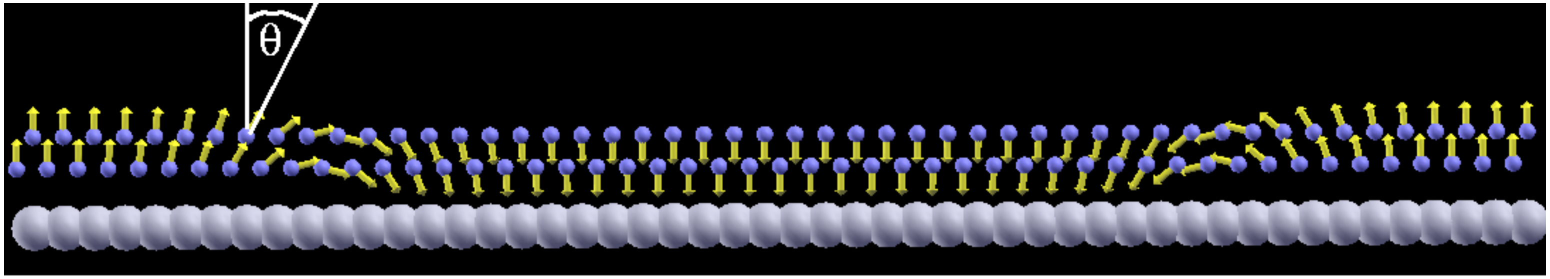
RKKY-type interaction: A. Fert and P. M. Levy, Phys. Rev. Lett. **44**, 1538 (1980).
Dzyaloshinskii-Moriya (DM) term, anisotropic exchange interaction.

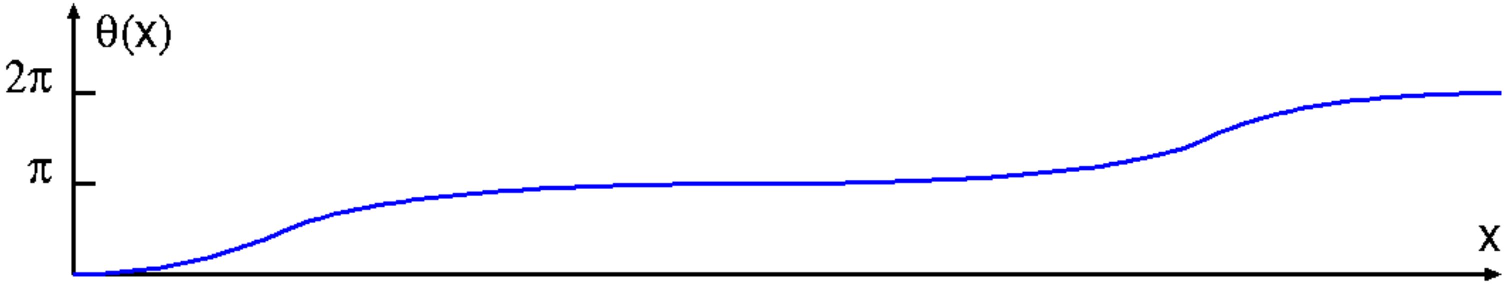
Dzyaloshinskii-Moriya interaction:

distinguish clockwise – counterclockwise rotations

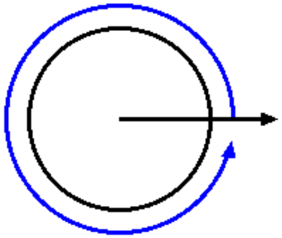


Simple 1D example: two domain walls



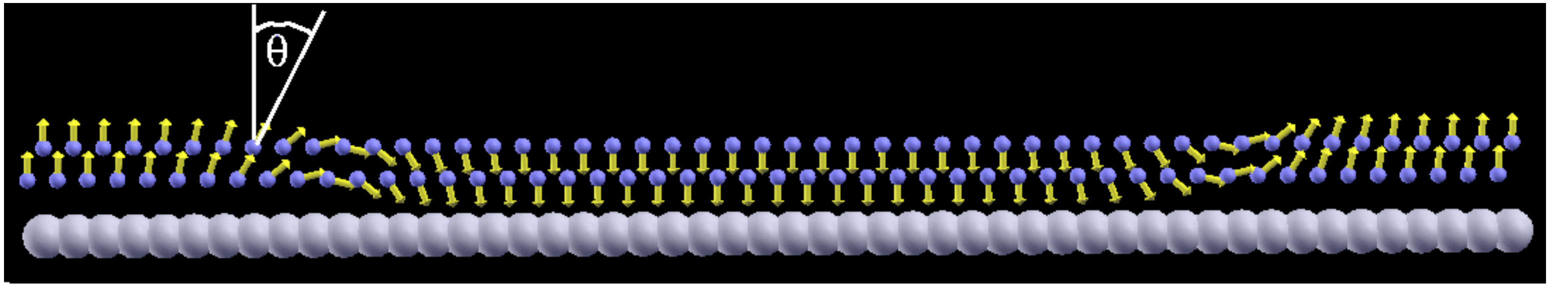


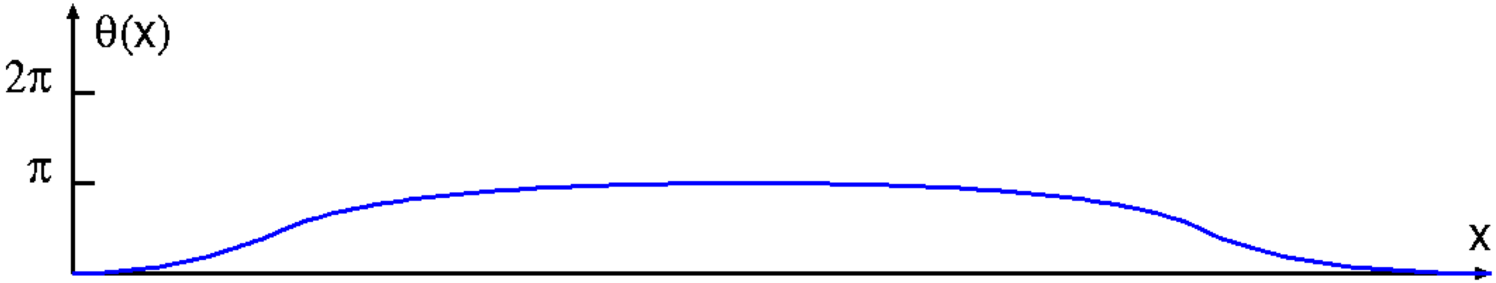
$$S = \frac{1}{2\pi}\int \frac{\partial\theta(x)}{\partial x}\,dx \; = 1$$



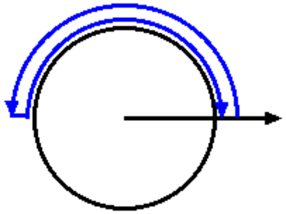
topological index, winding number

Simple 1D example: two domain walls



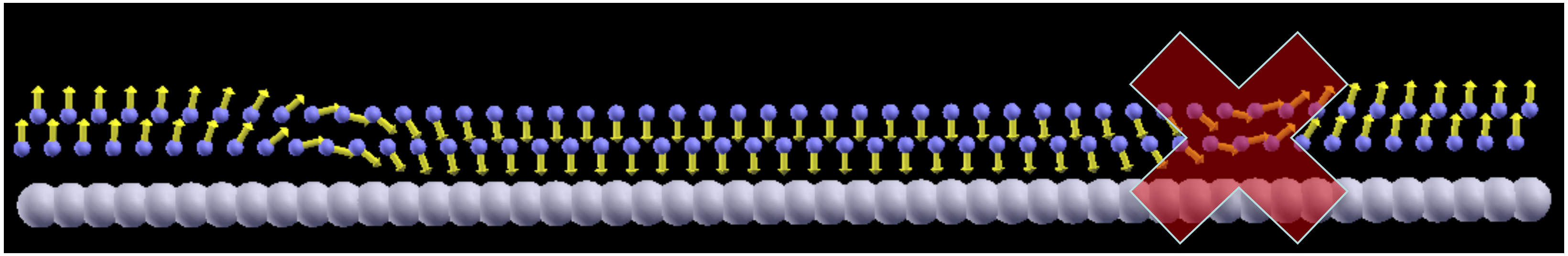


$$S = \frac{1}{2\pi}\int \frac{\partial\theta(x)}{\partial x}\,dx \;= 0$$



topologically trivial structure

Domain walls in 2 Fe / W(110)



Due to the Dzyaloshinskii-Moriya interaction this (Neél-type) domain-wall is stabilized

This domain wall does not exist!

Theory:
M. Heide, G. Bihlmayer and S. Blügel, Phys. Rev. B, 140403(R) (2008)

$$H = \underbrace{\sum_{ij} J_{ij}\vec{S}_i \cdot \vec{S}_j + \sum_{i} \vec{S}_i \underline{\underline{K}} \vec{S}_i}_{\text{Domain wall width}} + \underbrace{\sum_{ij} \vec{D}_{ij} \cdot \left(\vec{S}_i \times \vec{S}_j\right)}_{\text{rotational sense}}$$

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Exchange interactions:

2-spin terms:

$$H = \sum_{i<j} \vec{S}_i \underline{J}_{ij} \vec{S}_j$$

relativistic effects

on-site terms: i=j: trace(J)=Stoner I

symmetric, traceless part: magnetic anisotropy

intersite terms: trace(J)=Heisenberg-type exchange

symmetric, traceless part: quasi-dipolar exchange

antisymmetric part: Dzyaloshinskii-Moriya interaction

$$H = \sum_{i<j} \left[J_{ij} \vec{S}_i \cdot \vec{S}_j + \vec{D}_{ij} \cdot \left(\vec{S}_i \times \vec{S}_j \right) \right] + \sum_i \vec{S}_i^{\mathrm{T}} \mathcal{K}_i \vec{S}_i$$

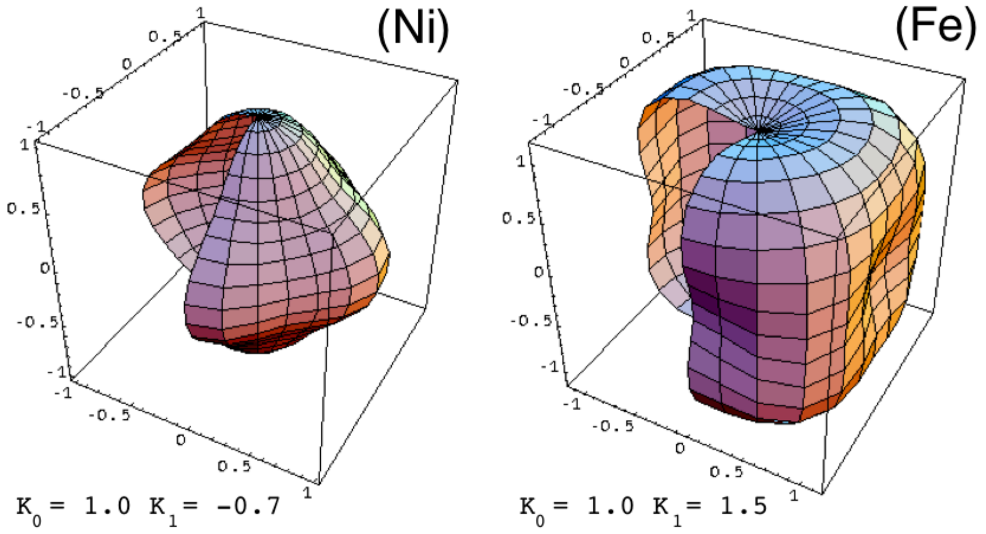
specify magnetization direction giving polar angles in the input!

```
<soc theta=“0.00” phi=“0.00” l_soc=T ....>
```

Magnetic Anisotropy:

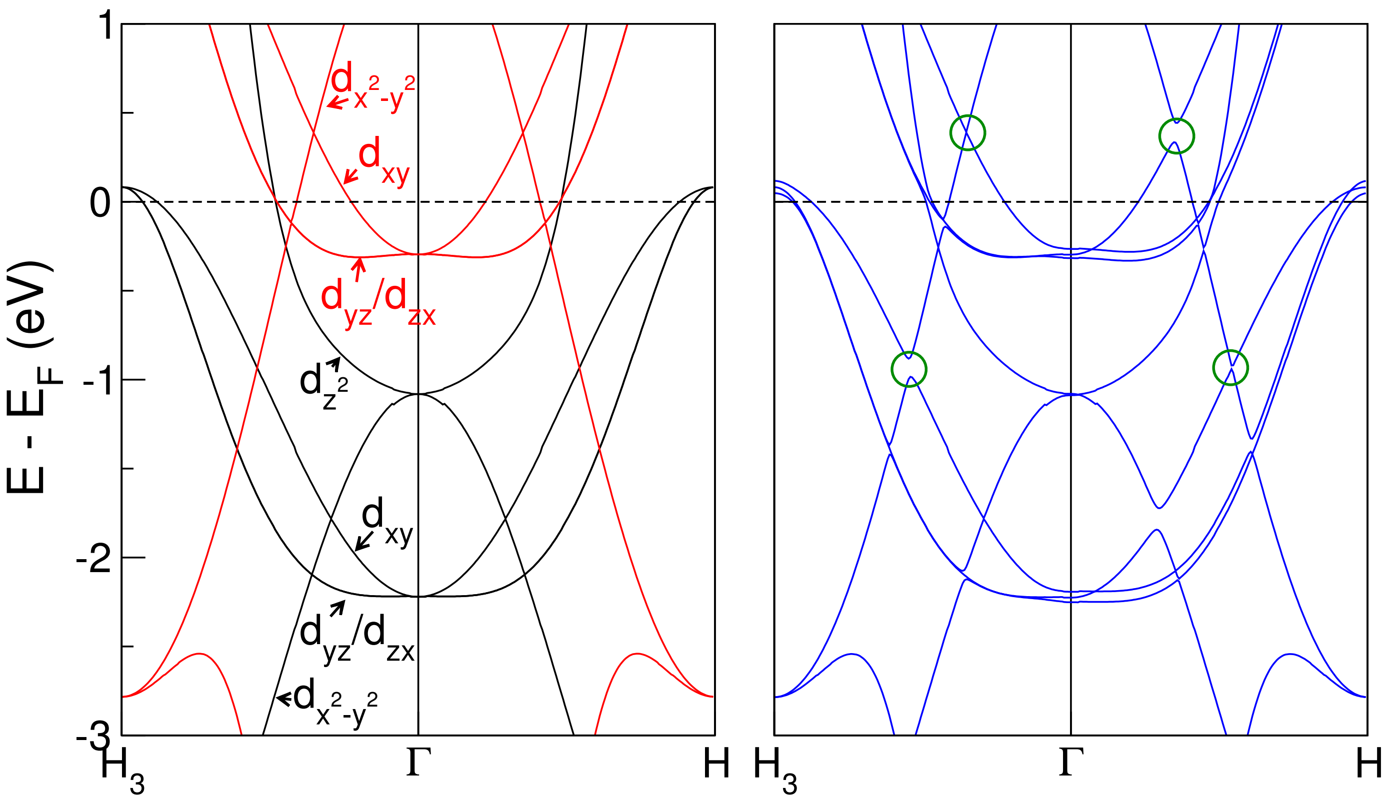
magnetization direction dependence of free energy of a cubic crystal:

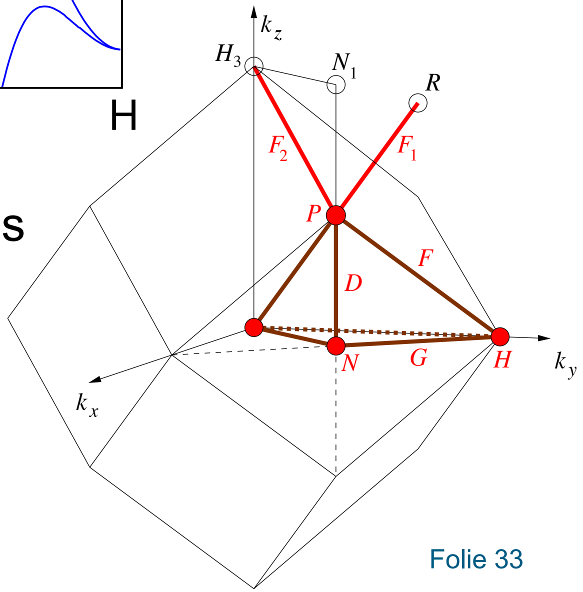
$$F(\hat{M}) = K_0 + \frac{K_1}{64}\{(3 - 4\cos 2\theta + \cos 4\theta)\,(1 - \cos 4\phi) + 8(1 - \cos 4\theta)\}$$



Uniaxial system: $F(\hat{M}) = K_0 + K_1 \sin^2\theta + K_2 sin^4\theta$

Effect of SOC on Fe band structure





Different band gaps open in formerly equivalent directions (depending on the magnetization direction)

E. Młyńczak et al., Phys. Rev. X **6**, 041048 (2016)

Magneto-crystalline anisotropy (MCA):

2nd order perturbation theory:

$$\delta E_{MCA} = \sum_{i,j} \frac{\langle \psi_i | \hat{H}_{SOC} | \psi_j \rangle \langle \psi_j | \hat{H}_{SOC} | \psi_i \rangle}{\varepsilon_i - \varepsilon_j} f(\varepsilon_i)\left[1 - f(\varepsilon_j)\right]$$

for a specific direction, $\hat{e}$, the matrix elements are:

$$\left\langle \psi_i | \hat{H}_{\mathrm{SOC}} | \psi_j \right\rangle \propto \left\langle \psi_i | \vec{L} \cdot \vec{S} | \psi_j \right\rangle \propto \left\langle \varphi_i | \vec{L} \cdot \hat{e} | \varphi_j \right\rangle$$

L•e	< zx |	< yz |	< xy |	< x^2-y^2 |	< $3z^2$-r^2 |
| zx >	0	-ie_z	ie_x	-ie_y	i√3e_y
| yz >	ie_z	0	-ie_y	-ie_x	-i√3e_x
| xy >	-ie_x	ie_y	0	2ie_z	0
| x^2-y^2 >	ie_y	ie_x	-2ie_z	0	0
| $3z^2$-r^2 >	-i√3e_y	i√3e_x	0	0	0

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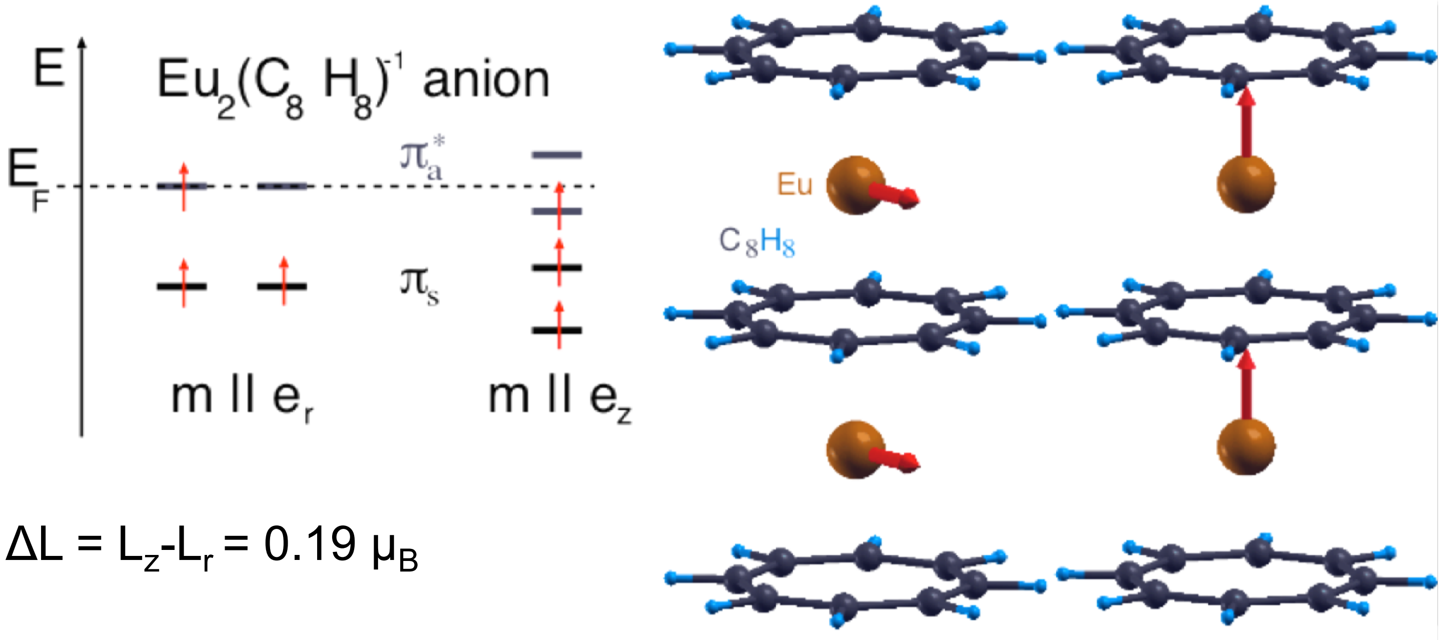
MCA of a molecular magnet:

dimer model: HOMO level determines easy axis



$\Delta L = L_z - L_r = 0.19\ \mu_B$

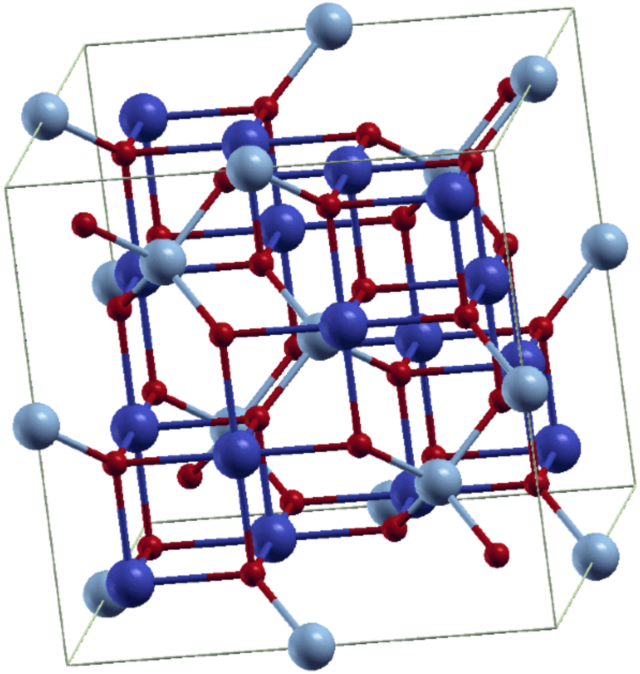
$\Delta E = E_z - E_r = -13.7$ meV

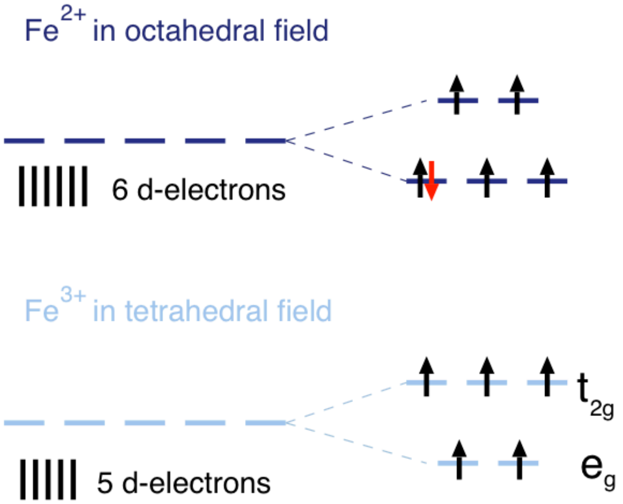
N. Atodiresei et al., Phys. Rev. Lett. **100**, 117207 (2008)

A solid example: Magnetite

Early compass:

images: Wikipedia





Fe^{2+} in octahedral field

6 d-electrons

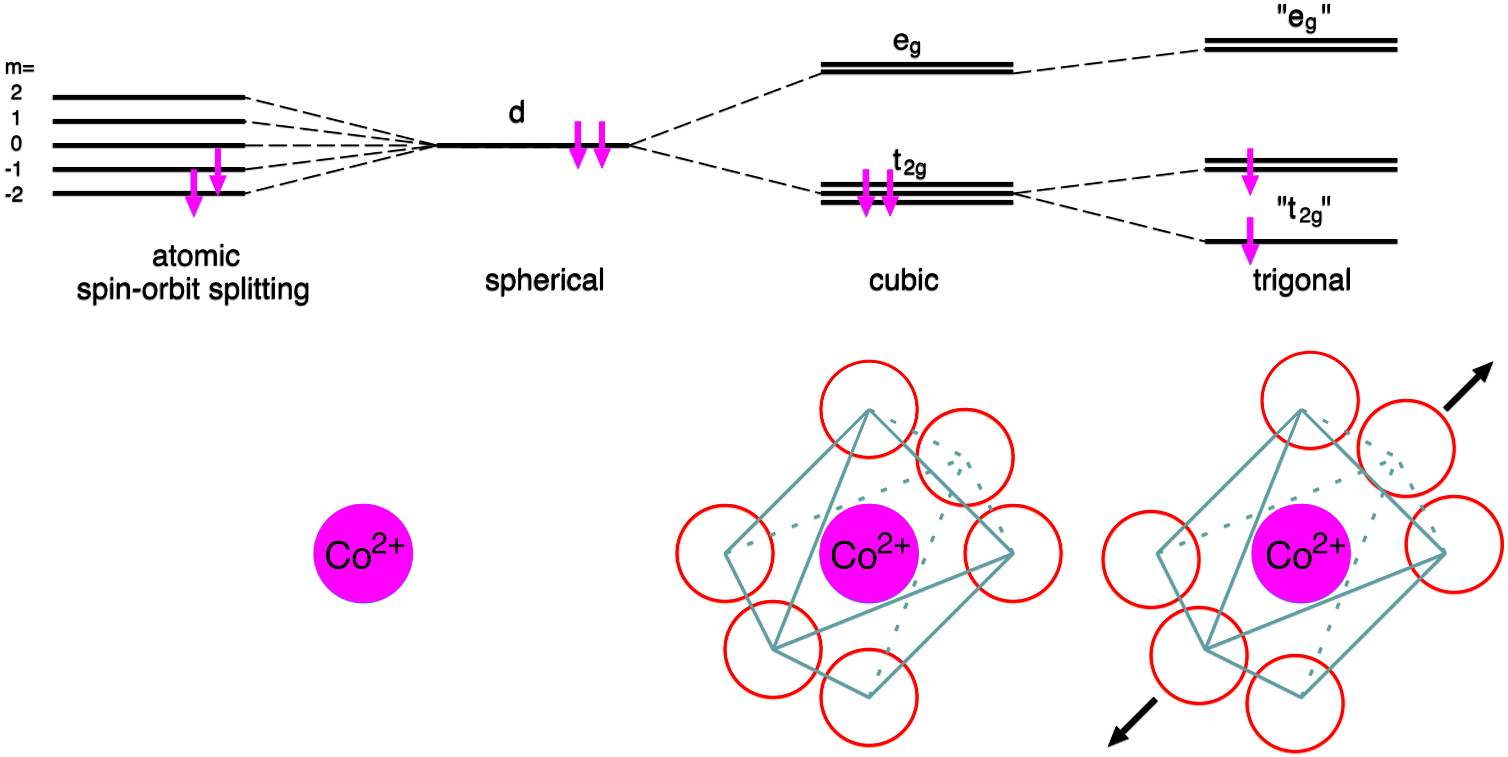
Fe^{3+} in tetrahedral field

5 d-electrons

Magnetite: larger MCA with Co doping

Fe_3O_4: $(Fe^{2+}O^{2-})(Fe_2^{3+}O_3^{2-})$ $K_1= -2 \bullet 10^4$ (J/m^{-3})

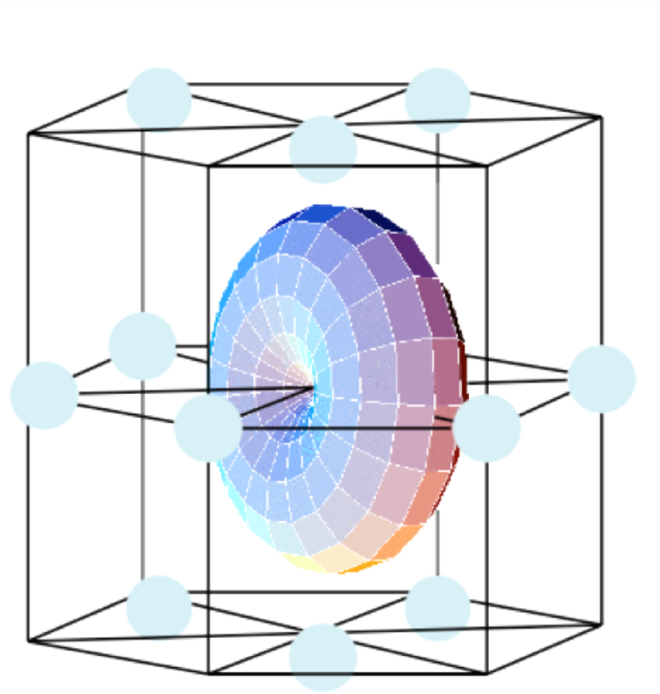
$CoFe_2O_4$: $(Co^{2+}O^{2-})(Fe_2^{3+}O_3^{2-})$ $K_1 \approx 10^6$ (J/m^{-3})

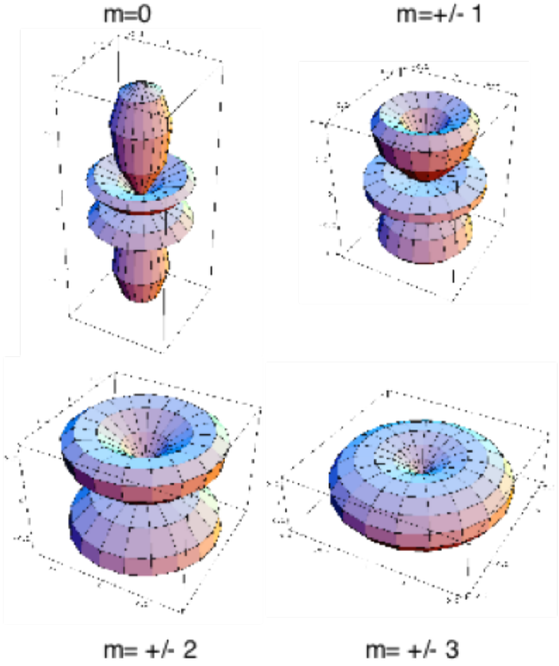


Single ion anisotropy:

Gd: K_1= -1.2•10^5 K_2= +8.0•10^4 (J/m^{-3})   conf: $6s^2\ 5d^1\ 4f^7$

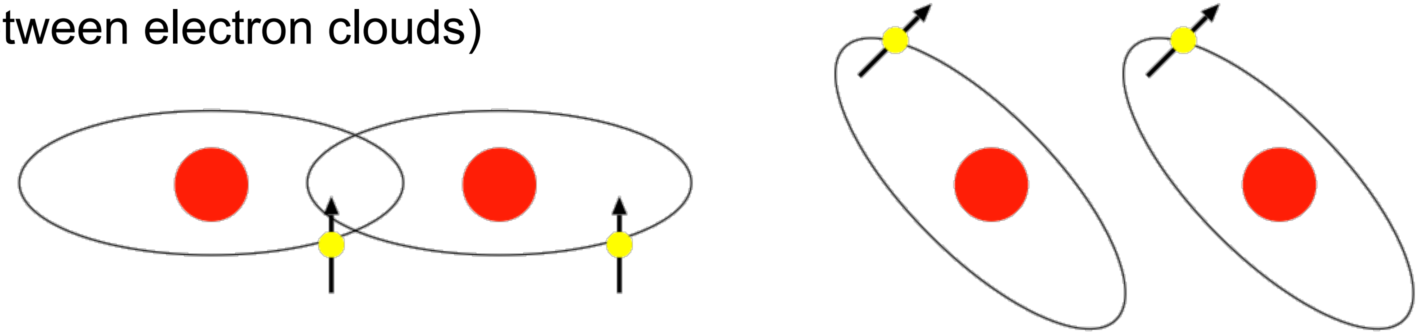
Tb: K_1= -5.7•10^7 K_2= -4.6•10^6 (J/m^{-3})   conf: $6s^2\ 5d^1\ 4f^8$





Other relativistic effects in magnetism:

- spin – other orbit coupling: $$H = \sum_{i,j} C_{i,j} \vec{S}_i \cdot \vec{L}_j$$
- spin – spin coupling (magnetic dipolar interaction between spin moments at the same ion)
- quadrupole – quadrupole interaction (electrostatic interaction between electron clouds)



Breit correction: captures relativistic 2-particle effects (dipole-dipole int.)

$$\left(E + \hat{H}_1 + \hat{H}_2 + \frac{e^2}{r_{12}} \right) \Psi = \frac{e^2}{2r_{12}} \left[\vec{\alpha}_1 \cdot \vec{\alpha}_2 + \frac{(\vec{\alpha}_1 \cdot \vec{r}_1)(\vec{\alpha}_2 \cdot \vec{r}_2)}{r_{12}^2} \right] \Psi$$

not captured in our DFT formalism!

Summary:

relativistic effects:

- single particle Dirac equation (can be studied with `l_soc="t"`)
  - scalar relativistic effects (d-band position Au, Ag)
  - spin-orbit effects
    - *T & S inversion symmetry ($p_{1/2}$-$p_{3/2}$ splitting)*
    - *T inversion symmetry (Rashba & Dresselhaus effect)*
    - *no T inversion symmetry (magneto-crystalline anisotropy)*
    - *no T & S (anisotropic exchange, Dzyaloshinskii-Moryia interaction)*
  - topological effects
    - *k-space: topological insulators*
    - *real space: magnetic skyrmions*
- two particle effects (Breit correction, dipole-dipole interaction)

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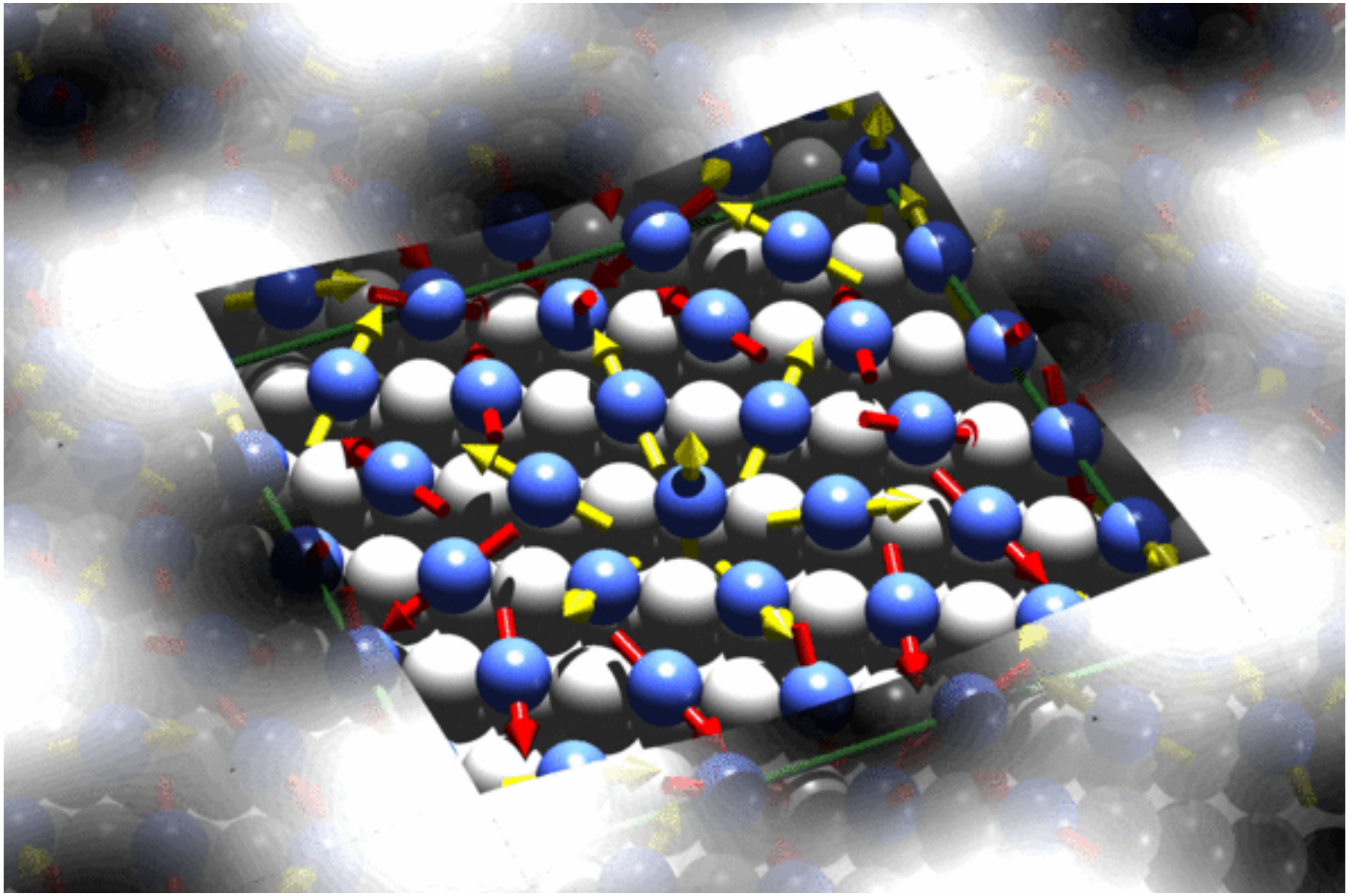
Now try it in practice!



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Orbital Moment:

2$^{\text{nd}}$ order perturbation theory:

$$\left\langle \vec{L} \right\rangle = \sum_{i,j} \frac{\left\langle \psi_i | \hat{L} | \psi_j \right\rangle \left\langle \psi_i | \hat{H}_{\text{SOC}} | \psi_j \right\rangle}{\varepsilon_i - \varepsilon_j} f(\varepsilon_i) \left[1 - f(\varepsilon_j)\right]$$

large orbital moments cause large energy changes due to SOC:

$$\delta E_{\text{SOC}} \approx -\frac{1}{4} \xi \vec{S} \cdot \left[\left\langle \vec{L}^{\uparrow} \right\rangle - \left\langle \vec{L}^{\downarrow} \right\rangle \right]$$

suppose a $d_{x^2-y^2}$ and d_{xy} orbital cross at Fermi level:

< xy | e•L | x^2-y^2 > = -2 i e_z

- largest orbital moment component is L_z
- easy axis points in z-direction

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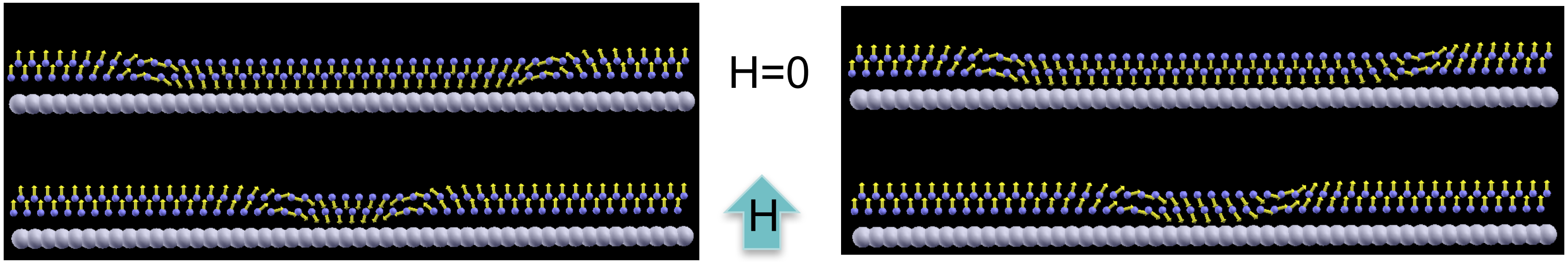
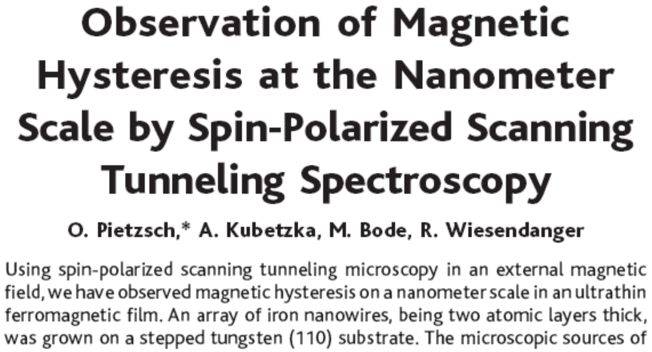
2 domain walls in magnetic field:



topologically protected:
H-field cannot destroy the
inner domain (in 1D case)

topologically trivial:
H-field destroys the inner
domain easily

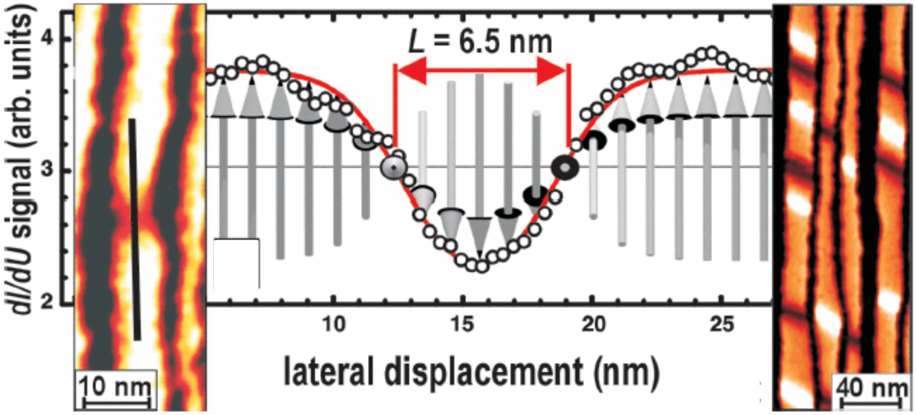
Example: Science **292**, 2053 (2001)



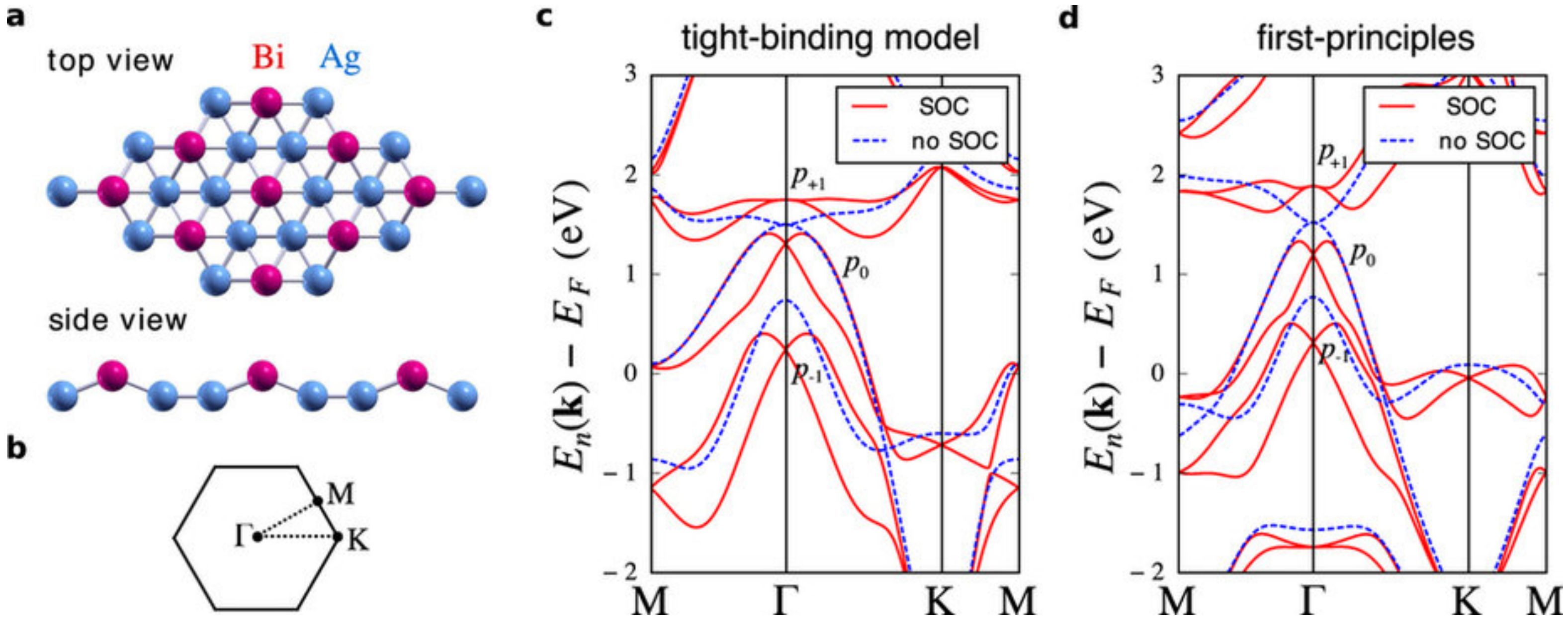
Observation of Magnetic Hysteresis at the Nanometer Scale by Spin-Polarized Scanning Tunneling Spectroscopy

O. Pietzsch,* A. Kubetzka, M. Bode, R. Wiesendanger

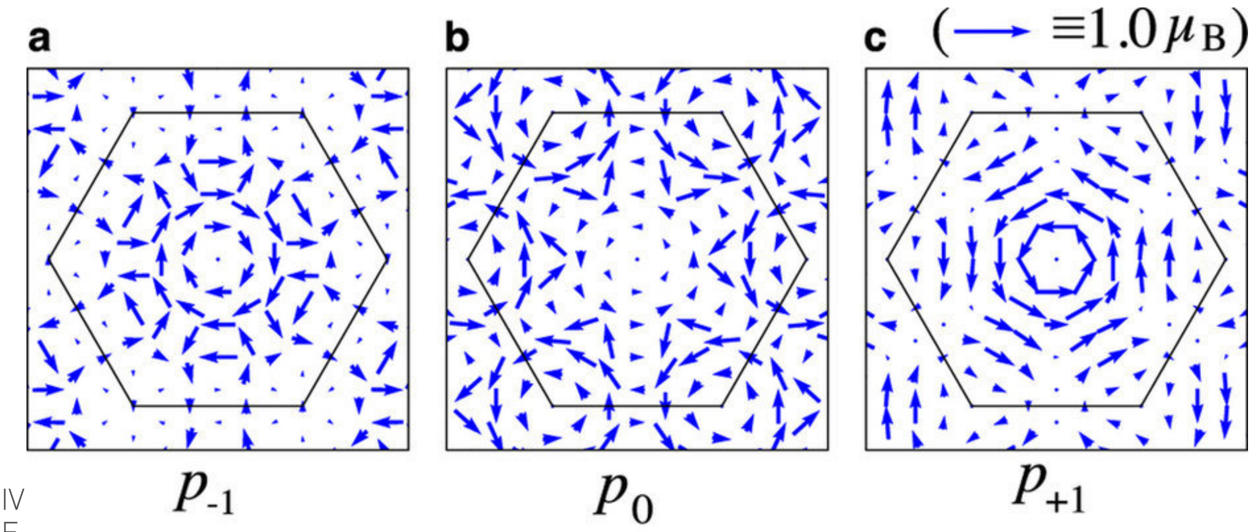
Using spin-polarized scanning tunneling microscopy in an external magnetic field, we have observed magnetic hysteresis on a nanometer scale in an ultrathin ferromagnetic film. An array of iron nanowires, being two atomic layers thick, was grown on a stepped tungsten (110) substrate. The microscopic sources of



Orbital moments (even without SOC)

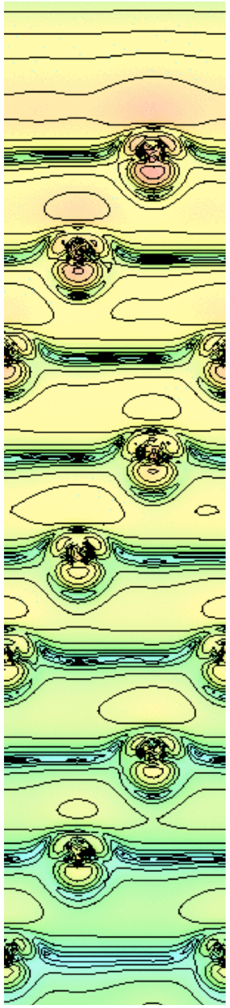


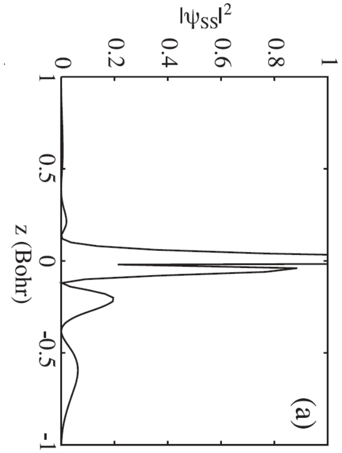
orbital
texture:

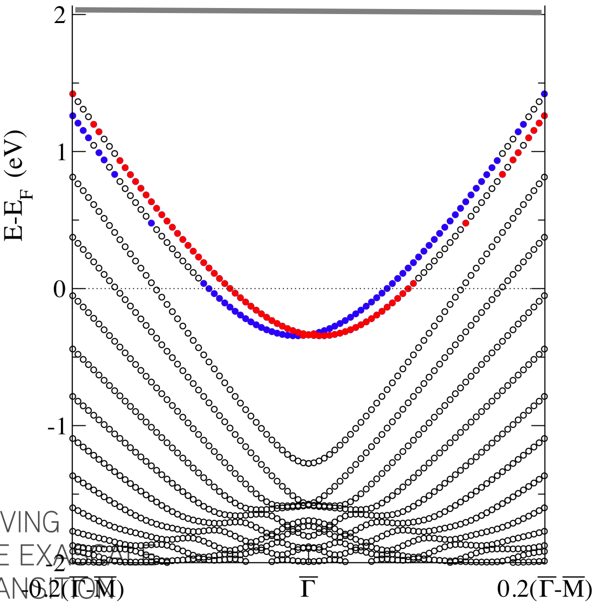


Go et al. Sci. Rep. 7, 46742 (2017)

Origin of the Rashba-splitting







needs:

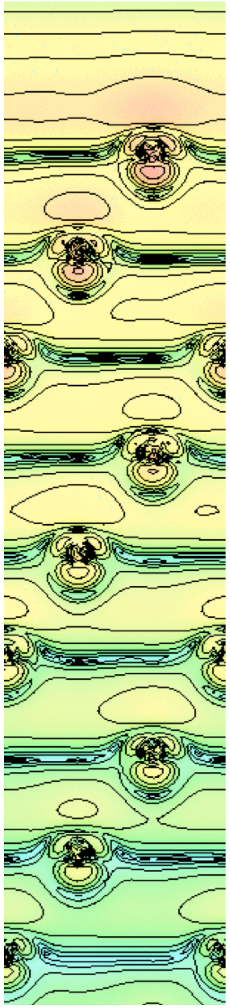
- strong spin-orbit coupling
- gradient of the wavefunction

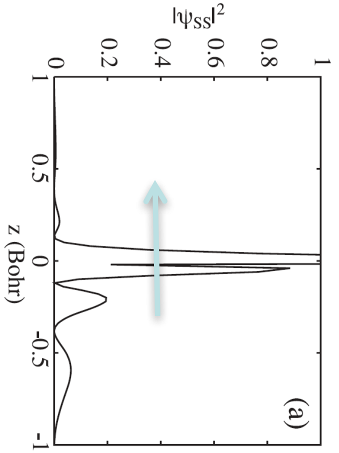
  asymmetry of $|\Psi_{SS}|^2$ at nucleus matters

[G. Bihlmayer et al., Surf. Sci. **600**, 3888 (2006)]

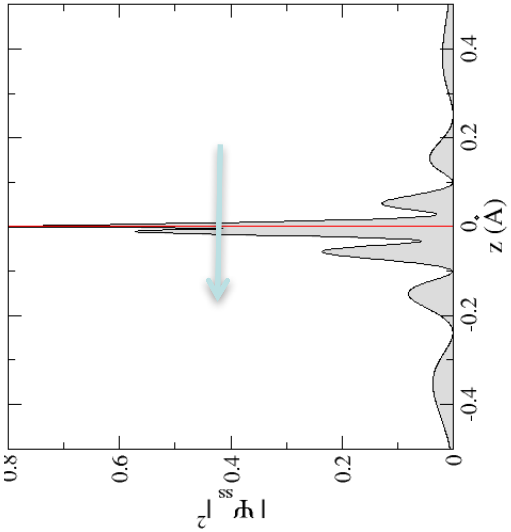
example: Au(111):
1D-plot through surface atom
[M. Nagano et al., J. Phys.: Cond. Matter **21**, 064239 (2009)]

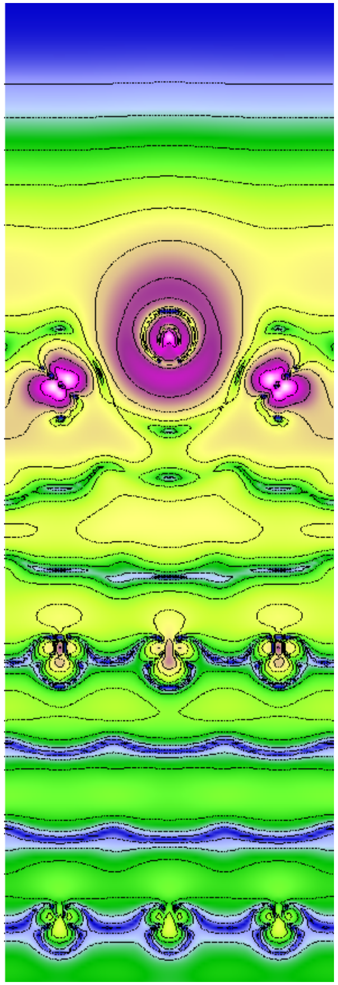
Origin of the Rashba-splitting



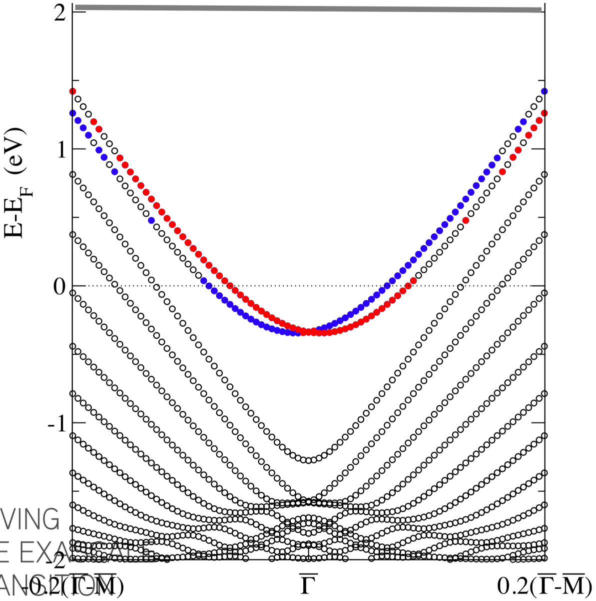


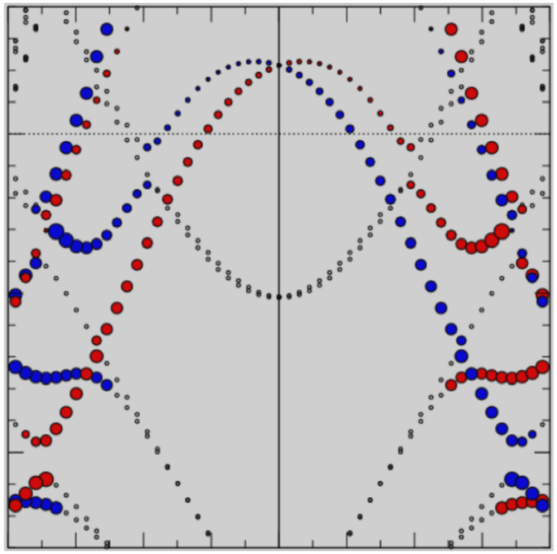
BiCu$_2$/Cu(111): Bentmann et al., Phys.Rev.B **84**, 115426 (2011)





sign reversal of α_R!





Introduction: Topological insulators

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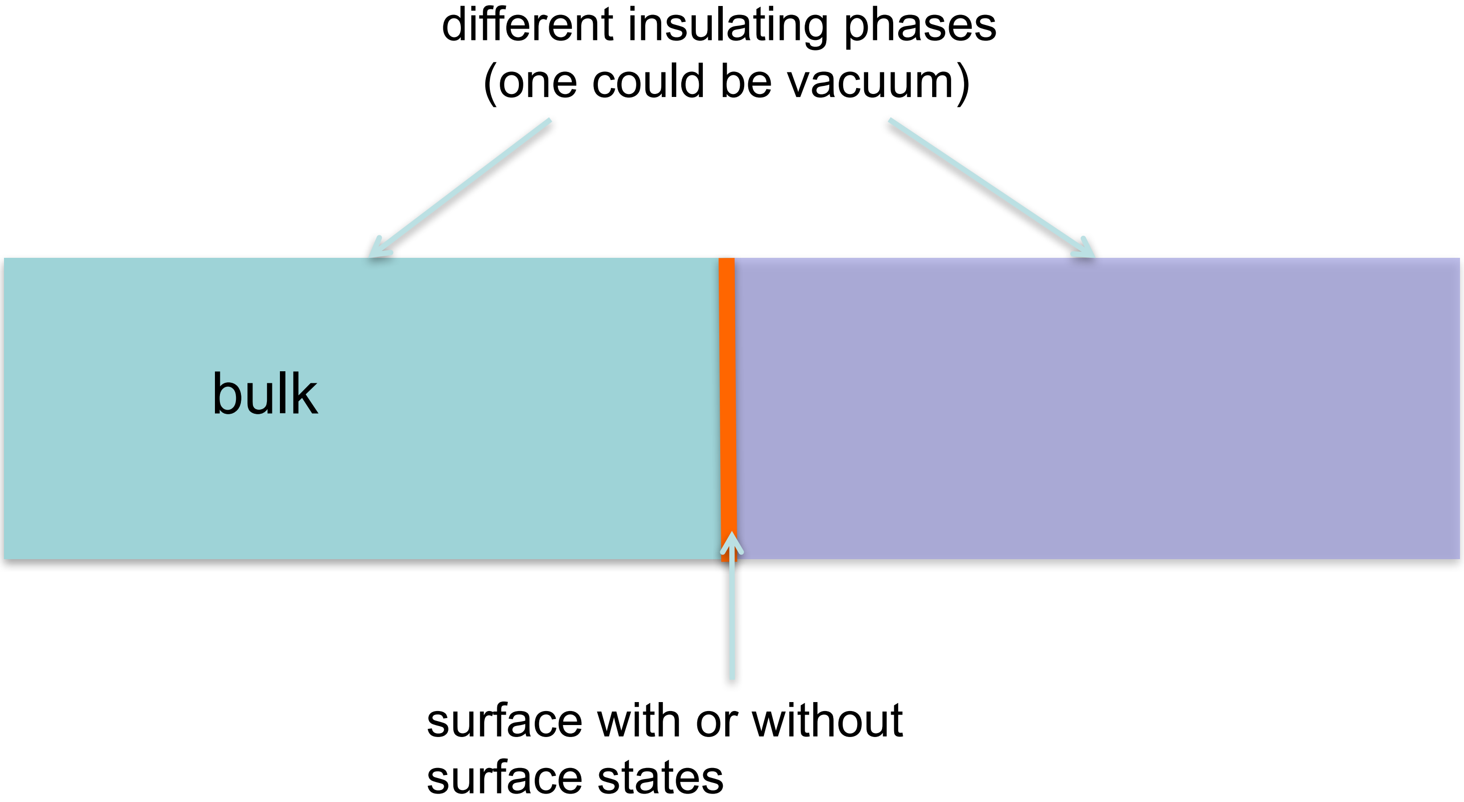
Surfaces & Interfaces of Insulators



different insulating phases
(one could be vacuum)

bulk

surface with or without
surface states

- Surface/interface states appear due to dangling bonds or or appropriate scattering conditions of the surface potential.
- They may be more or less spin-polarized (Rashba effect).

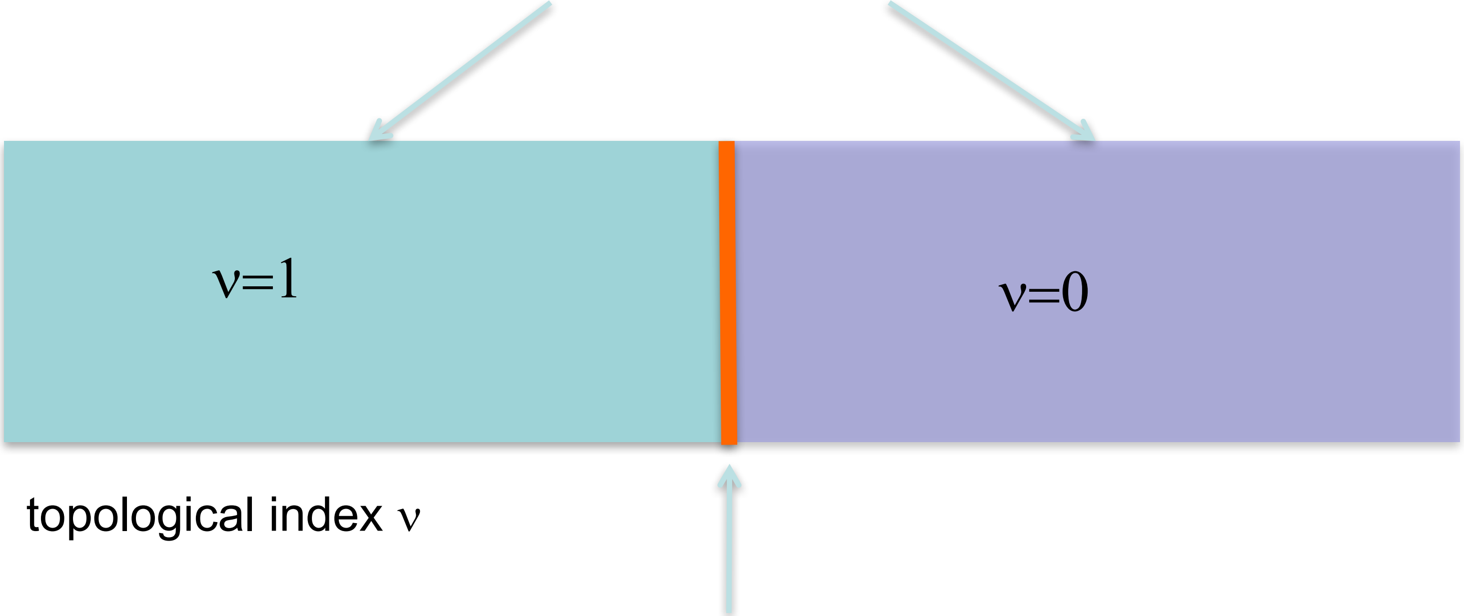
Topological Insulator

describe different insulating phases
with topological properties ν

topological index ν

Topological Insulator

describe different insulating phases
with topological properties ν



ν=1

ν=0

topological index ν

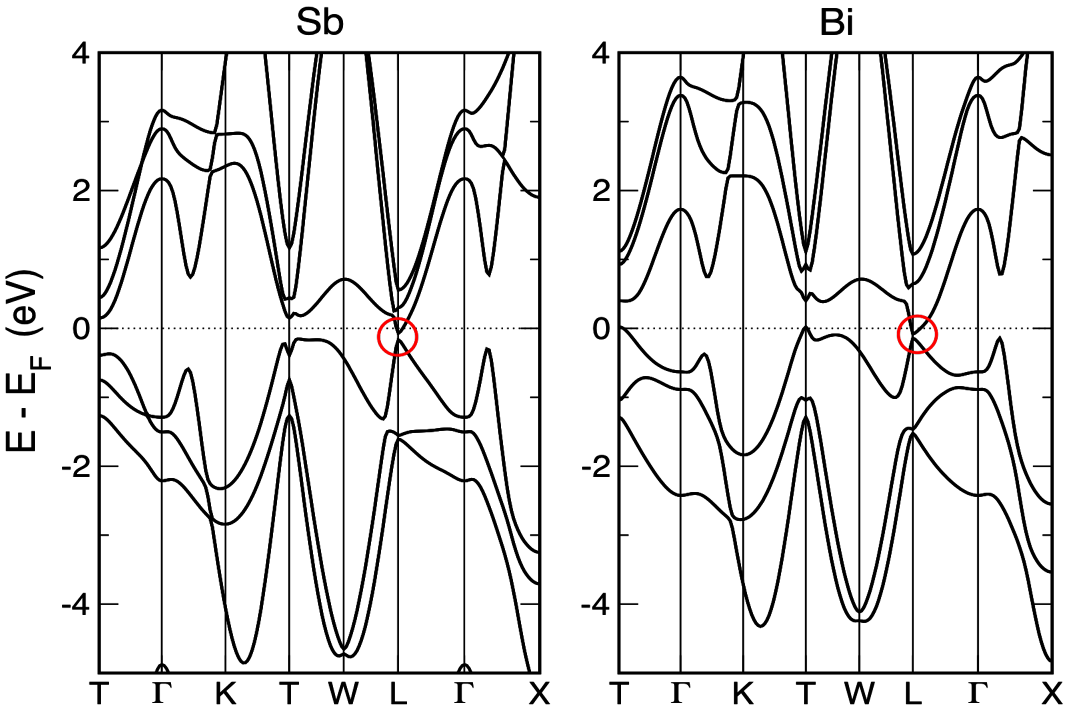
metallic boundary

metallic states are robust against perturbations that
- do not break time-reversal symmetry
- do not close the bulk-bandgap of the insulator

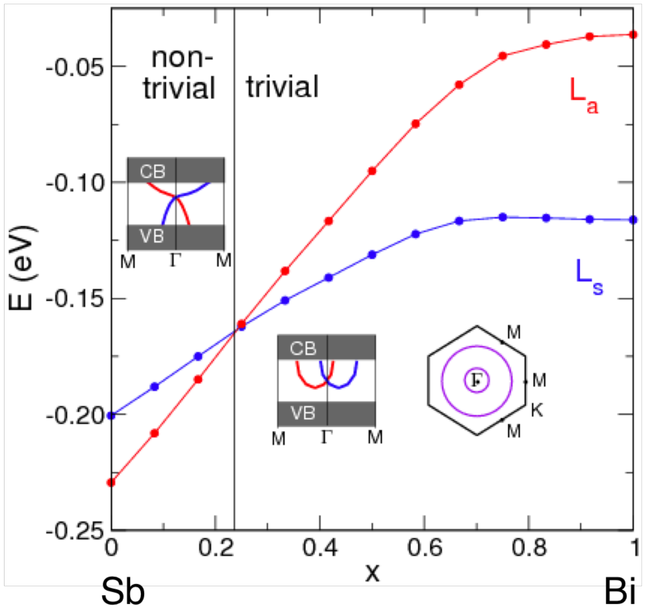
band inversion: Bi vs. Sb

bulk Bi: topologically trivial ν=(0;000)

bulk Sb: topological semimetal ν=(1;111)



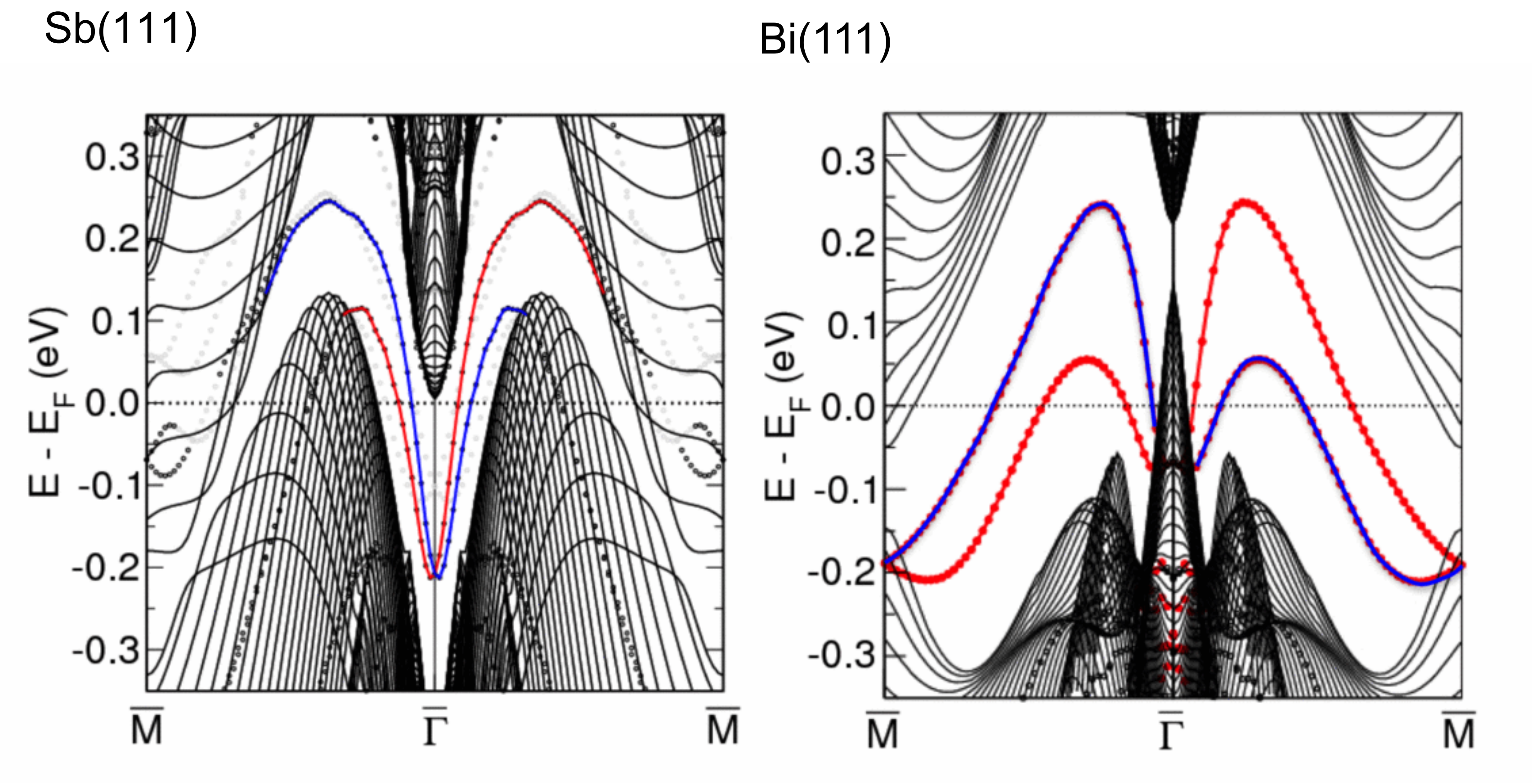
changing the SOC strength



- ○ bandgap at L-point inverted with decreasing SOC
- ○ for vanishing SOC: another band-inversion at T

analyze parity!

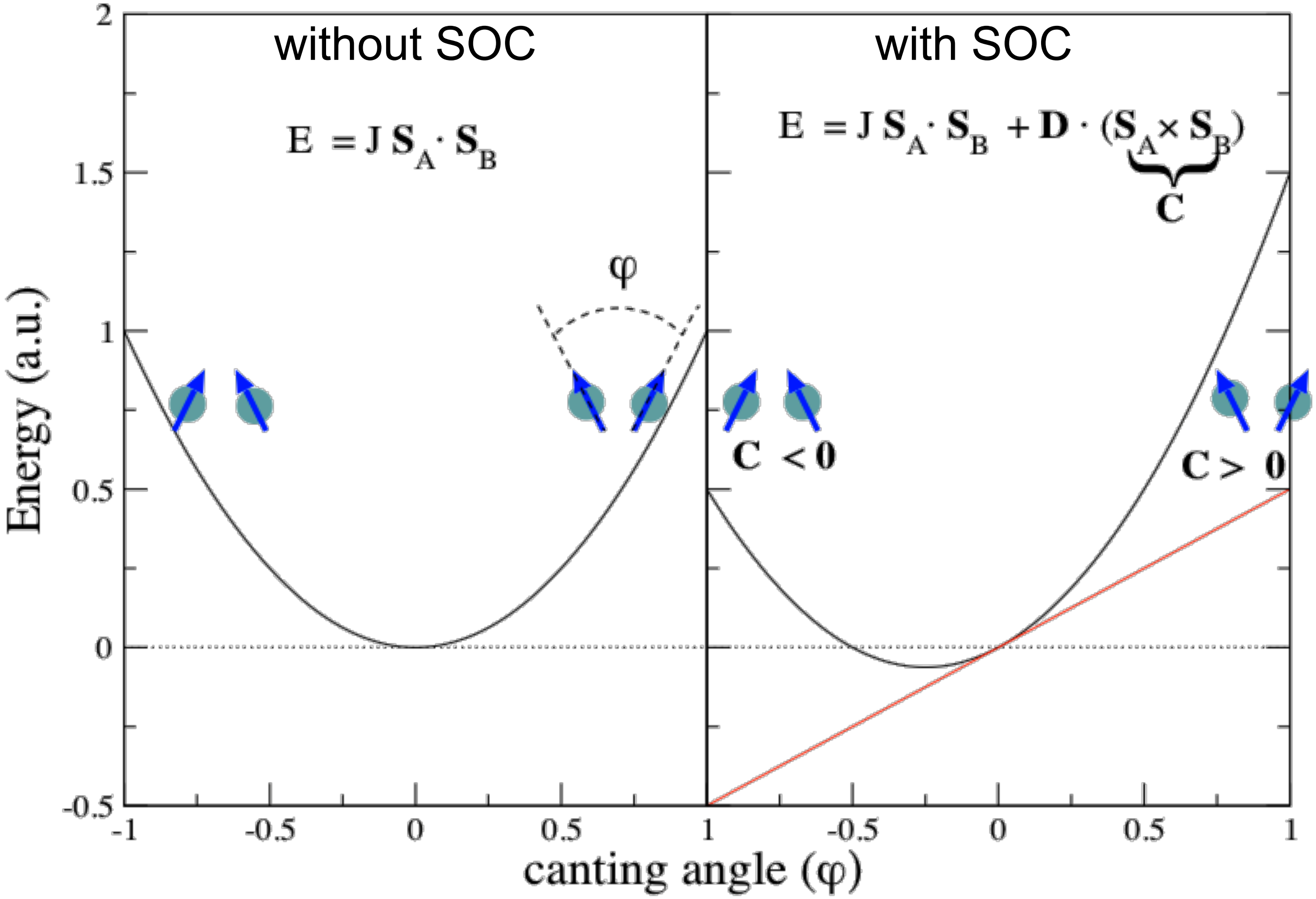
Sb and Bi surfaces:



- Sb: surface state connects valence and conduction band: $\nu=(1;111)$
- Bi: both spin-split branches return to valence band

Dzyaloshinskii-Moriya interaction:

distinguish clockwise – counterclockwise rotations



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