Spin-orbit coupling and non-collinear magnetism in Wien2k

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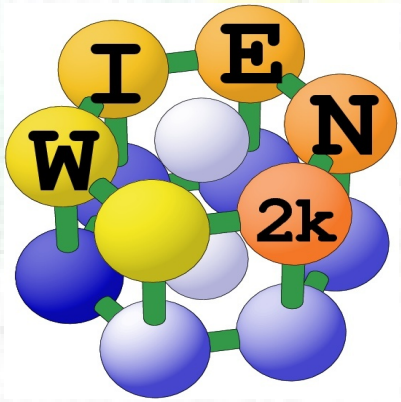


Dirac Hamiltonian

Dirac relativistic Hamiltonian provides a quantum mechanical description of electrons, consistent with the theory of special relativity.

$$H_D = c\,\vec{\alpha}\cdot\vec{p} + \beta\, m c^2 + V$$

$$\alpha_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix} \qquad \beta_k = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & \mathbf{-1} \end{pmatrix}$$

Pauli matrices:

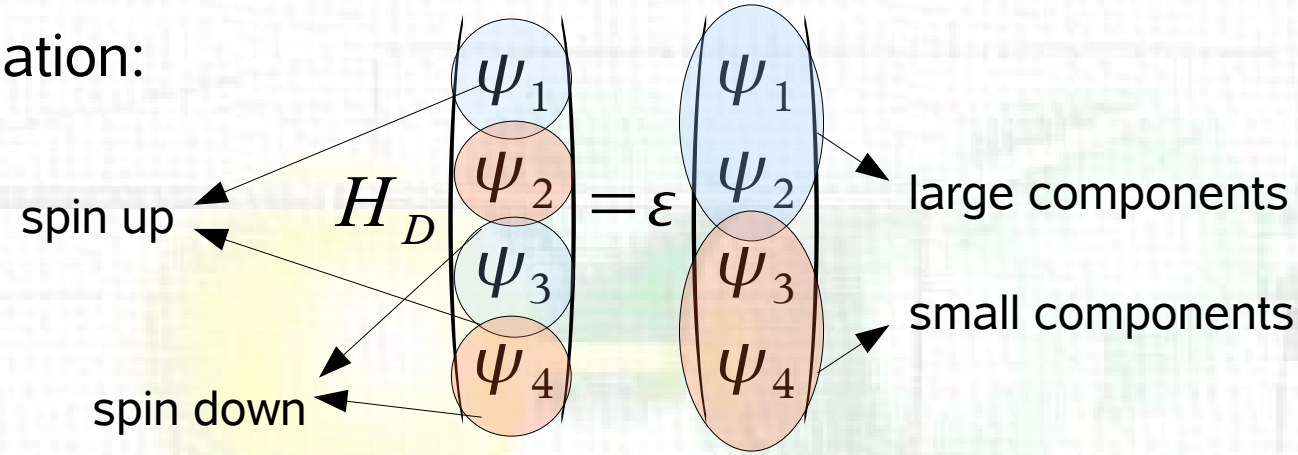
$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},$$

$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

H_D and the wave function are 4-dimensional objects

Dirac Hamiltonian

Dirac equation:



free particle:

$$\begin{pmatrix} \varepsilon-mc^2 & 0 & -\hat{p}_z & -(\hat{p}_x-i\hat{p}_y) \\ 0 & \varepsilon-mc^2 & -(\hat{p}_x+i\hat{p}_y) & \hat{p}_z \\ -\hat{p}_z & -(\hat{p}_x-i\hat{p}_y) & \varepsilon+mc^2 & 0 \\ -(\hat{p}_x+i\hat{p}_y) & \hat{p}_z & 0 & \varepsilon+mc^2 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} = 0$$

slow particle limit (p=0):

$mc^2, \begin{pmatrix} \psi \\ 0 \\ 0 \\ 0 \end{pmatrix}$ spin up $\quad mc^2, \begin{pmatrix} 0 \\ \psi \\ 0 \\ 0 \end{pmatrix}$ spin down

$-mc^2, \begin{pmatrix} 0 \\ 0 \\ \psi \\ 0 \end{pmatrix} \quad -mc^2, \begin{pmatrix} 0 \\ 0 \\ 0 \\ \psi \end{pmatrix}$ antiparticles, up, down

Dirac equation in spherical potential

Solution for spherical potential

$$\Psi = \begin{pmatrix} g_\kappa(r)\chi_{\kappa\sigma} \\ -i f_\kappa(r)\chi_{\kappa\sigma} \end{pmatrix}$$

combination of spherical harmonics and spinor

$$\kappa = -s(j+1/2)$$
$$j = l + s/2$$
$$s = +1, -1$$

insert Ψ into Dirac equation

$$\frac{dg_\kappa}{dr} = -\frac{(\kappa+1)}{r} g_\kappa + 2\mathrm{M}\mathrm{c} f_\kappa$$
$$\frac{df_\kappa}{dr} = \frac{1}{c}(V-E) g_\kappa + \frac{\kappa-1}{r} f_\kappa$$

Radial Dirac equation

substitute f from first eq. into the second eq.

$$-\frac{1}{2\mathrm{M}}\left[\frac{d^2 g_\kappa}{dr^2} + \frac{2}{r}\frac{dg_\kappa}{dr} - \frac{l(l+1)}{r^2} g_\kappa\right] - \frac{dV}{dr}\frac{dg_\kappa}{dr}\frac{1}{4\mathrm{M}^2 c^2} + V g_\kappa - \frac{\kappa-1}{r}\frac{dV}{dr}\frac{g_\kappa}{4\mathrm{M}^2 c^2} = E g_\kappa$$

scalar relativistic approximation

spin-orbit coupling

κ dependent term, for a constant *l*, κ depends on the sign of *s*

Implementation, core electrons

Core electrons are calculated with spin-compensated Dirac equation

for spin polarized potential – spin up and down are calculated separately, the density is averaged according to the occupation number specified in *case.inc* file

$1s^{1/2}$

$2p^{1/2}$

$2p^{3/2}$

```
   9 0.00
1,-1,2        ( N,KAPPA,OCCUP)
2,-1,2        ( N,KAPPA,OCCUP)
2, 1,2        ( N,KAPPA,OCCUP)
2,-2,4        ( N,KAPPA,OCCUP)
3,-1,2        ( N,KAPPA,OCCUP)
3, 1,2        ( N,KAPPA,OCCUP)
3,-2,4        ( N,KAPPA,OCCUP)
3, 2,4        ( N,KAPPA,OCCUP)
3,-3,6        ( N,KAPPA,OCCUP)
```

case.inc for Ru atom

		j=l+s/2		κ=-s(j+½)		occupation	
	l	s=-1	s=+1	s=-1	s=+1	s=-1	s=+1
s	0		1/2		-1		2
p	1	1/2	3/2	1	-2	2	4
d	2	3/2	5/2	2	-3	4	6
f	3	5/2	7/2	3	-4	6	8

Implementation, valence electrons

Valence electrons inside atomic spheres are treated within scalar relativistic approximation (*Koelling and Harmon, J. Phys C 1977*) if *RELA* is specified in struct file

$$\frac{dP}{dr} - \frac{1}{r} P = 2\mathrm{McQ}$$

$$\frac{dQ}{dr} - \frac{1}{r} Q = \left[l\frac{(l+1)}{2\mathrm{Mcr}^2} + \frac{(V-\epsilon)}{c} \right] P$$

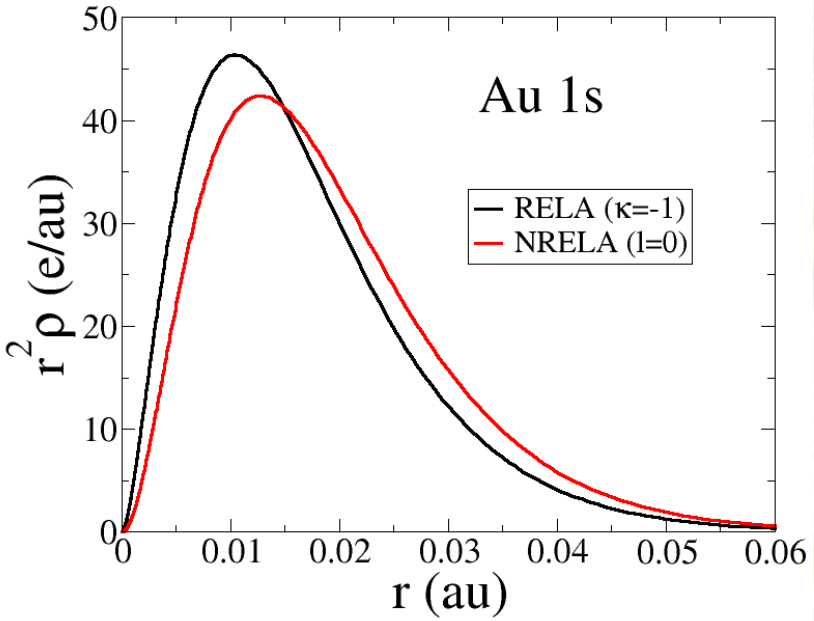
radial equations of Koelling and Harmon (spherical potential)

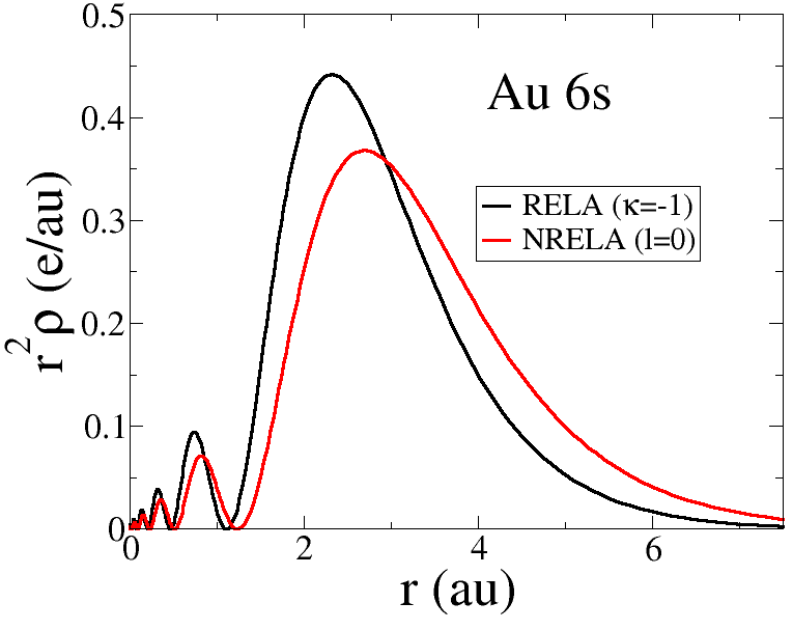
- no κ dependency of the wave function, (l,m,s) are good quantum numbers
- all relativistic effects are included except SOC
- small component enters normalization and calculation of charge inside spheres
- augmentation with large component only
- SOC can be included in "second variation"

Valence electrons in interstitial region are treated classically

Effects of *RELA*

- contraction of Au s orbitals





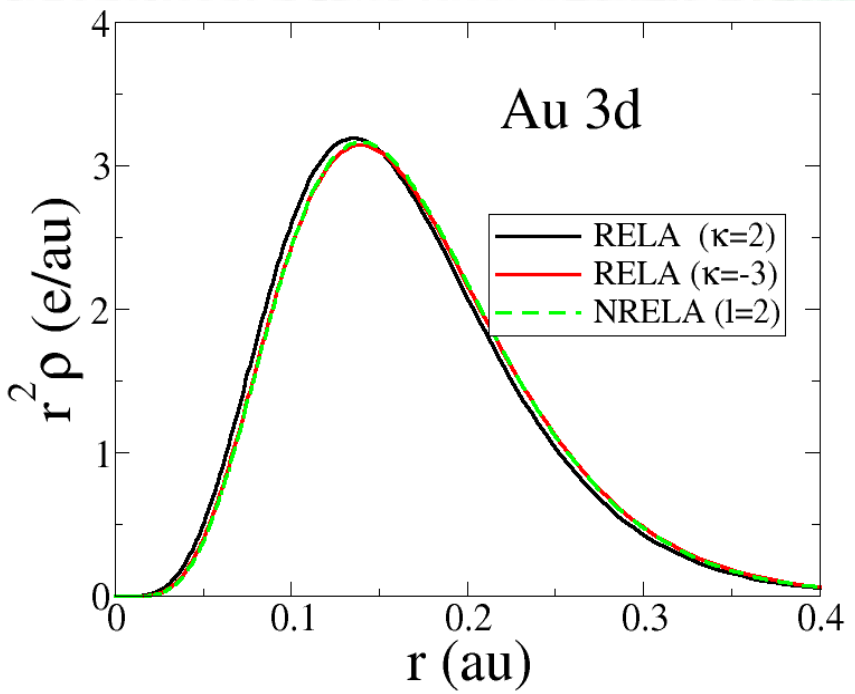
- 1s contracts due to relativistic mass enhancement
- 2s - 6s contract due to orthogonality to 1s

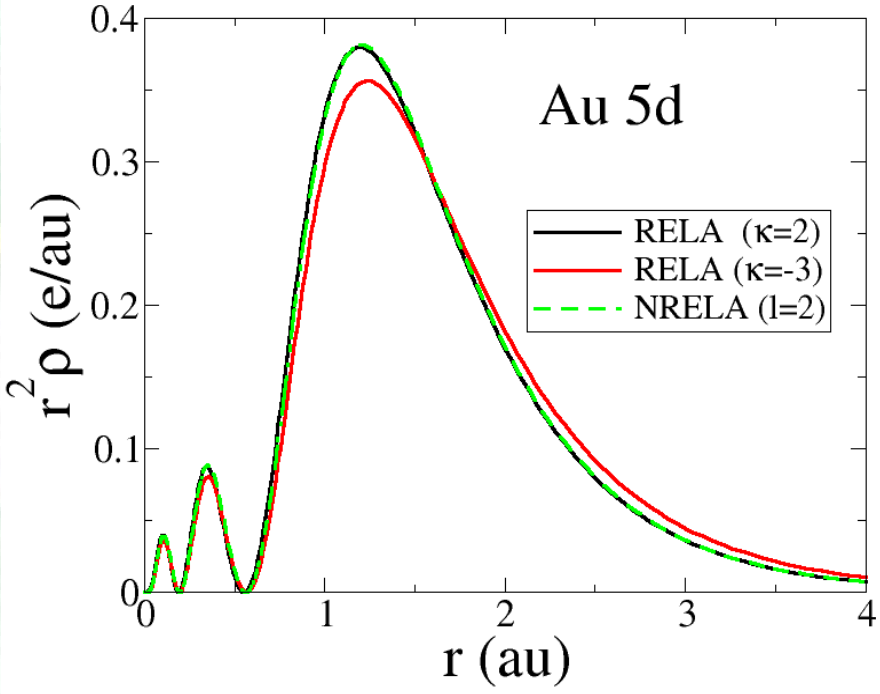
$$M = m/\sqrt{1-(v/c)^2}$$

v is proportional to Z: Gold: Z = 79;M = 1.2 m

Effects of *RELA*

- orbital expansion of Au d orbitals





- Higher l-quantum number states expand due to better shielding of core charge from contracted s-states (effect is larger for higher states).

Spin orbit-coupling

$$H_{MT}\,\phi_{lms} = \epsilon\,\phi_{lms} + H_{SO}\,\phi_{lms}$$

$$H_{SO} = \frac{1}{2\mathrm{Mc}^2}\,\frac{1}{r^2}\,\frac{dV_{MT}(r)}{dr}\begin{bmatrix} P\,\sigma\cdot L\,Y_{lm}\,\chi_s \\ 0 \end{bmatrix}$$

- SOC is active only inside atomic spheres, only spherical potential (V_{MT}) is taken into account, in the polarized case spin up and down parts are averaged
- eigenstates are not pure spin states, SOC mixes up and down spin states
- off-diagonal term of the spin density matrix is ignored, it means that in each SCF cycle the magnetization is projected on the chosen direction (from *case.inso*)

- SOC is added in a second variation (*lapwso*):

first diagonalization (lapw1)

$$H_1\psi_1 = \varepsilon_1\psi_1$$

$$\left(H_1 + H_{SO}\right)\psi = \varepsilon\,\psi$$

second diagonalization (lapwso)

second eq. is expanded in the basis of first eigenvectors

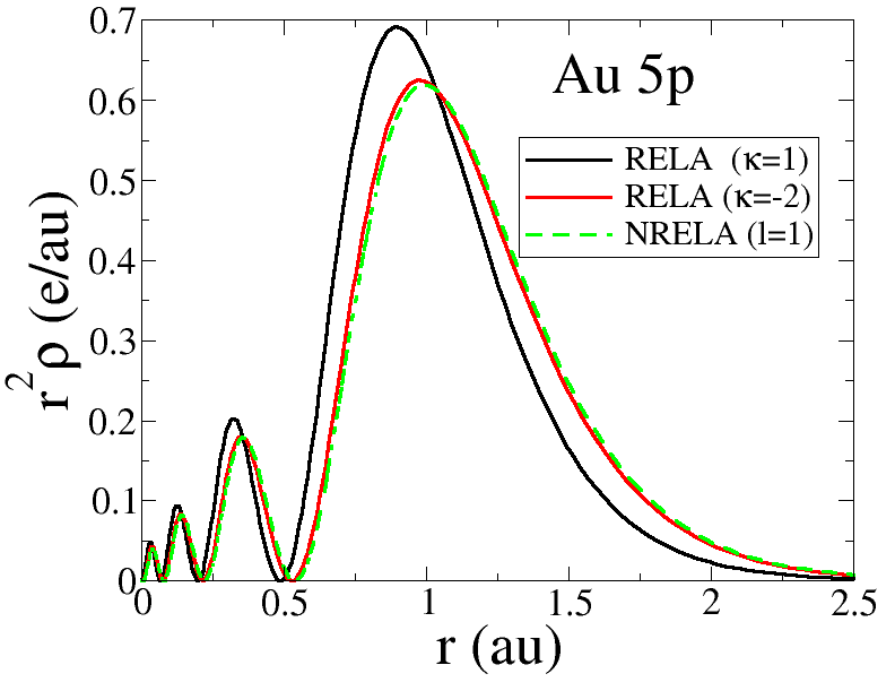
$$\sum_i^N \left(\delta_{ij}\,\varepsilon_1^j + \left\langle \psi_1^j \middle| H_{SO} \middle| \psi_1^i \right\rangle\right)\left\langle \psi_1^i \middle| \psi \right\rangle = \varepsilon \left\langle \psi_1^j \middle| \psi \right\rangle$$

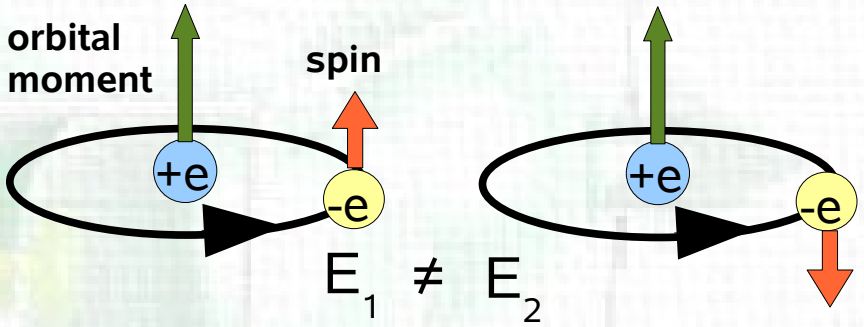
sum includes both up/down spin states

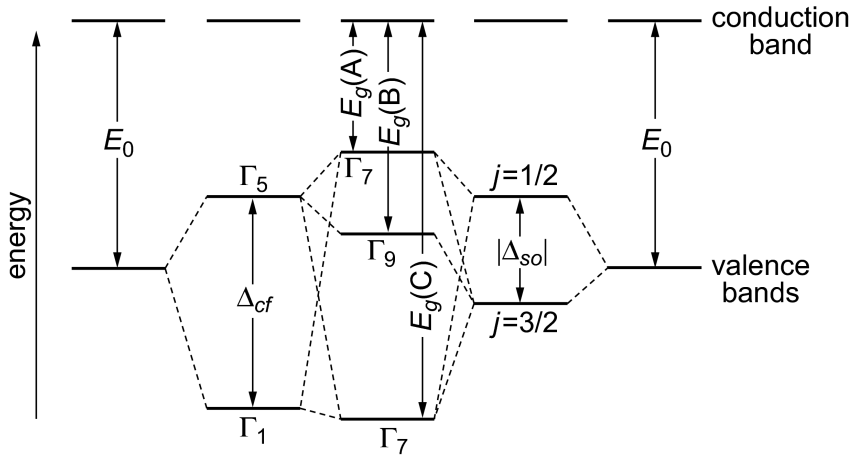
N is much smaller then the basis size in lapw1!!

SOC splitting of p states

- Spin Orbit splitting of l-quantum number.







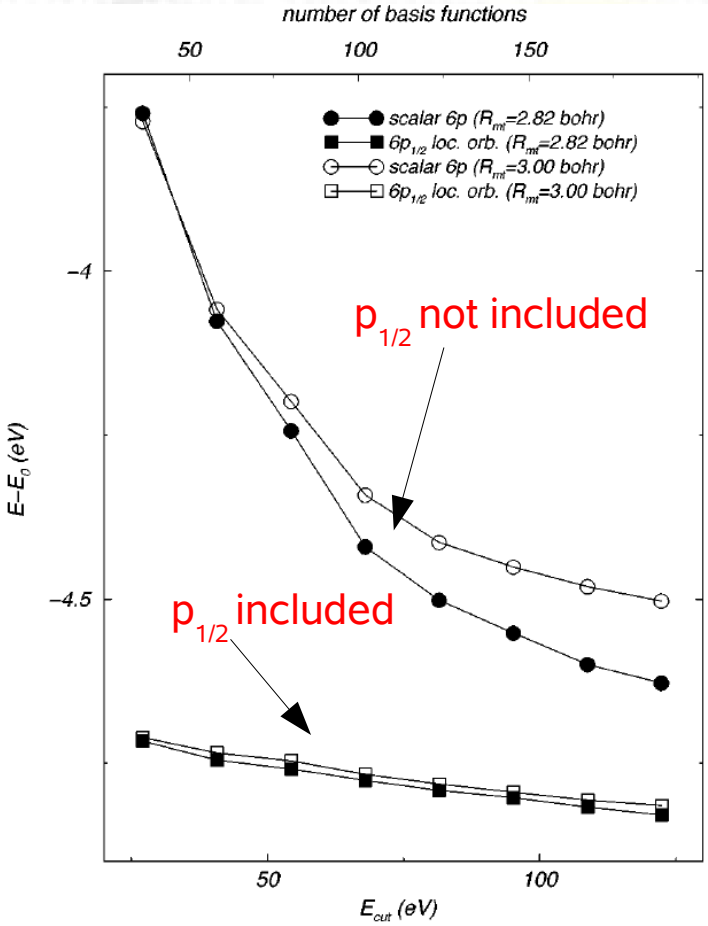
band edge at Γ in ZnO

- $p_{1/2}$ (κ=1), markedly different behavior than non-relativistic p-state (density is diverging at nucleus), thus there is a need for extra basis function ($p_{1/2}$ orbital)

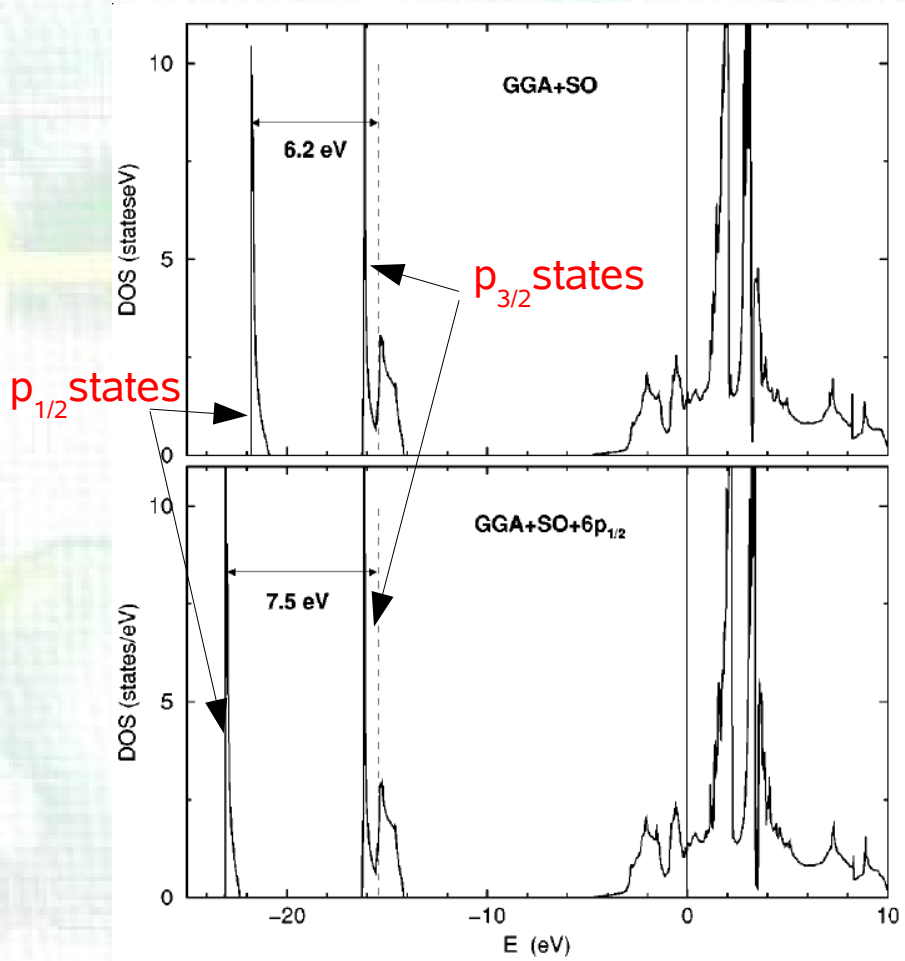
$p_{1/2}$ orbitals

Electronic structure of fcc Th, SOC with $6p_{1/2}$ local orbital

PRB, 64, 1503102 (2001)

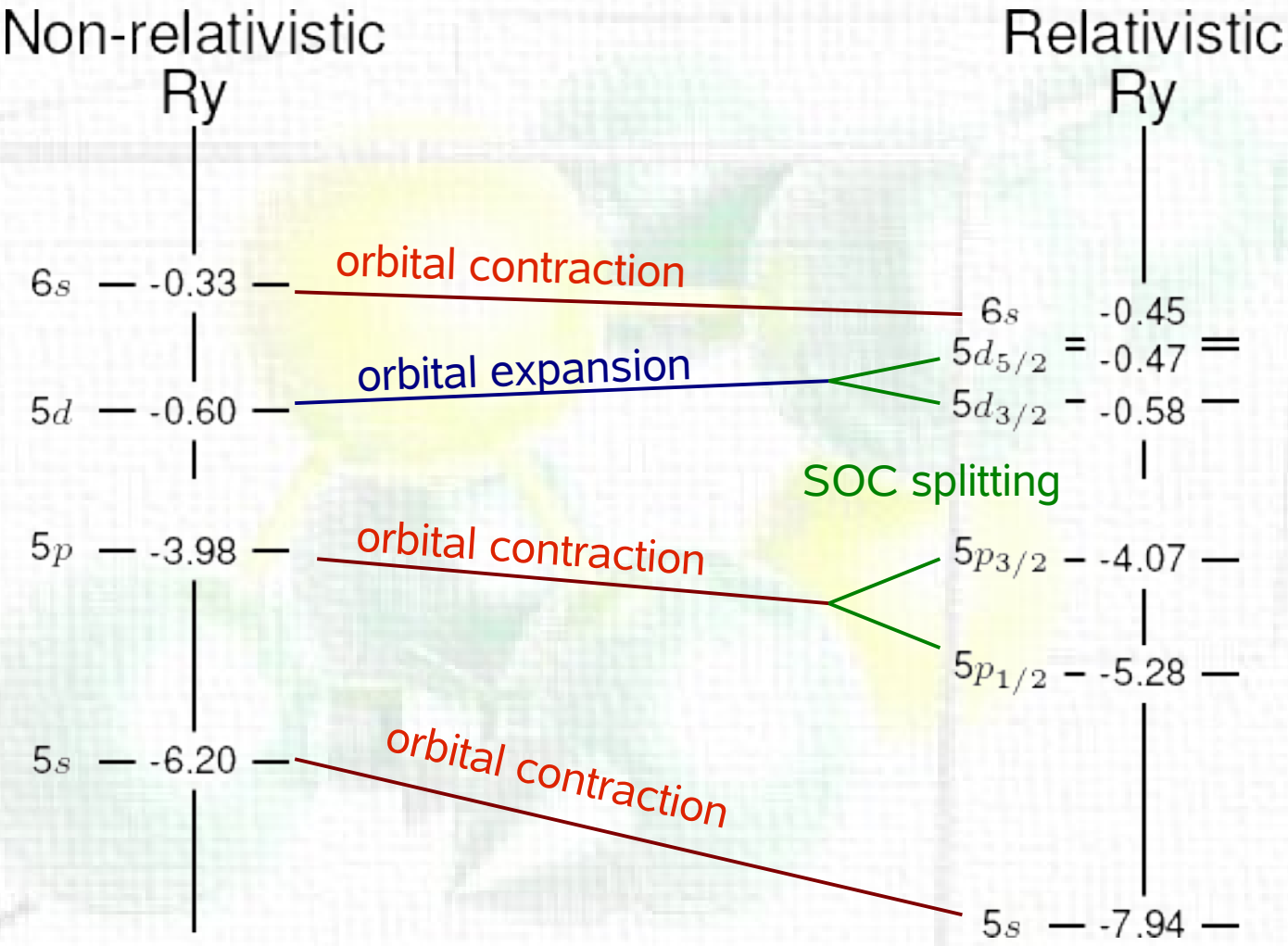


energy vs. basis size



DOS with and without $p_{1/2}$

Au atomic spectra

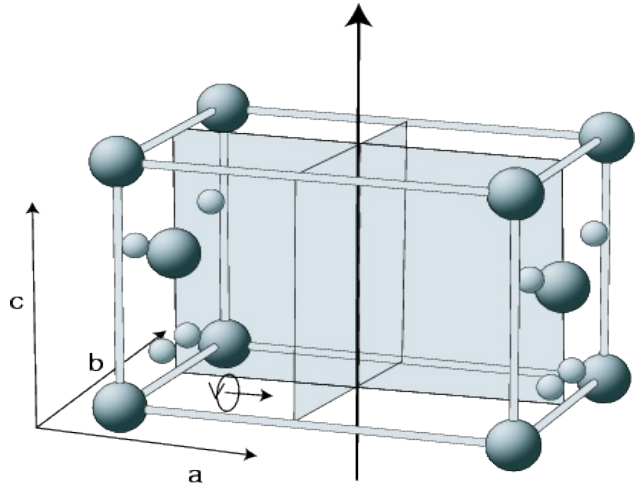


SOC in magnetic systems

- **SOC couples magnetic moment to the lattice**
  - direction of the exchange field matters (input in `case.inso`)
- **symmetry operations acts in real and spin space**
  - number of symmetry operations may be reduced (reflections act differently on spins than on positions)
  - time inversion is not symmetry operation (do not add an inversion for k-list)
  - *initso_lapw* (must be executed) detects new symmetry setting

direction of magnetization

sym. operation	[100]	[010]	[001]	[110]
1	A	A	A	A
m_a	A	B	B	-
m_b	B	A	B	-
2_c	B	B	A	B



SOC in Wien2k

- run(sp)_lapw -so script:

```
x lapw1          (increase E-max for more eigenvectors in second diag.)
x lapwso         (second diagonalization)
x lapw2    so    (SOC ALWAYS needs complex lapw2 version)
```

- `case.inso` file:

```
WFFIL
4  1  0                    llmax,ipr,kpot
-10.0000   1.50000         emin,emax (output energy window)
 0.  0.  1.                direction of magnetization (lattice vectors)
1                          number of atoms for which RLO is added
2   -0.97      0.005       atom number,e-lo,de (case.in1), repeat NX times
0 0 0 0 0                  number of atoms for which SO is switched off; list of atoms
```

$p_{1/2}$ orbitals, use with caution !!

Pauli Hamiltonian

$$H_P = -\frac{\hbar}{2m}\nabla^2 + V_{ef} + \mu_B \vec{\sigma}\cdot\vec{B}_{ef} + \zeta(\vec{\sigma}\cdot\vec{l}) \ldots$$

- 2x2 matrix in spin space, due to Pauli spin operators
- wave function is a 2-component vector (spinor)

spin up component

$$H_P \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \varepsilon \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$$

spin down component

Pauli matrices:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Pauli Hamiltonian

$$H_P = -\frac{\hbar}{2m}\nabla^2 + V_{ef} + \mu_B \vec{\sigma}\cdot\vec{B}_{ef} + \zeta(\vec{\sigma}\cdot\vec{l})\ldots$$

electrostatic potential

magnetic field

spin-orbit coup.

$$V_{ef} = V_{ext} + V_H + V_{xc}$$

Hartee term

exchange-correlation potential

$$B_{ef} = B_{ext} + B_{xc}$$

exchange-correlation field

- exchange-correlation potential V_{xc} and magnetic field B_{xc} are defined within DFT LDA or GGA

Exchange and correlation

- from DFT LDA exchange-correlation energy:

$$E_{xc}(n,\vec{m}) = \int n\,\epsilon_{xc}(n,\vec{m})\,dr^3$$

local function of n and m

- definition of V_{cx} and B_{xc}:

$$V_{xc} = \frac{\partial E_{xc}(n,\vec{m})}{\partial n} \qquad \vec{B}_{xc} = \frac{\partial E_{xc}(n,\vec{m})}{\partial \vec{m}}$$

functional derivatives

- LDA expression for V_{cx} and B_{xc}:

B_{xc} and m are parallel

$$V_{xc} = \epsilon_{xc}(n,\vec{m}) + n\frac{\partial \epsilon_{xc}(n,\vec{m})}{\partial n}$$

$$\vec{B}_{xc} = n\frac{\partial \epsilon_{xc}(n,\vec{m})}{\partial m}\hat{m}$$

Non-collinear case

$$H_P = -\frac{\hbar}{2\mathrm{m}}\nabla^2 + V_{ef} + \mu_B \vec{\sigma}\cdot\vec{B}_{ef} + \zeta(\vec{\sigma}\cdot\vec{l})\ \ldots$$

- direction of magnetization vary in space
- spin-orbit coupling is present

$$\begin{pmatrix} -\frac{\hbar}{2\mathrm{m}}\nabla^2 + V_{ef} + \mu_B B_z + \ldots & \mu_B\left(B_x - iB_y\right) \\ \mu_B\left(B_x + iB_y\right) & -\frac{\hbar}{2\mathrm{m}}\nabla^2 + V_{ef} + \mu_B B_z + \ldots \end{pmatrix} \psi = \varepsilon\,\psi$$

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}, \quad \psi_1, \psi_2 \neq 0$$

- solutions are non-pure spinors
- non-collinear magnetic moments

Collinear case

$$H_P = -\frac{\hbar}{2m}\nabla^2 + V_{ef} + \mu_B \vec{\sigma}\cdot\vec{B}_{ef} + \cancel{\zeta(\vec{\sigma}\cdot\vec{l})} \ldots$$

- magnetization in Z direction, B_x and B_y=0
- spin-orbit coupling is not present

$$\begin{pmatrix} -\frac{\hbar}{2m}\nabla^2 + V_{ef} + \mu_B B_z + \ldots & 0 \\ 0 & -\frac{\hbar}{2m}\nabla^2 + V_{ef} + \mu_B B_z + \ldots \end{pmatrix} \psi = \varepsilon\,\psi$$

$$\psi_\uparrow = \begin{pmatrix} \psi_1 \\ 0 \end{pmatrix},\ \psi_\downarrow = \begin{pmatrix} 0 \\ \psi_2 \end{pmatrix},\quad \varepsilon_\uparrow \neq \varepsilon_\downarrow$$

- solutions are pure spinors
- collinear magnetic moments

Non-magnetic case

$$H_P = -\frac{\hbar}{2m}\nabla^2 + V_{ef} + \mu_B \vec{\sigma}\cdot\vec{B}_{ef} + \zeta(\vec{\sigma}\cdot\vec{l})\ldots$$

- no magnetization present, B_x, B_y and B_z=0
- spin-orbit coupling is not present

$$\begin{pmatrix} -\frac{\hbar}{2m}\nabla^2 + V_{ef} + \ldots & 0 \\ 0 & -\frac{\hbar}{2m}\nabla^2 + V_{ef} + \ldots \end{pmatrix} \psi = \varepsilon\,\psi$$

$$\psi_\uparrow = \begin{pmatrix} \psi \\ 0 \end{pmatrix},\ \psi_\downarrow = \begin{pmatrix} 0 \\ \psi \end{pmatrix},\ \ \varepsilon_\uparrow = \varepsilon_\downarrow$$

- solutions are pure spinors
- degenerate spin solutions

Magnetism and Wien2k

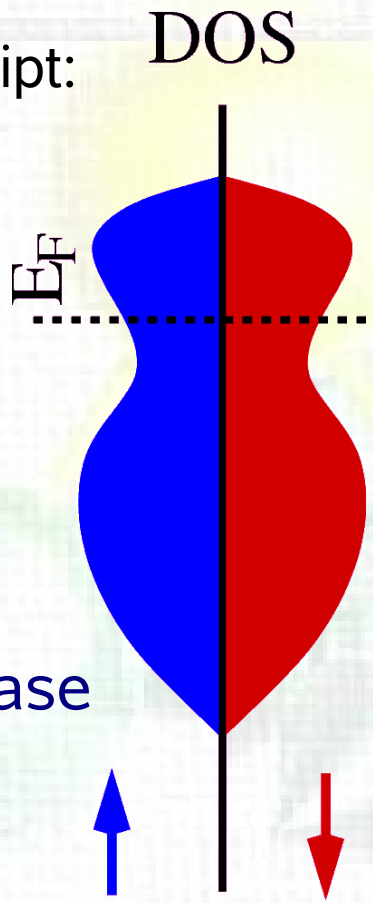
- Wien2k can only handle collinear or non-magnetic cases

run_lapw script:

```
x lapw0
x lapw1
x lapw2
x lcore
x mixer
```

non-magnetic case

$$m = n_\uparrow - n_\downarrow = 0$$

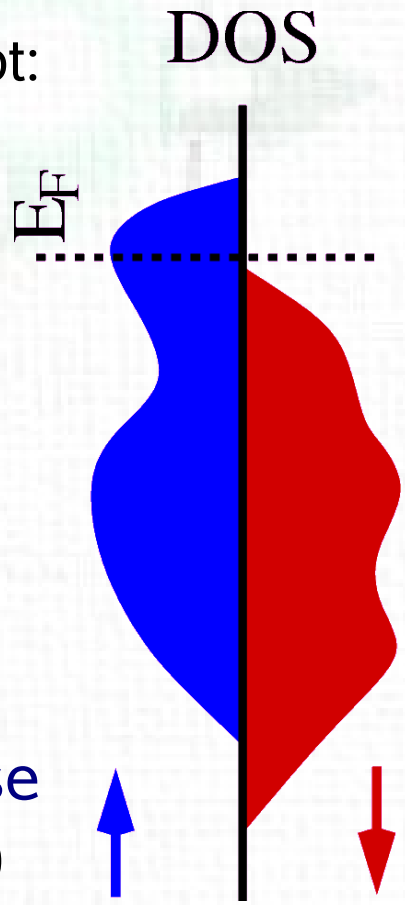


runsp_lapw script:

```
x lapw0
x lapw1 -up
x lapw1 -dn
x lapw2 -up
x lapw2 -dn
x lcore -up
x lcore -dn
x mixer
```

magnetic case

$$m = n_\uparrow - n_\downarrow \neq 0$$



Magnetism and Wien2k

- in NCM case both part of the spinor are treated simultaneously

runncm_lapw script:

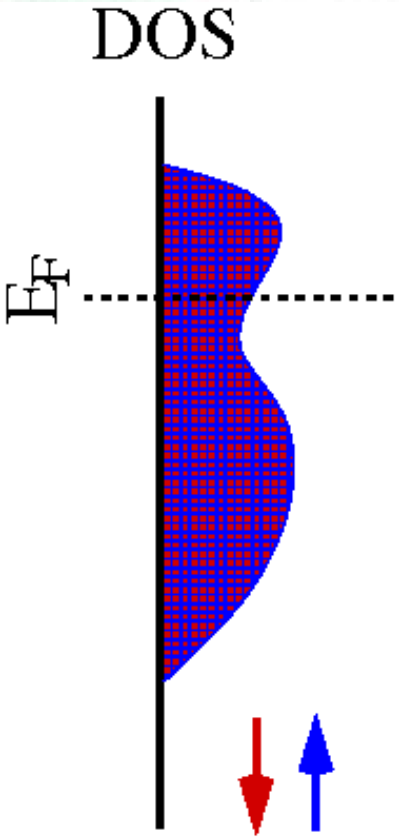
```
xncm lapw0
xncm lapw1
xncm lapw2
xncm lcore
xncm mixer
```

$$\hat{n} = \sum_{nk} \begin{pmatrix} \psi_{\uparrow nk} \\ \psi_{\downarrow nk} \end{pmatrix}^{*} \left(\psi_{\uparrow nk} \psi_{\downarrow nk} \right)$$

$$m_z = n_{\uparrow\uparrow} - n_{\downarrow\downarrow} \neq 0$$

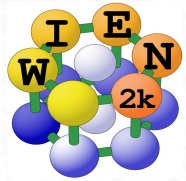
$$m_x = \frac{1}{2}\left(n_{\uparrow\downarrow} + n_{\downarrow\uparrow} \right) \neq 0$$

$$m_x = i\frac{1}{2}\left(n_{\uparrow\downarrow} - n_{\downarrow\uparrow} \right) \neq 0$$



NCM case

Non-collinear calculations



- **in the case of non-collinear arrangement of spin moment WienNCM (Wien2k clone) has to be used**
  - code is based on Wien2k (available for Wien2k users)
  - structure and usage philosophy similar to Wien2k
  - independent source tree, independent installation
- **WienNCM properties:**
  - real and spin symmetry (simplifies SCF, less k-points)
  - constrained or unconstrained calculations (optimizes magnetic moments)
  - SOC is applied in the first variational step, LDA+U
  - spin spirals are available

WienNCM - implementation

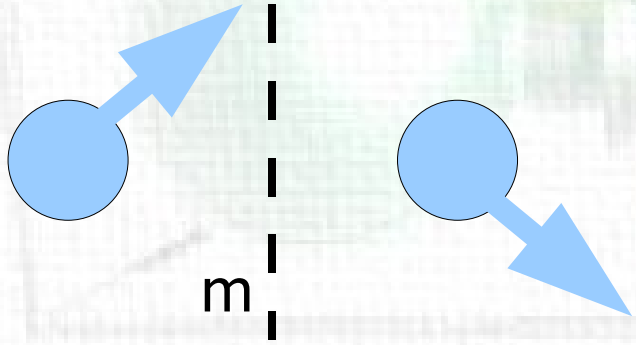
- **basis set – mixed spinors** (Yamagami, PRB (2000); Kurtz PRB (2001)

interstities: $\varphi_{\vec{G}\sigma} = e^{i(\vec{G}+\vec{k})\cdot\vec{r}}\chi_\sigma \qquad \chi_\sigma = \begin{pmatrix}1\\0\end{pmatrix}, \begin{pmatrix}0\\1\end{pmatrix}$

spheres: $\varphi^{APW}_{\vec{G}\sigma} = \sum_{\sigma_\alpha}\sum_{lm}\left(A^{\vec{G}\sigma\sigma_\alpha}_{lm}u^{\sigma_\alpha}_l + B^{\vec{G}\sigma\sigma_\alpha}_{lm}\dot{u}^{\sigma_\alpha}_l\right)Y_{lm}\chi_{\sigma_\alpha}$

$\varphi^{APW}_{\vec{G}\sigma_\alpha} = \left(A^{\vec{G}\sigma\sigma_\alpha}_{lm}u^{\sigma_\alpha}_l + B^{\vec{G}\sigma\sigma_\alpha}_{lm}\dot{u}^{\sigma_\alpha}_l + C^{\vec{G}\sigma\sigma_\alpha}_{lm}u^{\sigma_\alpha}_{2,l}\right)Y_{lm}\chi_{\sigma_\alpha}$

- **real and spin space parts of symmetry op. are not independent**



- symmetry treatment like for SOC always on
- tool for setting up magnetic configuration
- concept of magnetic and non-magnetic atoms

WienNCM implementation

- Hamiltonian inside spheres:

$$\hat{H} = -\frac{\hbar}{2\mathrm{m}}\nabla^2 + \hat{V} + \hat{H}_{so} + \hat{H}_{orb} + \hat{H}_c$$

AMA and full NC calculation

$$\hat{V}_{FULL} = \begin{pmatrix} V_{\uparrow\uparrow} & V_{\downarrow\uparrow} \\ V_{\uparrow\downarrow} & V_{\downarrow\downarrow} \end{pmatrix} \qquad \hat{V}_{AMA} = \begin{pmatrix} V_{\uparrow\uparrow} & 0 \\ 0 & V_{\downarrow\downarrow} \end{pmatrix}$$

SOC in first diagonalization

$$\hat{H}_{so} = \xi\,\vec{\sigma}\cdot\vec{l} = \xi \begin{pmatrix} \hat{l}_z & \hat{l}_x - i\,\hat{l}_y \\ \hat{l}_x + i\,\hat{l}_y & -\hat{l}_z \end{pmatrix}$$

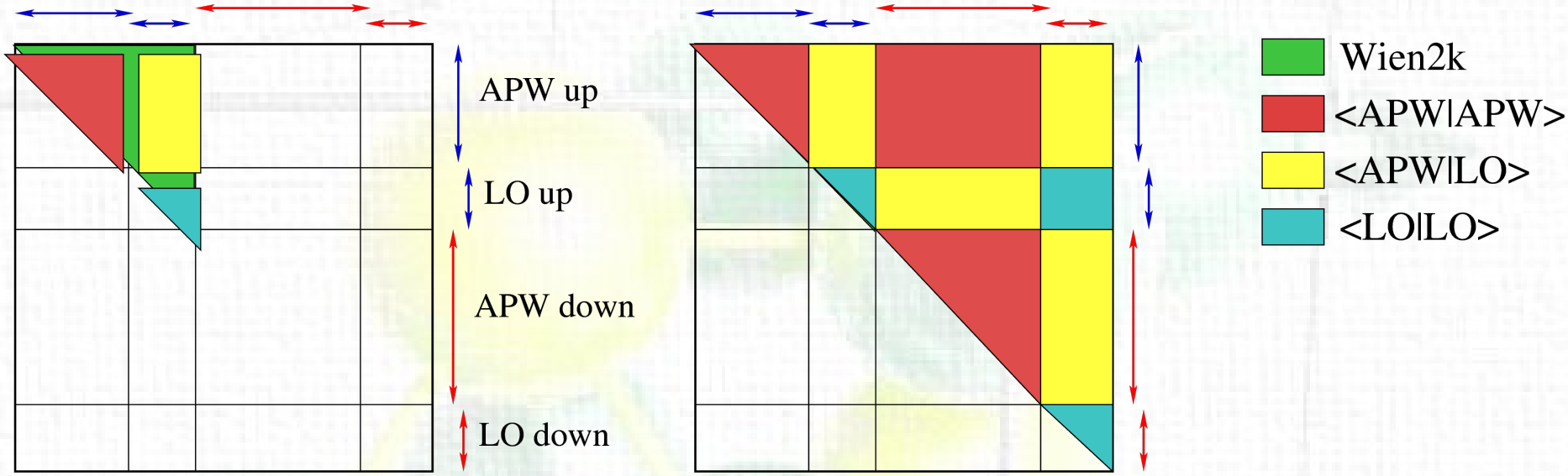
diagonal orbital field

$$\hat{H}_{orb} = \sum_{m\,m'} \begin{pmatrix} |m\rangle V^{\uparrow}_{mm'} \langle m'| & 0 \\ 0 & |m\rangle V^{\downarrow}_{mm'} \langle m'| \end{pmatrix}$$

constraining field

$$\hat{H}_c = \mu_B\,\vec{\sigma}\cdot\vec{B}_c = \begin{pmatrix} 0 & \mu_B\left(B_{cx} - iB_{cy}\right) \\ \mu_B\left(B_{cx} + iB_{cy}\right) & 0 \end{pmatrix}$$

NCM Hamiltonian

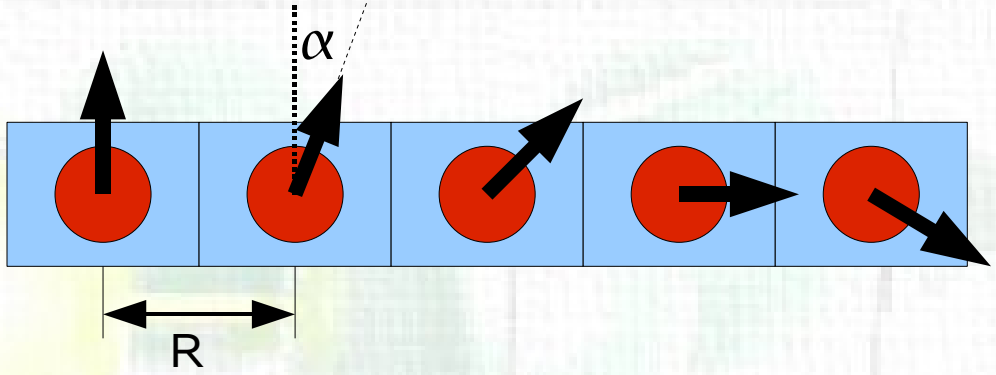


- size of the Hamiltonian/overlap matrix is doubled comparing to Wien2k
- computational cost increases !!!

WienNCM – spin spirals

- transverse spin wave

$$\alpha = \vec{R} \cdot \vec{q}$$



$$\vec{m}^n = m\left(\cos(\vec{q}\cdot\vec{R}^n), \sin(\vec{q}\cdot\vec{R}^n)\sin(\theta), \cos(\theta)\right)$$

- spin-spiral is defined by a vector **q** given in reciprocal space and,
- an angle **Θ** between magnetic moment and rotation axis
- rotation axis is arbitrary (no SOC), hard-coded as Z

Translational symmetry is lost !!!

WienNCM – spin spirals

- generalized Bloch theorem
  - generalized translations are symmetry operation of the H

$$T_n = \left\{ -\vec{q}\cdot\vec{R}_n \middle| \epsilon \middle| \vec{R}_n \right\}$$

$$T_n^{\dagger} H(\vec{r}) T_n = U^{\dagger}(-\vec{q}\cdot\vec{R}_n) H(\vec{r}+\vec{R}_n) U(-\vec{q}\cdot\vec{R}_n)$$

group of T_n is Abelian

$$\psi_{\vec{k}}(\vec{r}) = e^{i(\vec{k}\cdot\vec{r})} \begin{pmatrix} e^{\frac{i\vec{q}\cdot\vec{r}}{2}} u^{\uparrow}(\vec{r}) \\ e^{\frac{-i\vec{q}\cdot\vec{r}}{2}} u^{\downarrow}(\vec{r}) \end{pmatrix}$$

$$T_n \psi_{\vec{k}}(\vec{r}) = U(-\vec{q}\cdot\vec{R}) \psi_{\vec{k}}(\vec{r}+\vec{R}) = e^{i\vec{k}\cdot\vec{r}} \psi_{\vec{k}}(\vec{r})$$

1-d representations, Bloch Theorem

- efficient way for calculation of spin waves, only one unit cell is necessary for even incommensurate wave

Usage

- generate atomic and magnetic structure

  1) create atomic structure

  2) create magnetic structure

     need to specify only directions of magnetic atoms

     use utility programs: **ncmsymmetry**, **polarangles**, ...

- run **initncm** (initialization script)
- **xncm** (WienNCM version of **x** script)
- **runncm** (WienNCM version of **run** script)
- find more in manual

WienNCM – case.inncm file

- `case.inncm` – magnetic structure file

```
FULL
  0.000   0.000   0.000
 45.00000   54.73561    0
135.00000  125.26439    0
-135.00000   54.73561    0
 -45.00000  125.26439    0
 45.00000   54.73561    0
 45.00000   54.73561    0
315.00000  125.26439    0
315.00000  125.26439    0
135.00000  125.26439    0
135.00000  125.26439    0
225.00000   54.73561    0
225.00000   54.73561    0
  0.50000
```

q spiral vector

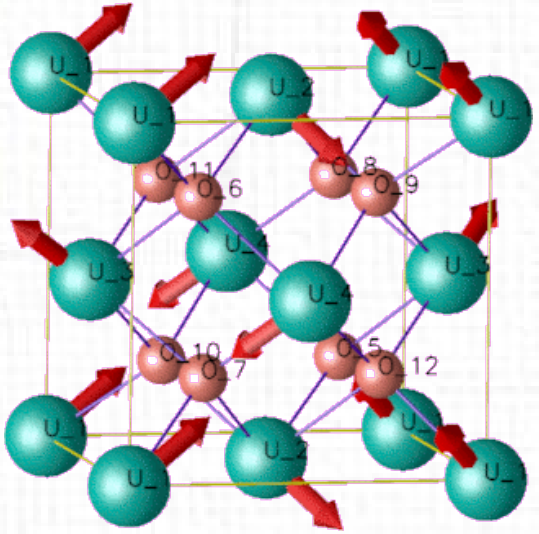
polar angles of mm

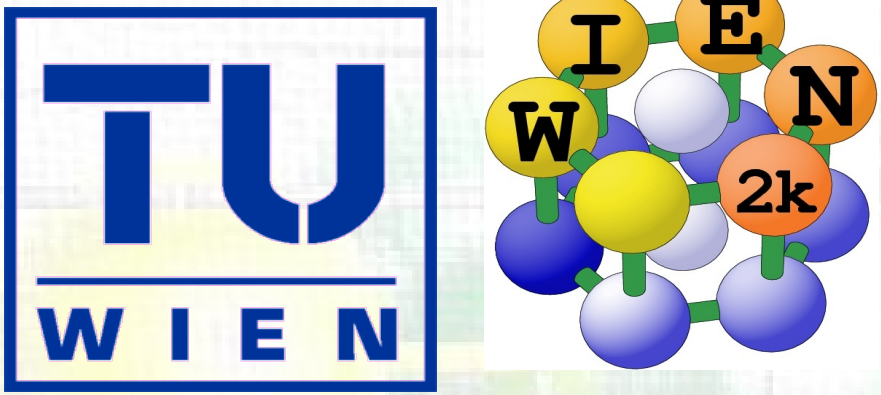
optimization switch

U, magnetic atoms

O, non-magnetic atoms

mixing for constraining field

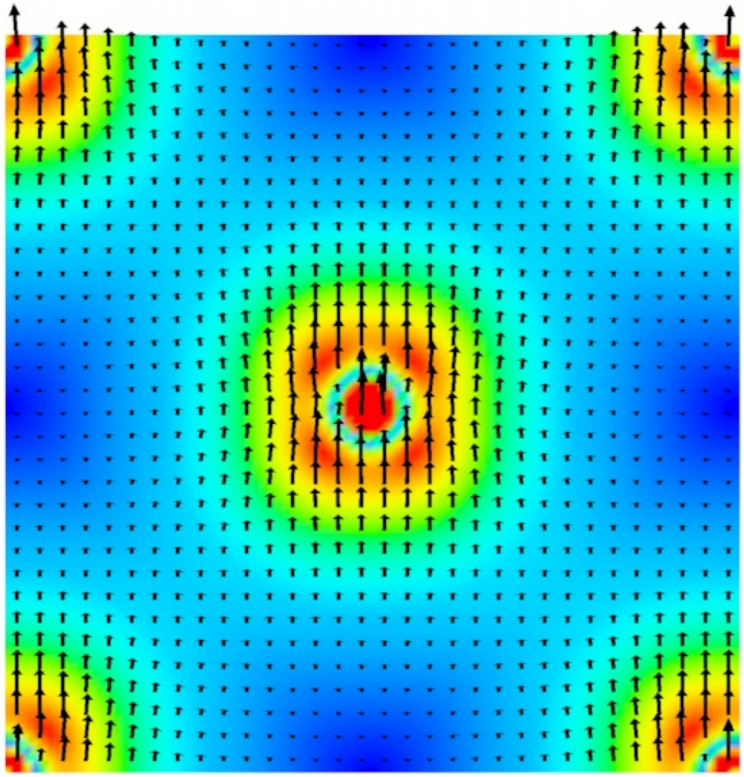




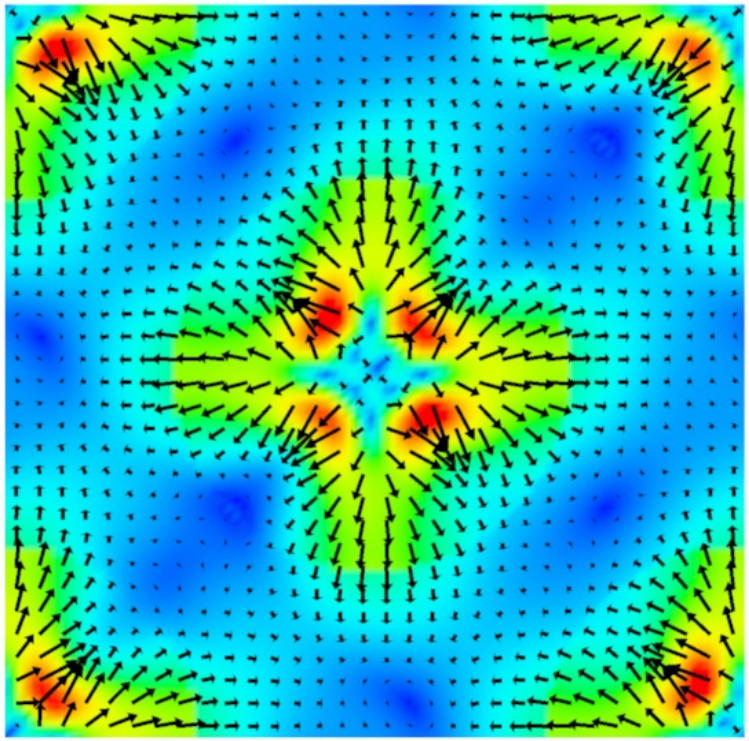
Thank you for your attention

Intra-atomic non collinearity in Pu

- magnetization density (colors encode magnitude, arrows – direction and magnitude)
- runncm -so -orb

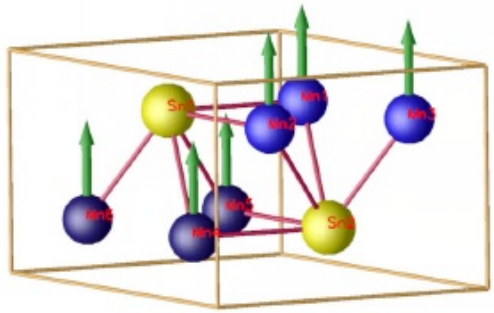


plane x=0

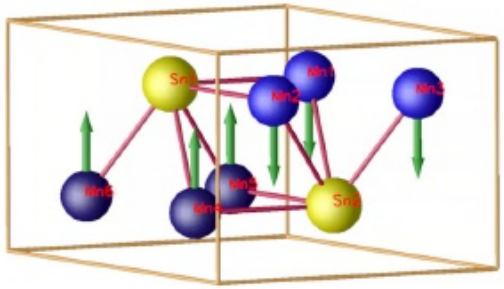


plane z=1/10

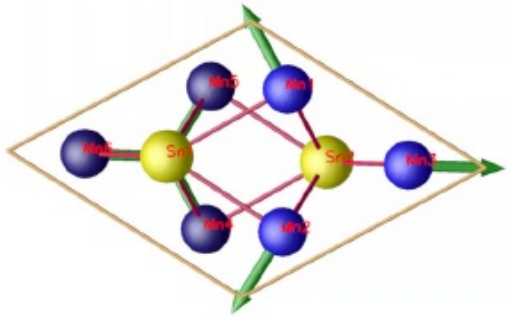
Magnetic structure of Mn_3Sn



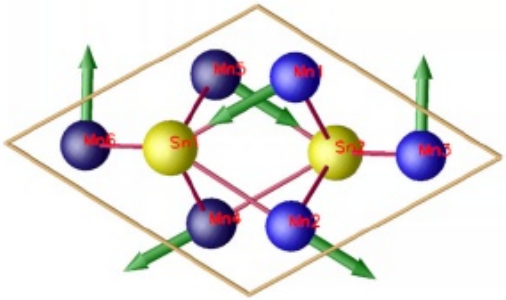
fm



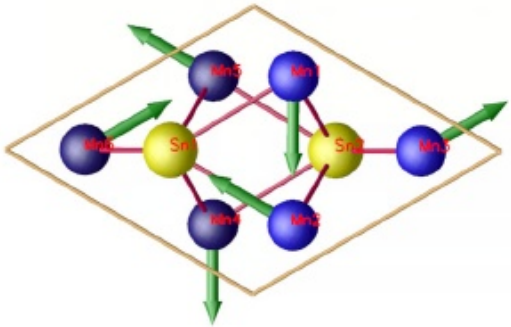
afm



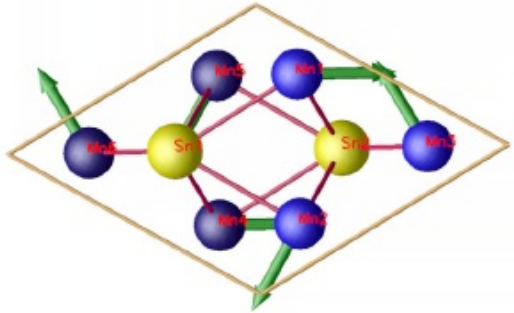
ncm 1



ncm 2



ncm 3



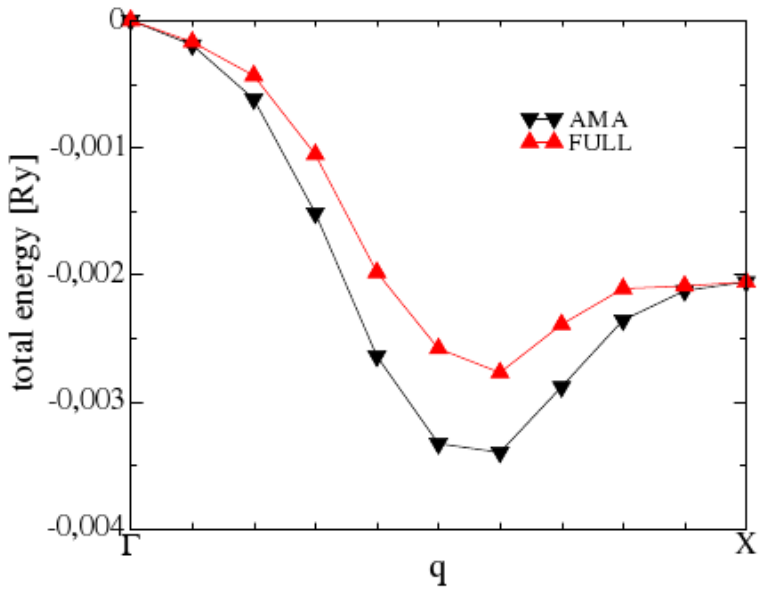
ncm 4

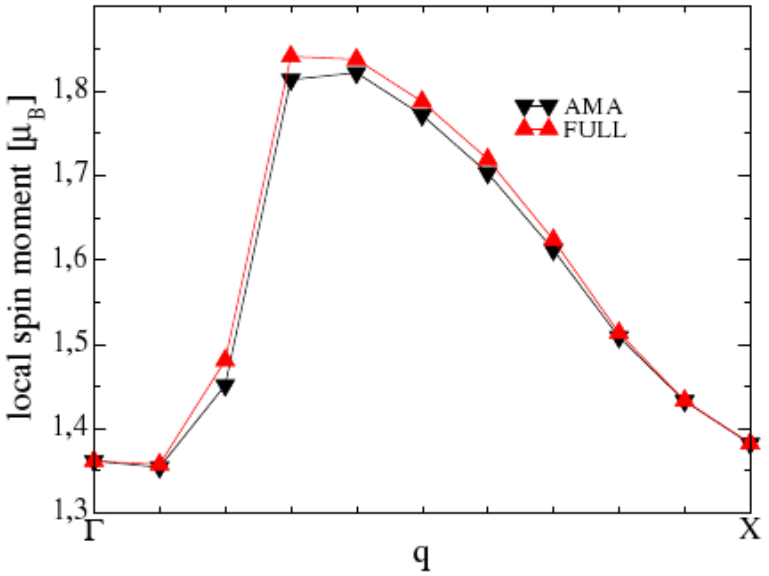
Mn_3Sn cd.

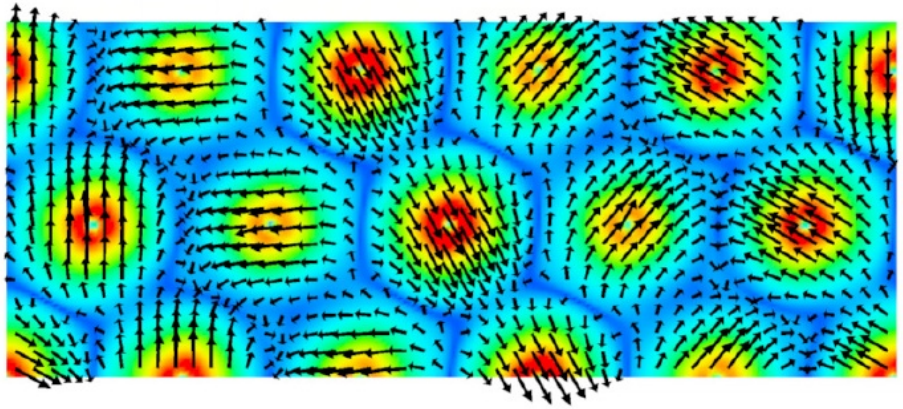
	so	fm	afm	ncm 1	ncm 2	ncm 3	ncm 4
$E_{fm} - E\ [Ry]$	-	0.0	0.0131	0.0444	0.0444	0.0444	0.0444
	+	0.0	0.0133	0.0441	0.0439	0.0444	0.0445
$M_s\ [\mu_B]$	-	3.012	2.684	3.037	3.037	3.037	3.037
	+	3.008	2.679	3.034	3.034	3.038	3.037
efg on Mn	-	-1.657	-2.111	-0.894	-0.894	-0.894	-0.894
$[10^{21}V/m^2]$	+	-1.661	-2.119	-0.892	-0.899	-0.891	-0.894
						-0.898	-0.881
hff on Mn	-	-309.9	-153.1	31.2	31.2	31.2	31.2
$[kGauss]$	+	-309.6	-152.9	31.1	31.5	31.5	30.9
						32.2	32.1

- in non-so case all ncm structures are symmetry equivalent
- with so ncm structures become inequivalent, additionally for ncm3 and ncm4 Mn_2 and Mn_5 are nolonger equivalent to the rest of Mn's

γ Fe, spin spiral



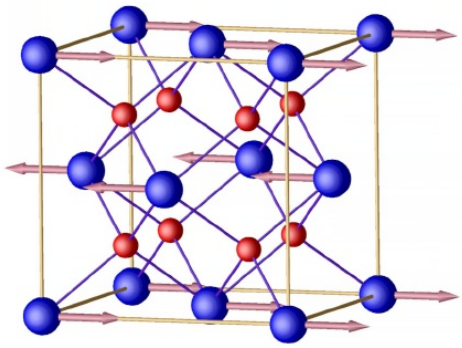




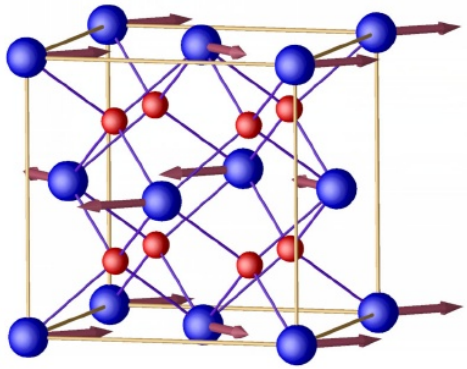
Spin density maps
for q = 0.6 (0-Γ, 1-X)

Magnetic structure of UO_2

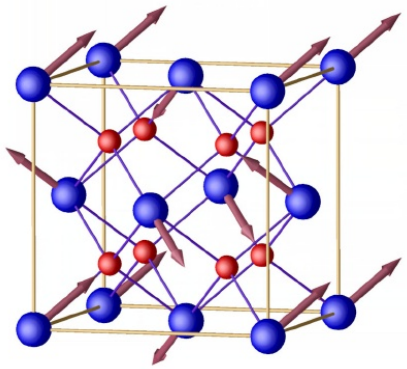
1-k

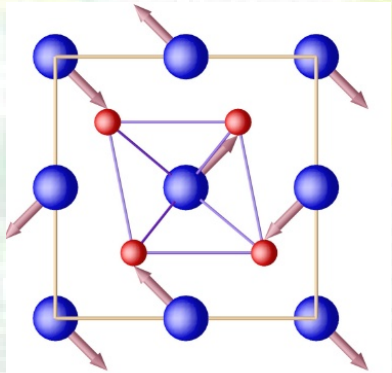


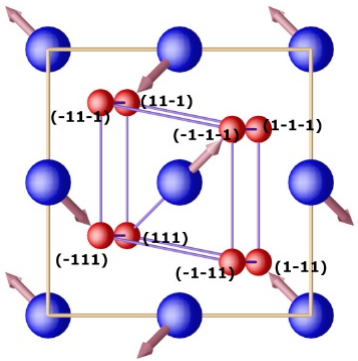
2-k



3-k







oxygen cage deformation

Magnetic structure of UO2

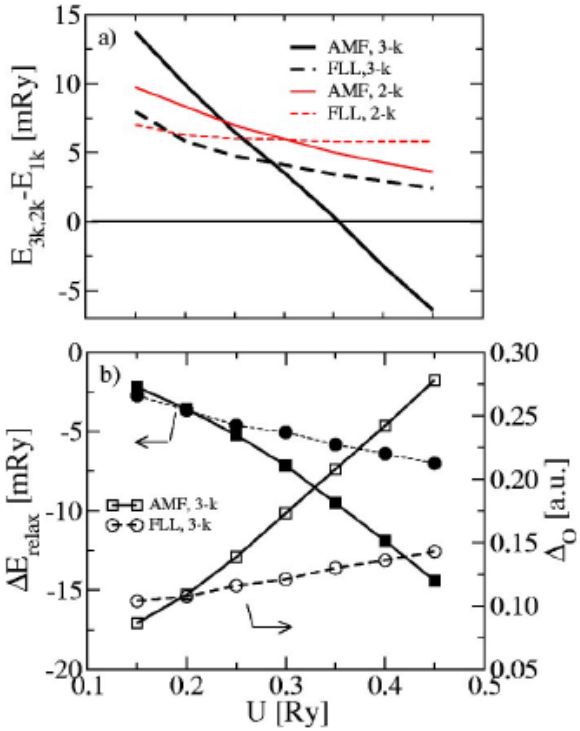


FIG. 1. (a) Total-energy differences (per four UO_2) between noncollinear and collinear structures vs the effective Coulomb interaction U. (b) Energy gain E_{relax} by relaxing the oxygen positions (closed symbols, left scale) and equilibrium oxygen displacements Δ_O from the ideal fluorite position calculated for the 3-**k** magnetic ordering (open symbols, right scale). The squares and circles are AMF and FLL-DCC calculations, respectively.

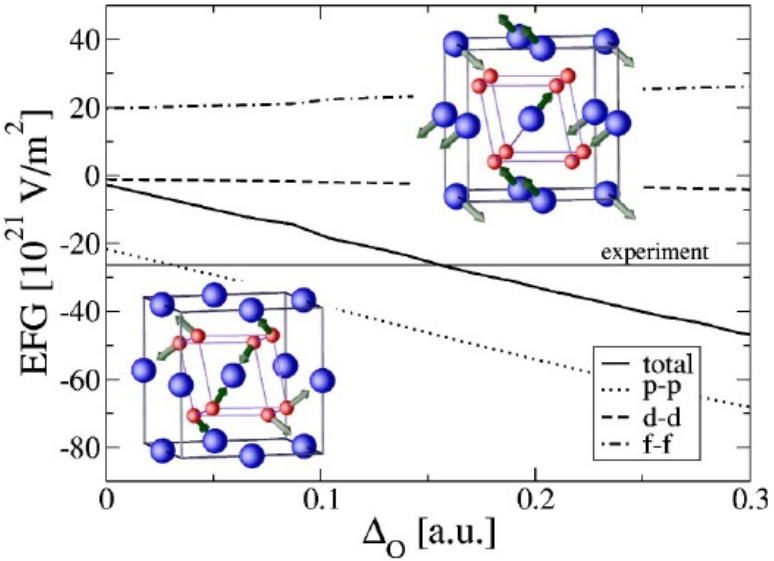


FIG. 2. Total U-EFG for the 3-**k** structure and its main angular contributions: p-p, d-d, and f-f as a function of O displacement. The s-d and p-f contributions are negligible. The upper inset presents the magnetic moments on U (large spheres) and the lower one the directions of oxygen displacements (small spheres).

R. Laskowski, et al PRB 69, 140408R 2004

Magnetic ground state Eu

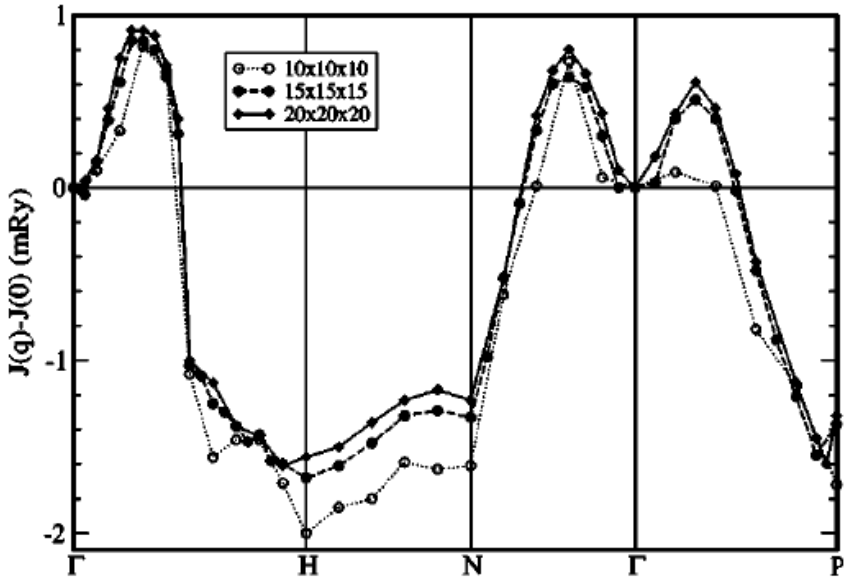


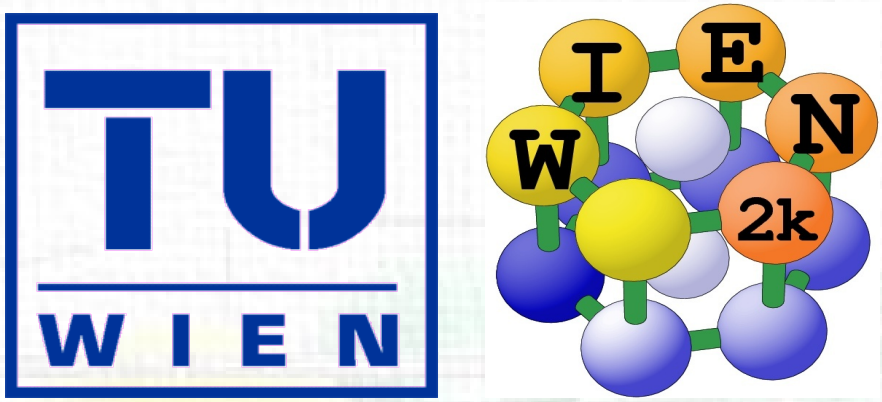
FIG. 2. The **q**-dependent exchange parameter calculated using the spin-spiral approach. Comparison of the results for different k-point samplings indicates that the $15 \times 15 \times 15$ mesh is reasonably well converged.

$$E(\mathbf{q}) = \sin^2(\theta)[J(\mathbf{q}) - J(0)] + J(0) + E_0$$

$$k_B T_N^{MF} = \frac{2}{3} J(\mathbf{Q})$$

$$(k_B T_N^{RPA})^{-1} = \frac{3}{4}\frac{1}{N}\sum_{\mathbf{q}} \left\{ [J(\mathbf{Q}) - J(\mathbf{q})]^{-1} + \left[J(\mathbf{Q}) - \frac{1}{2} J(\mathbf{q}+\mathbf{Q}) - \frac{1}{2} J(\mathbf{q}-\mathbf{Q}) \right]^{-1} \right\}$$

Kuneš et. al. PRB 70, 174415 (2004)



Thank you for your attention