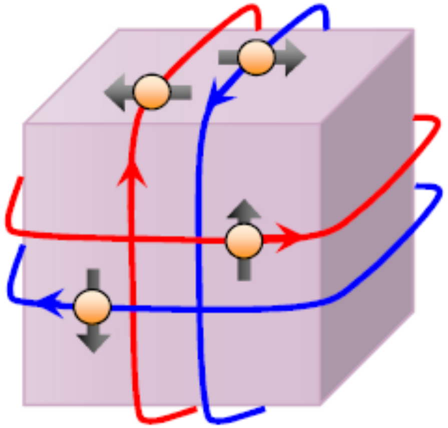

SPIN ORBIT COUPLING AND OTHER RELATIVISTIC EFFECTS

13.04.2021 I G. BIHLMAYER

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FORSCHUNGSZENTRUM JÜLICH AND JARA, 52425 JÜLICH, GERMANY

OVERVIEW

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

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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: $\Psi = \begin{pmatrix}\psi \\ \chi\end{pmatrix}$

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

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

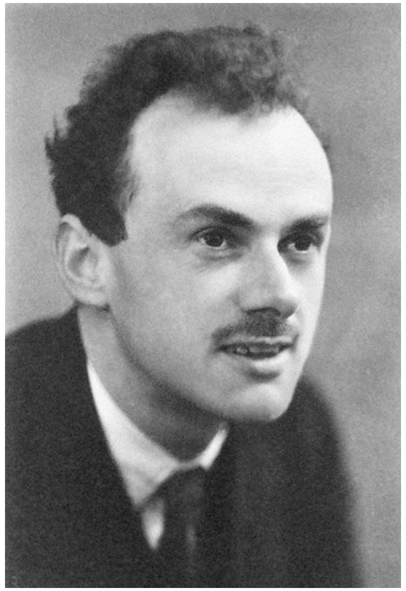

image: Wikipedia

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:

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

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

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

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

mass-velocity term

Darwin term

spin-orbit coupling

magnetic field int.

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

SCALAR RELATIVISTIC CALCULATIONS:

- block-diagonal equation in spin:

$$\left(E + eV(\vec{r}) - \frac{\vec{p}^{\,2}}{2m} - \frac{e\hbar}{2mc} B_z(\vec{r}) \boldsymbol{\sigma}_z + \frac{1}{2mc^2} \left(E + eV(\vec{r}) \right)^2 + i \frac{e\hbar}{(2mc)^2} \vec{E}(\vec{r}) \cdot \vec{p} \right) \psi = 0$$

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

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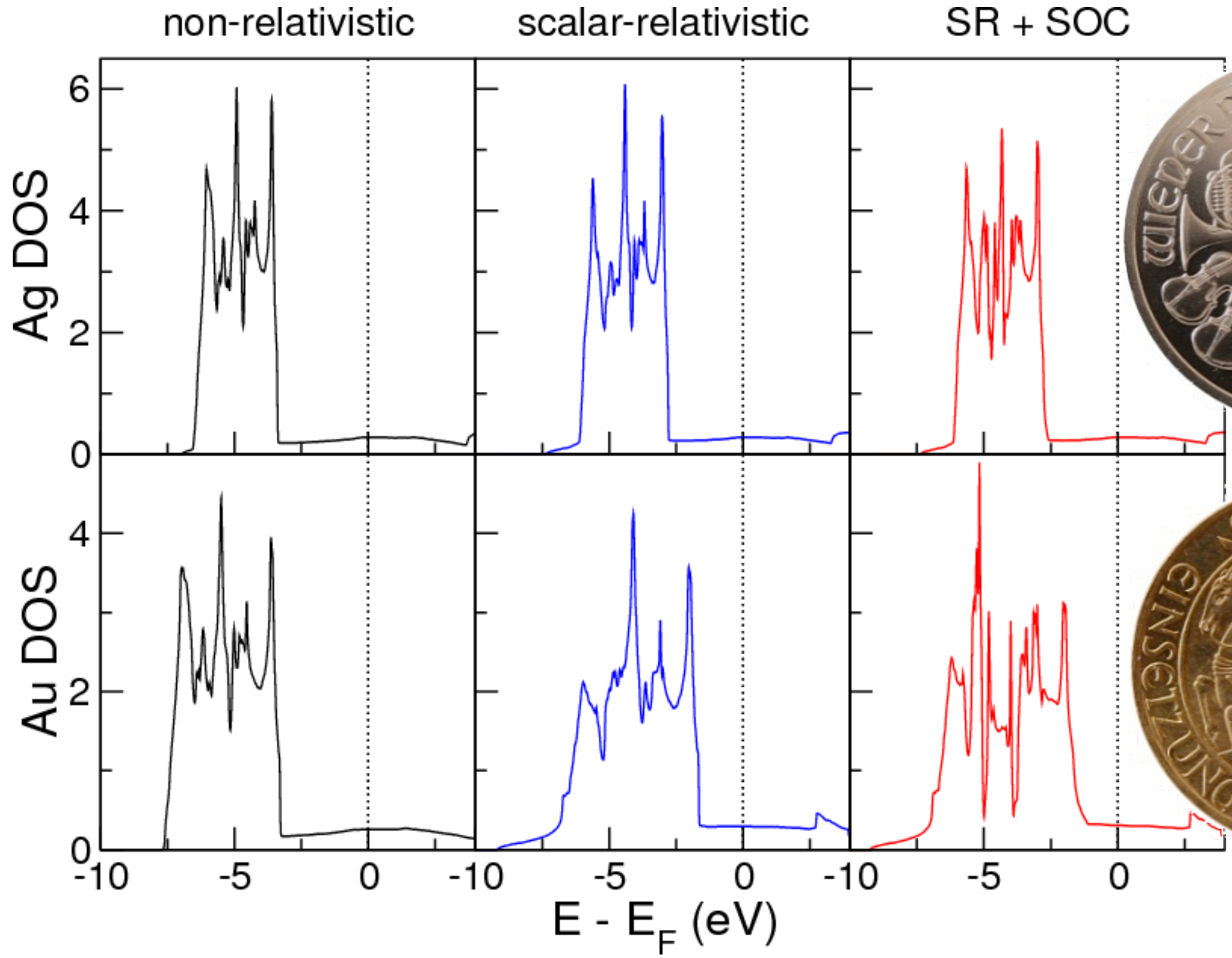
RELATIVISTIC EFFECTS IN AG AND AU

- density of states (DOS):



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Fleur

MAX

SPIN-ORBIT COUPLING

- interaction with an (internal) magnetic field:

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

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!

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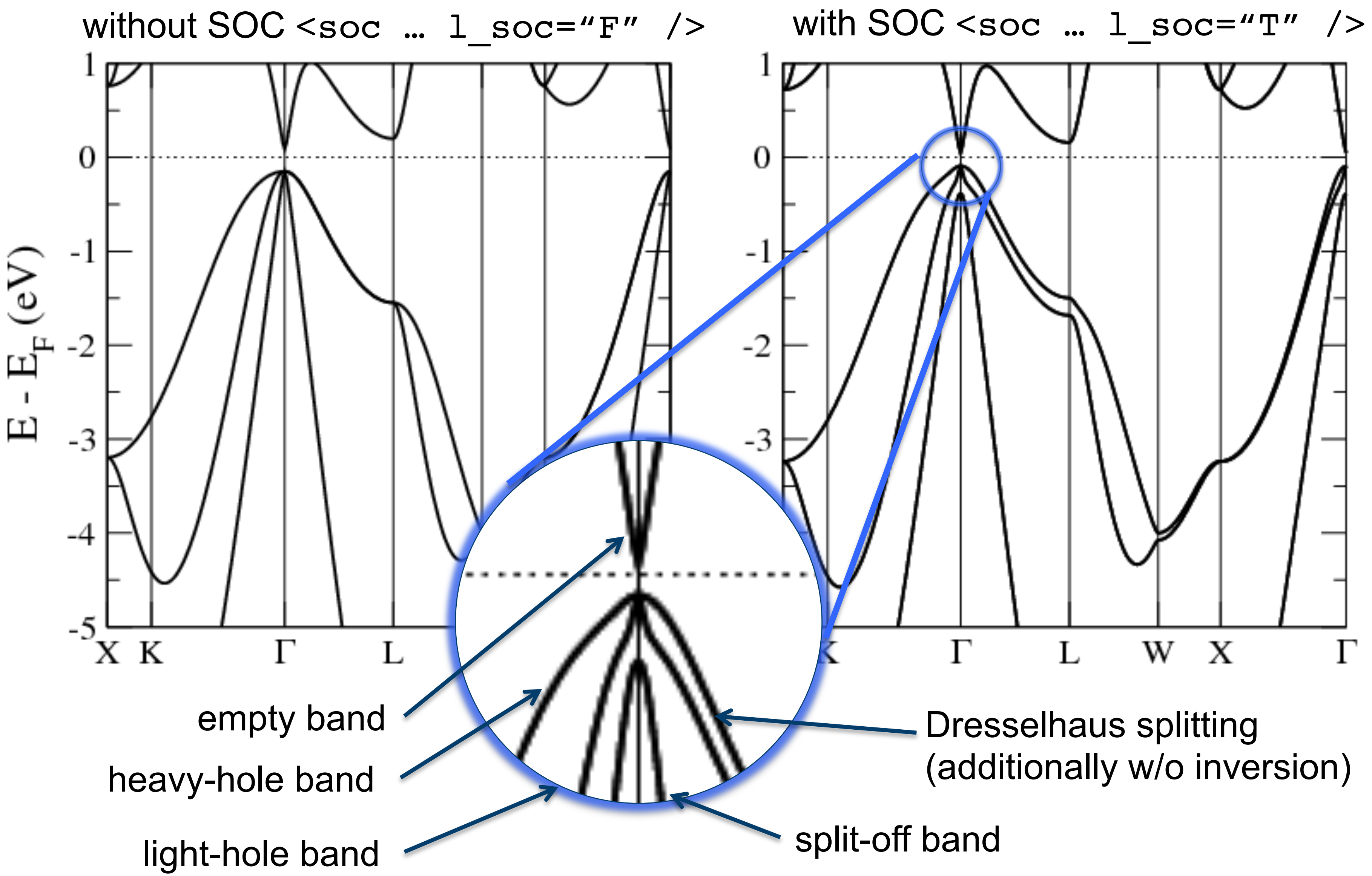
SPIN-ORBIT COUPLING EFFECTS IN NON-MAGNETIC SOLIDS

A TYPICAL SEMICONDUCTOR: GE



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RASHBA EFFECT AT A SURFACE

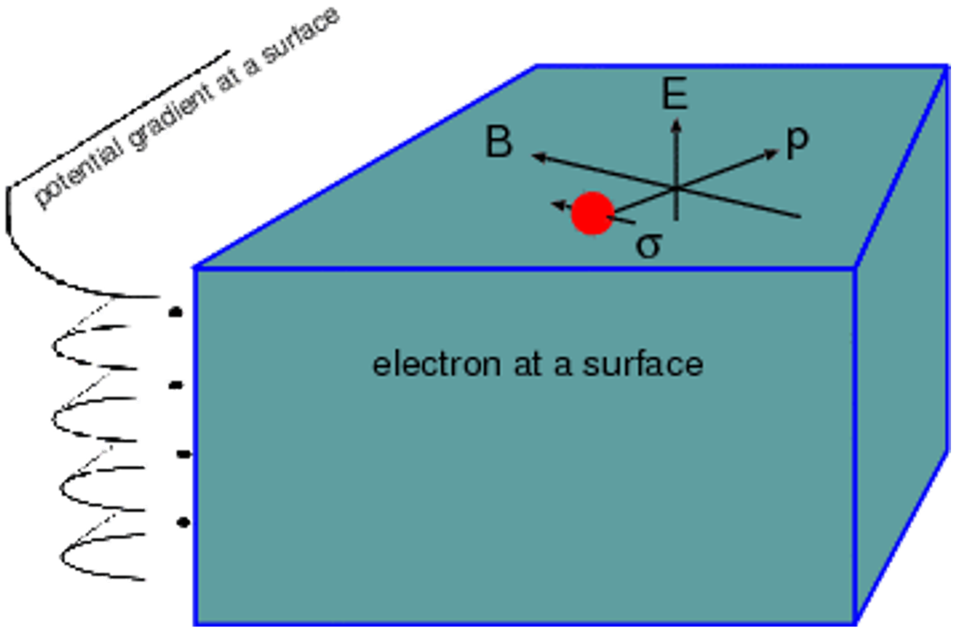
- Free electron gas in electric field:

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

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

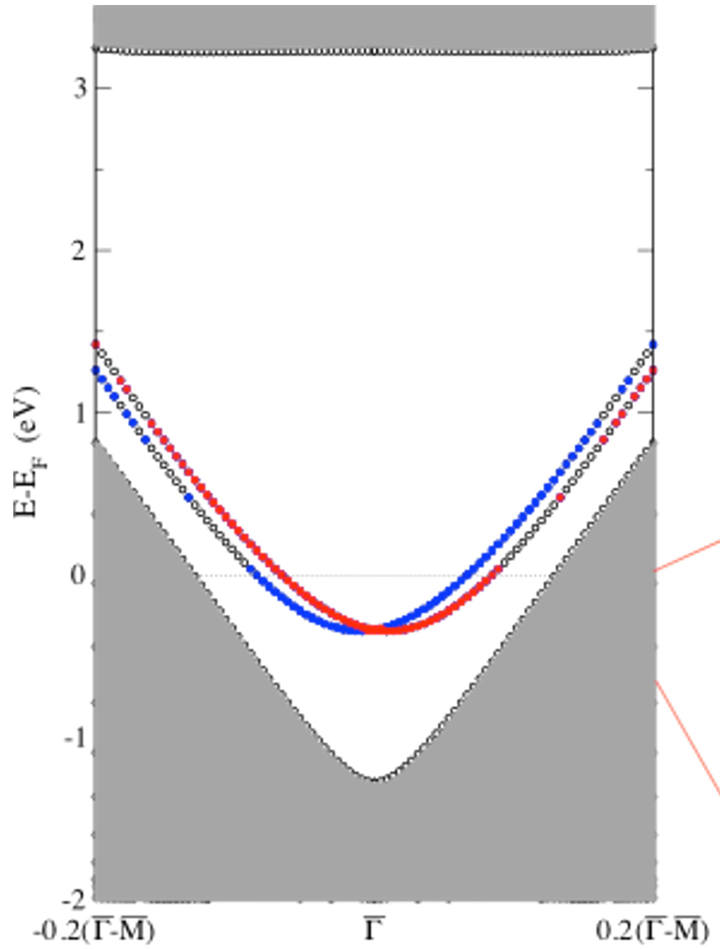
$$\left[-\frac{1}{2}\nabla^2 + \alpha_R\vec{\sigma}\cdot\left(\vec{k}_{\|}\times\vec{e}_z\right)\right]\psi_i = \varepsilon_i\psi_i$$

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



EXAMPLE: COINAGE METAL SURFACES

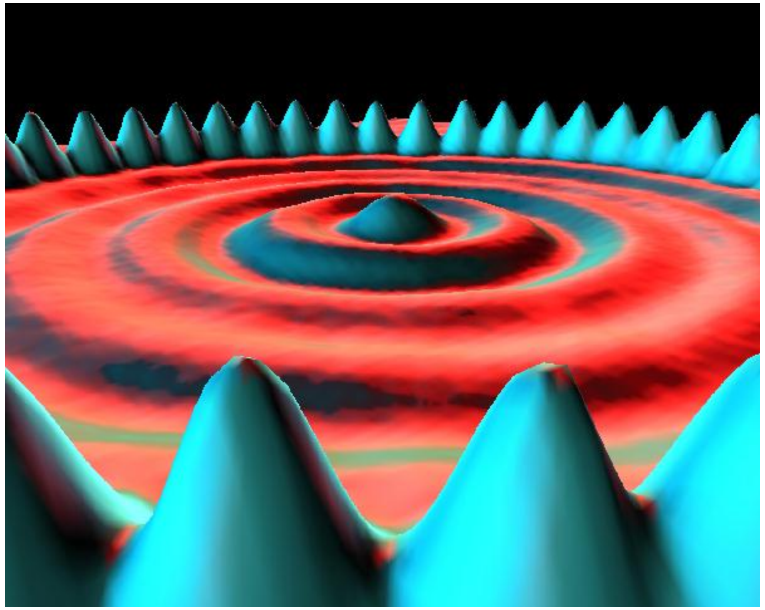
- (111) surface states

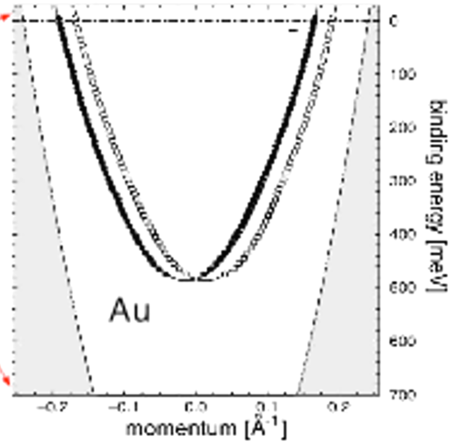


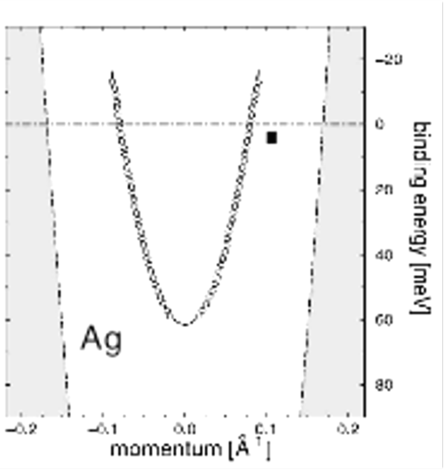
Z(Cu) = 29

Z(Ag) = 47

Z(Au) = 79







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

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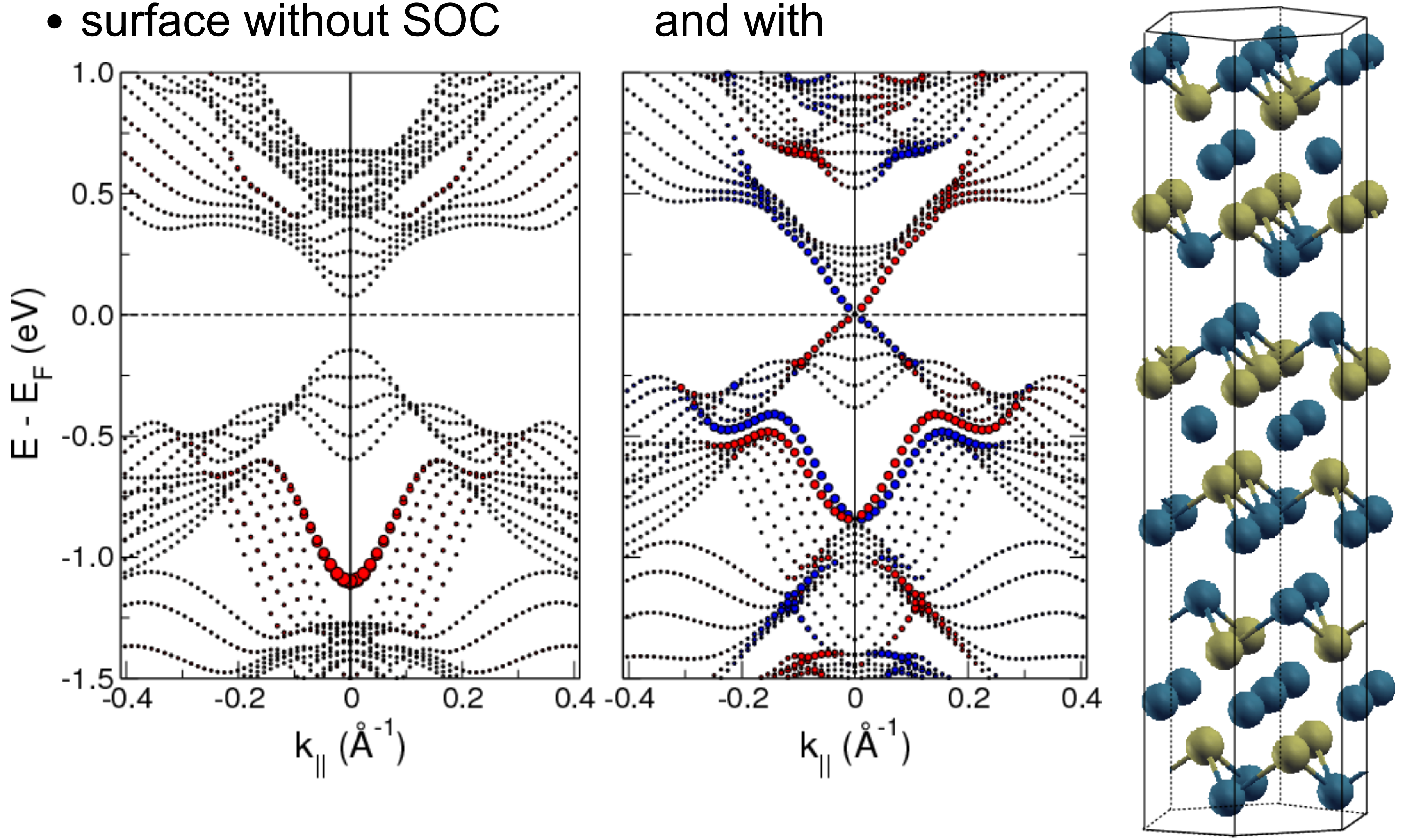
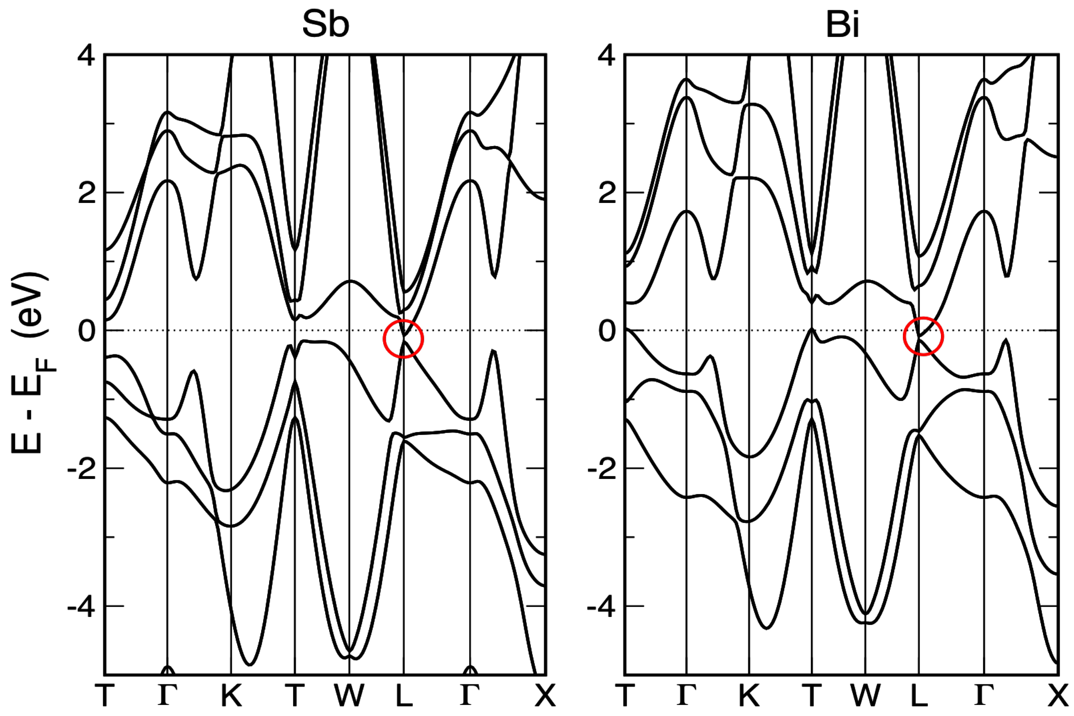
Topological Insulator: Sb_2Te_3

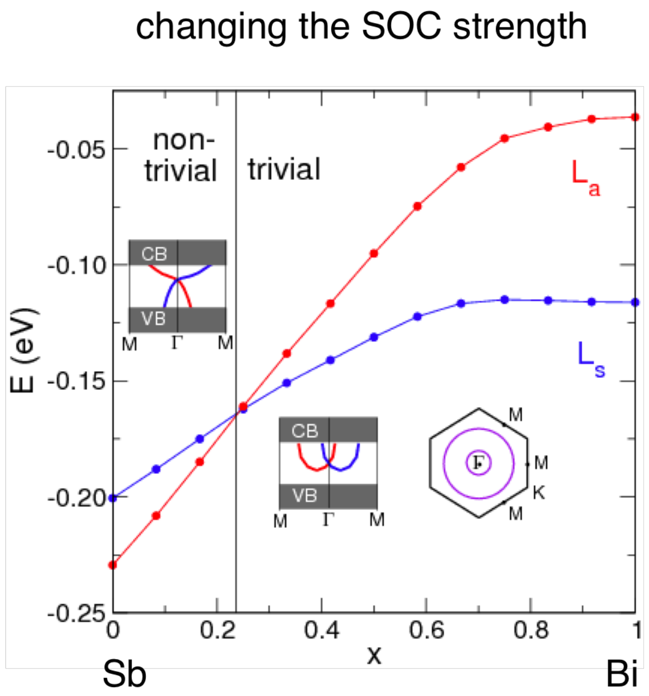
- surface without SOC and with



BAND INVERSION: BI VS. SB

- bulk Bi: topologically trivial ν=(0;000)
- bulk Sb: topological semimetal ν=(1;111)





○ bandgap at L-point inverted with decreasing SOC

○ for vanishing SOC: another band-inversion at T

e.g.
`socscale="0.4"`

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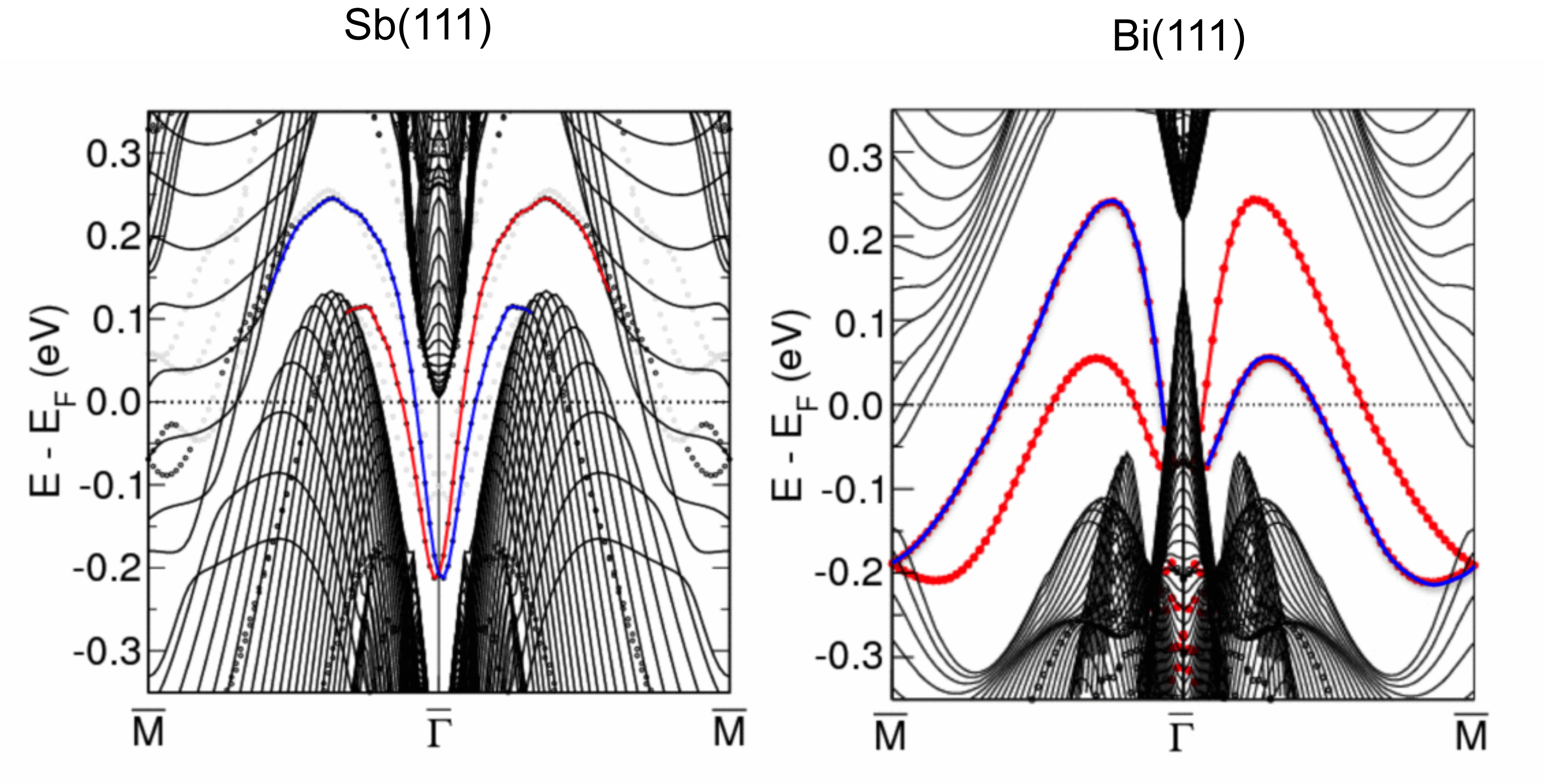
Sb and Bi surfaces:



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

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

non-relativistic effects

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

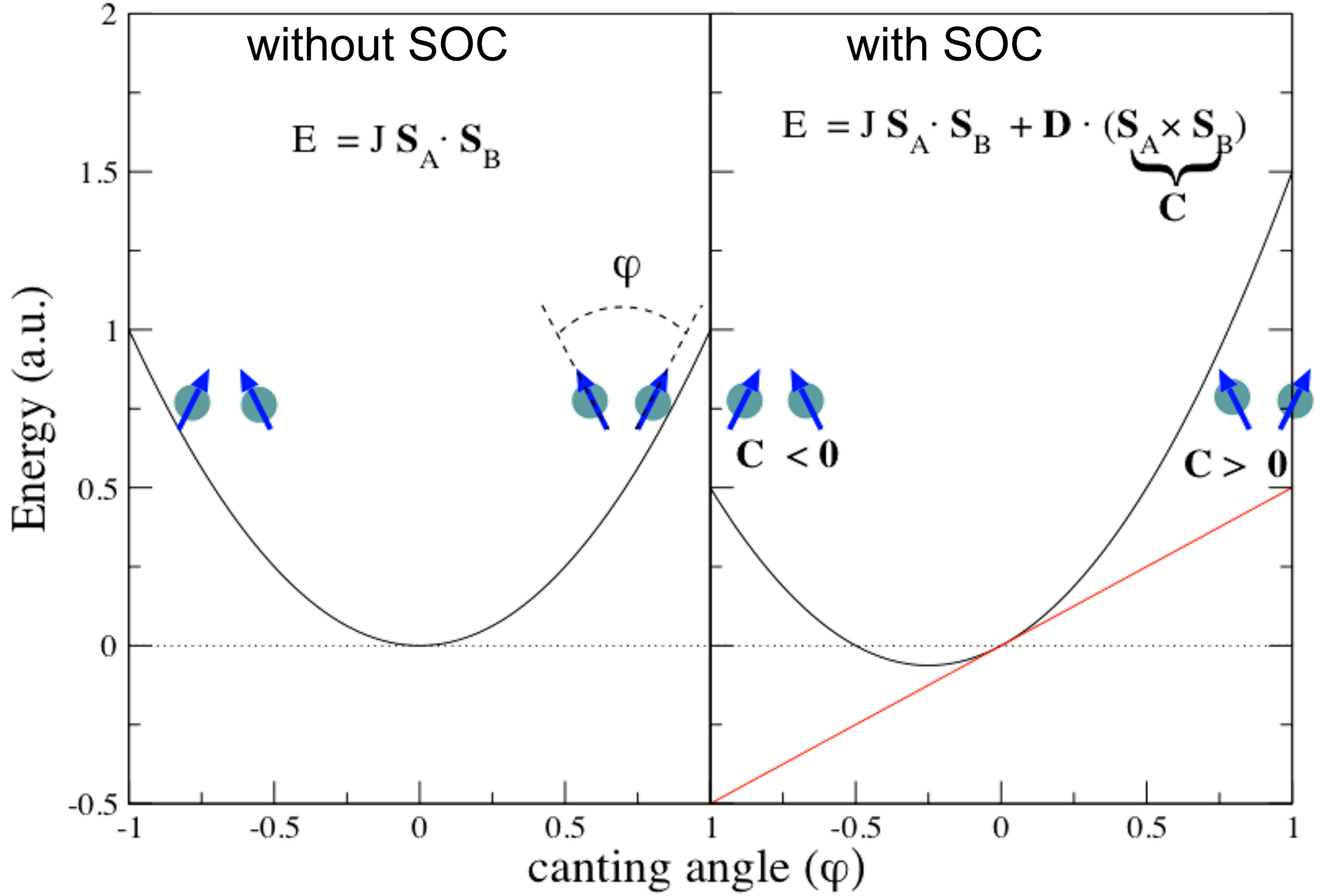
leads to $\vec{D} \cdot \left(\vec{S}_i \times \vec{S}_j\right)$

$$\underline{J}_{ij}^A \propto \left(\frac{\Delta g}{g}\right) J \quad ; \quad \underline{J}_{ij}^S \propto \left(\frac{\Delta g}{g}\right)^2 J$$

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

Dzyaloshinskii-Moriya Interaction:

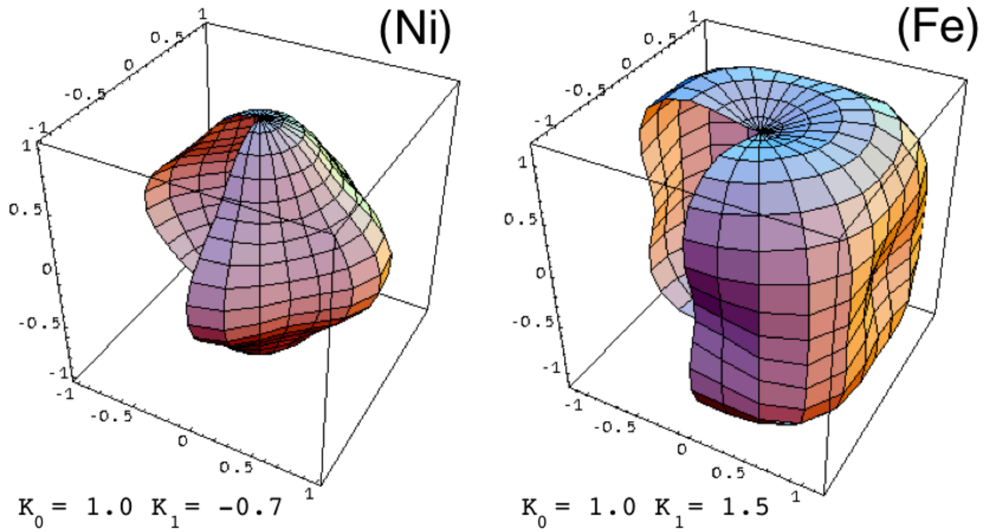
- symmetry dependent, leads e.g. to formation of skyrmions



MAGNETIC ANISOTROPY:

- phenomenology:
  magnetization direction dependence of free energy of a cubic crystal:

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



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

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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	$\langle zx \vert$	$\langle yz \vert$	$\langle xy \vert$	$\langle x^2-y^2 \vert$	$\langle 3z^2-r^2 \vert$
$\vert zx \rangle$	0	$-ie_z$	ie_x	$-ie_y$	$i\sqrt{3}e_y$
$\vert yz \rangle$	ie_z	0	$-ie_y$	$-ie_x$	$-i\sqrt{3}e_x$
$\vert xy \rangle$	$-ie_x$	ie_y	0	$2ie_z$	0
$\vert x^2-y^2 \rangle$	ie_y	ie_x	$-2ie_z$	0	0
$\vert 3z^2-r^2 \rangle$	$-i\sqrt{3}e_y$	$i\sqrt{3}e_x$	0	0	0

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ORBITAL MOMENT:

- 2^{nd} order perturbation theory:

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

large orbital moments cause large energy changes due to SOC:

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

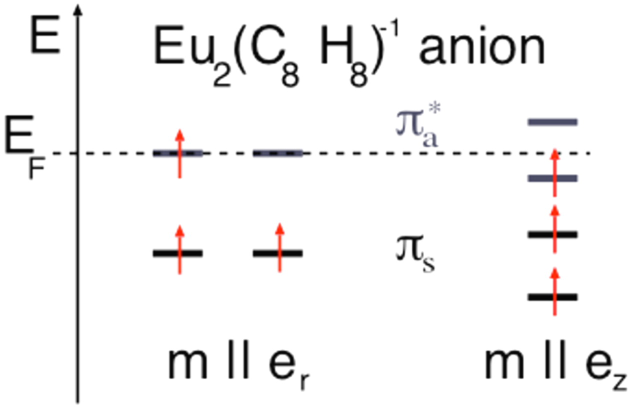
suppose a $d_{x^2-y^2}$ and d_{xy} orbital cross at Fermi level:

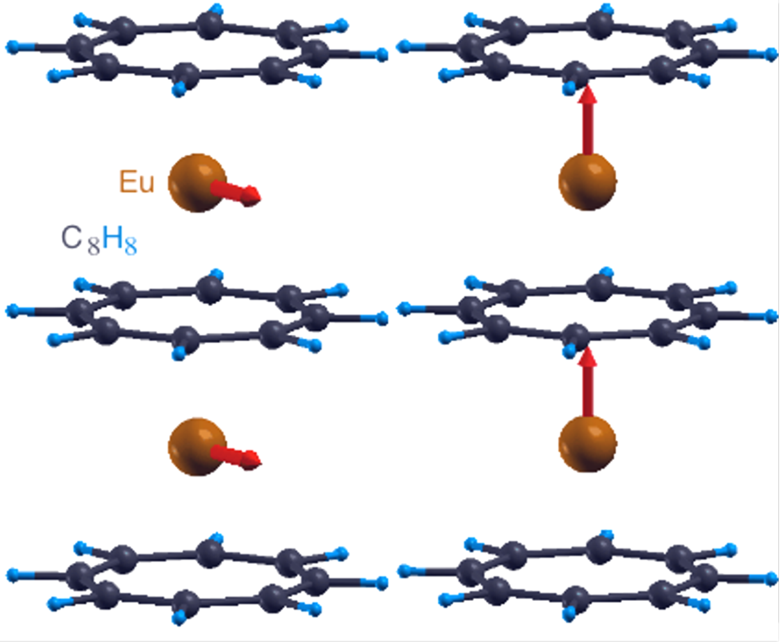
$< xy \mid e \bullet L \mid x^2-y^2 > = -2\, i\, e_z$

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

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

```
<soc
theta="0.5pi"
phi="0.0"
l_soc="T" />
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<soc
theta="0.0"
phi="0.0"
l_soc="T" />
```

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

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SUMMARY:

- single particle Dirac equation
  - 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 effect)
    - no T inversion symmetry (magneto-crystalline anisotropy)
    - no T & S (anisotropic exchange, Dzyaloshinskii-Moryia interaction)

Thank you for your attention !