Magnetism (FM, AFM, FSM)

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Localized vs. itinerant systems

- In localized systems (e.g. some rare earth) the magnetism is mainly governed by the atom (Hund‘s rule)

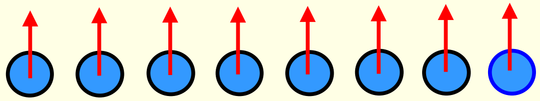
- In itinerant (delocalized) systems (many transition metals) magnetism comes from partial occupation of states, which differ between spin-up and spin-down.

- Boarderline cases (some f-electron systems)

  details of the structure (e.g. lattice spacing) determine whether or not some electrons are localized or itinerant.

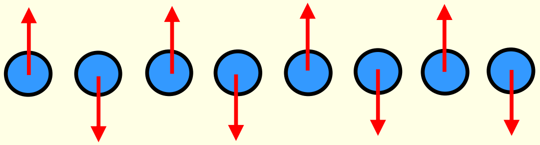
Ferro-, antiferro-, or ferri-magnetic

- Ferromagnetic (FM) (e.g. bcc Fe)



M > 0

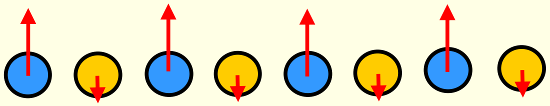
- Antiferromagnetic (AFM) (e.g. Cr)



M = 0

- Ferrimagnetic cases

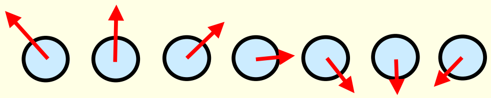
  the moments at different atoms are antiparallel but of different magnitude



M > 0

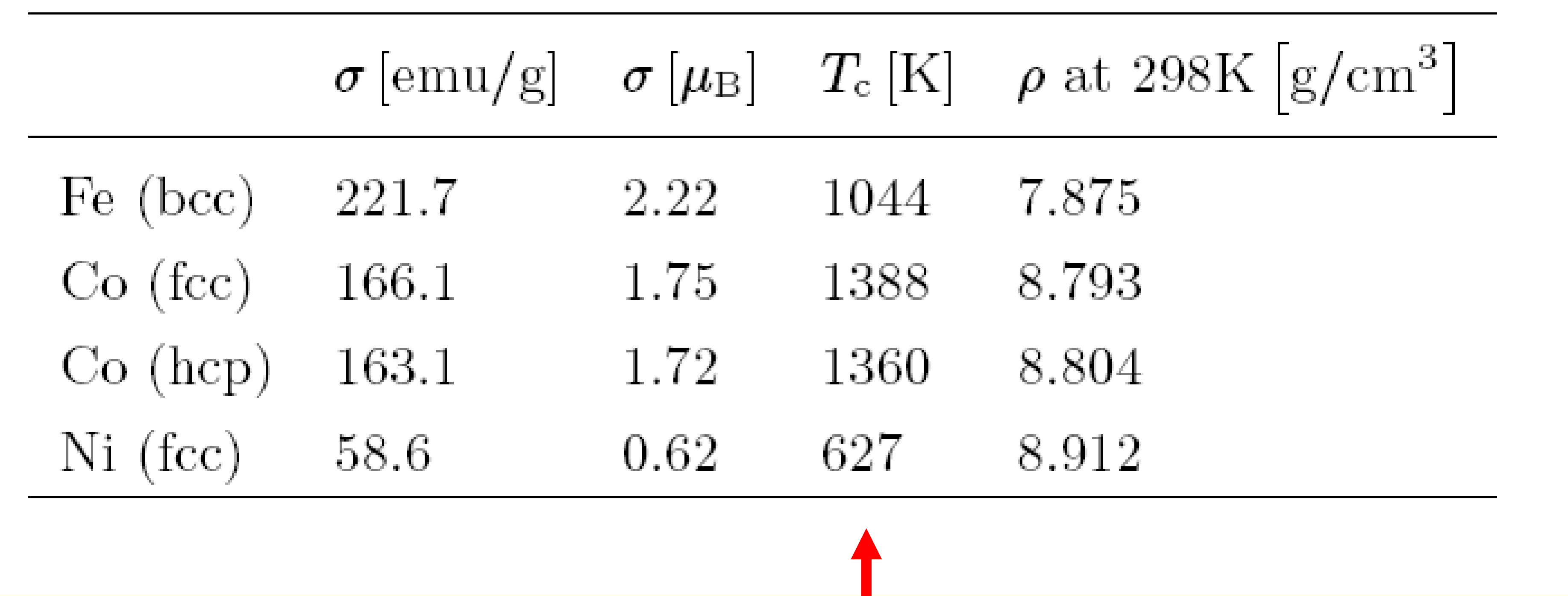
- Non-collinear magnetism (NCM)

  the magnetic moments are not ligned up parallel.



Itinerant electron magnetism

Experimental facts:



	σ [emu/g]	σ [μ_B]	T_c [K]	ρ at 298K $\left[\mathrm{g/cm^3}\right]$
Fe (bcc)	221.7	2.22	1044	7.875
Co (fcc)	166.1	1.75	1388	8.793
Co (hcp)	163.1	1.72	1360	8.804
Ni (fcc)	58.6	0.62	627	8.912

Curie
temperature

Stoner theory of itinerant electron magnetism

1. The carriers of magnetism are the unsaturated spins in the d-band.
2. Effects of exchange are treated with a molecular field term.
3. One must conform to Fermi statistics.

Stoner, 1936

Stoner model for itinerant electrons

In a

- non magnetic (NM) case

  $N_\uparrow = N_\downarrow$ (spin-up and spin-down)

- ferromagnetic (FM) case

  $N_\uparrow > N_\downarrow$ (majority and minority spin)

  the moments at all sites are parallel (collinear)

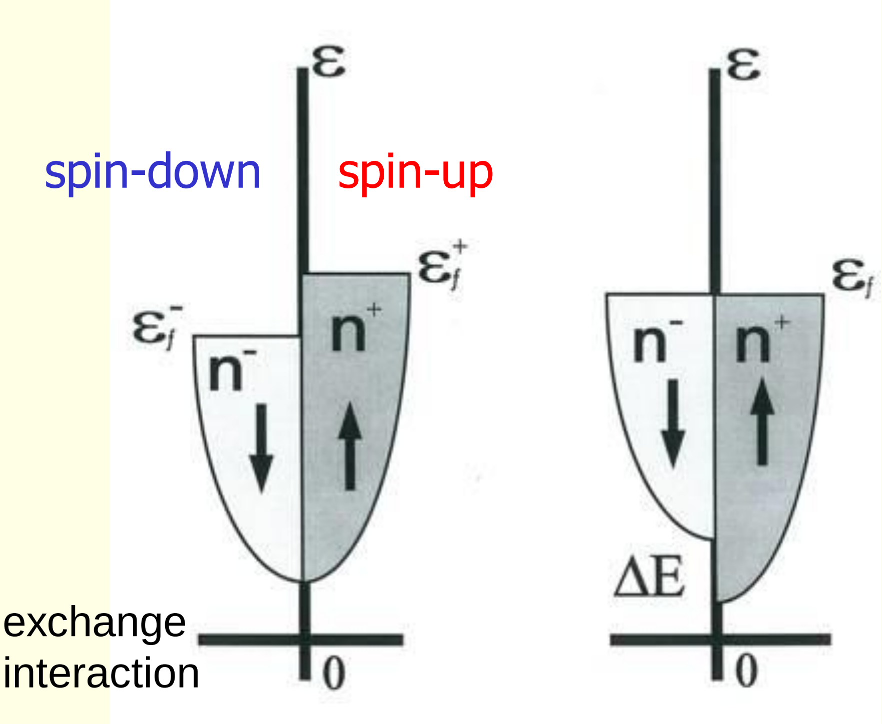
- the (spin) magnetic moment **m**
  - ***$m = N_\uparrow - N_\downarrow$***
  - its orientation with respect to the crystal axes is only defined by **spin orbit coupling**.

- there can also be an orbital moment

  it is often suppressed in 3d transition metals

$$\chi = \frac{\chi_P}{1 - 2\mu_B^2 I_s \mathcal{N}(\varepsilon_F)} = \chi_P \; S$$

Exchange splitting



$$E_b = \int_0^{\varepsilon_F} \varepsilon \mathcal{N}(\varepsilon)\,d\varepsilon - \int_{\varepsilon^-}^{\varepsilon_F} \varepsilon \mathcal{N}(\varepsilon)\,d\varepsilon + \int_0^{\varepsilon_F} \varepsilon \mathcal{N}(\varepsilon)\,d\varepsilon + \int_{\varepsilon_F}^{\varepsilon^+} \varepsilon \mathcal{N}(\varepsilon)\,d\varepsilon - \frac{I_s M^2}{2} \; .$$

Stoner criterion $2\mu_B^2 I_s \mathcal{N}(\varepsilon_F) > 1$

Stoner model for itinerant electrons

- The existence of ferromagnetism (FM) is governed by the

- Stoner criterion

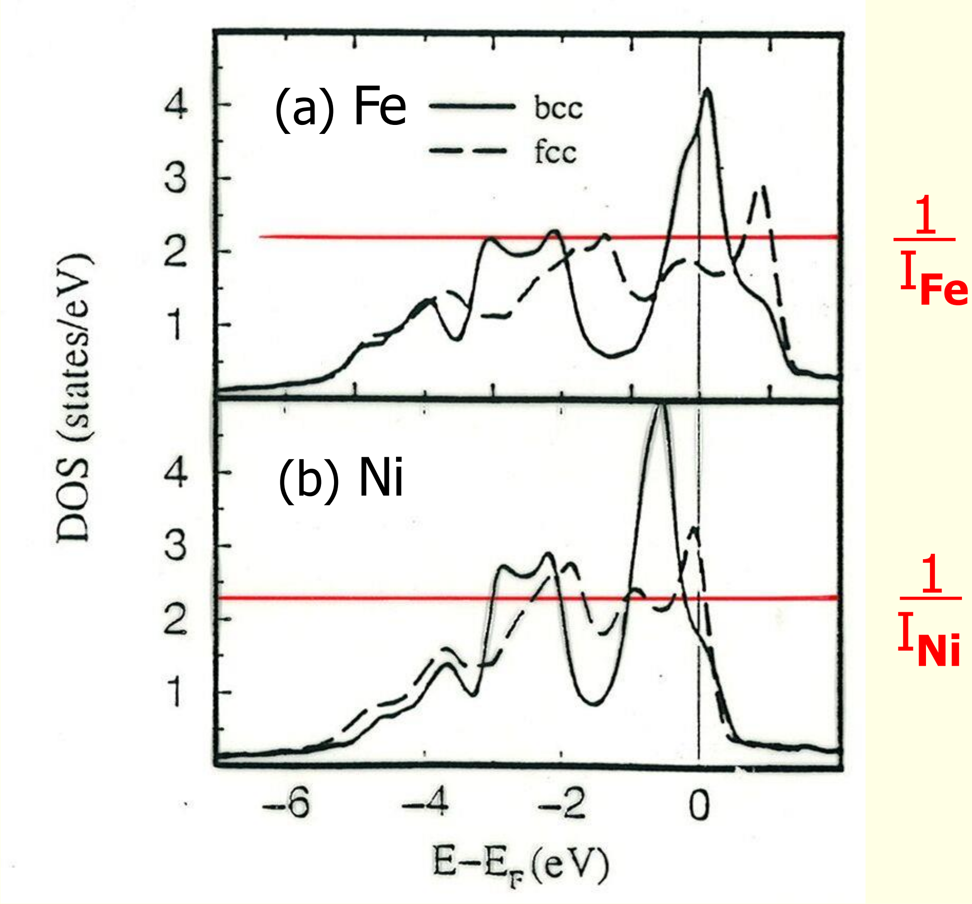
$$\boxed{I \,.\, N(E_F) \;>\; 1}$$

$N(E_F)$ DOS at E_F (of NM case)

I Stoner parameter

~ independent of structure

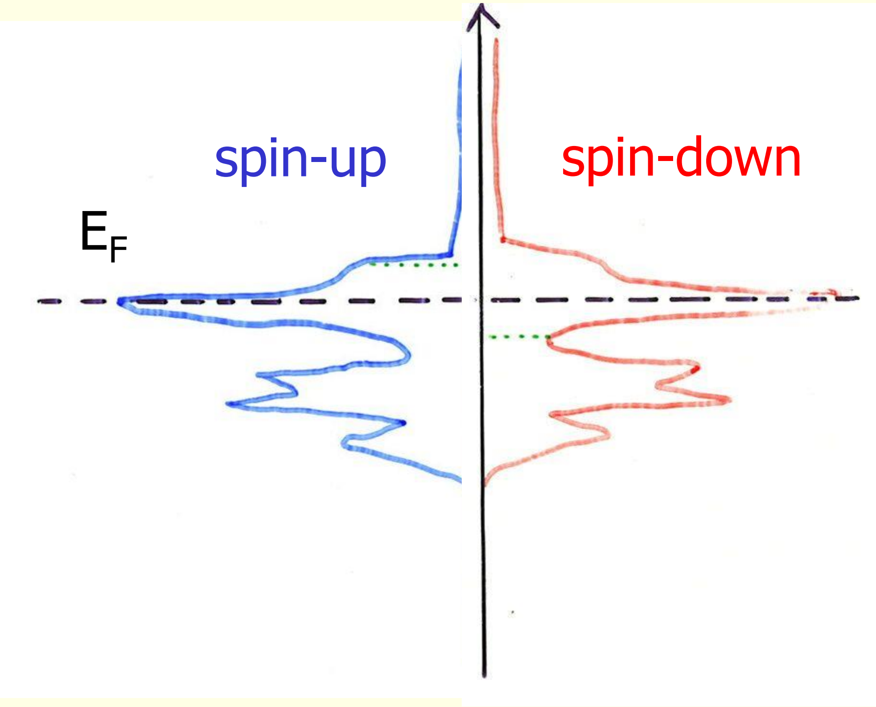
- Ferromagnetism appears when the **gain** in exchange energy is larger than the **loss** in kinetic energy



P.James, O.Eriksson, B.Johansson, I.A.Abrikosov,
Phys.Rev.B **58**, ... (1998)

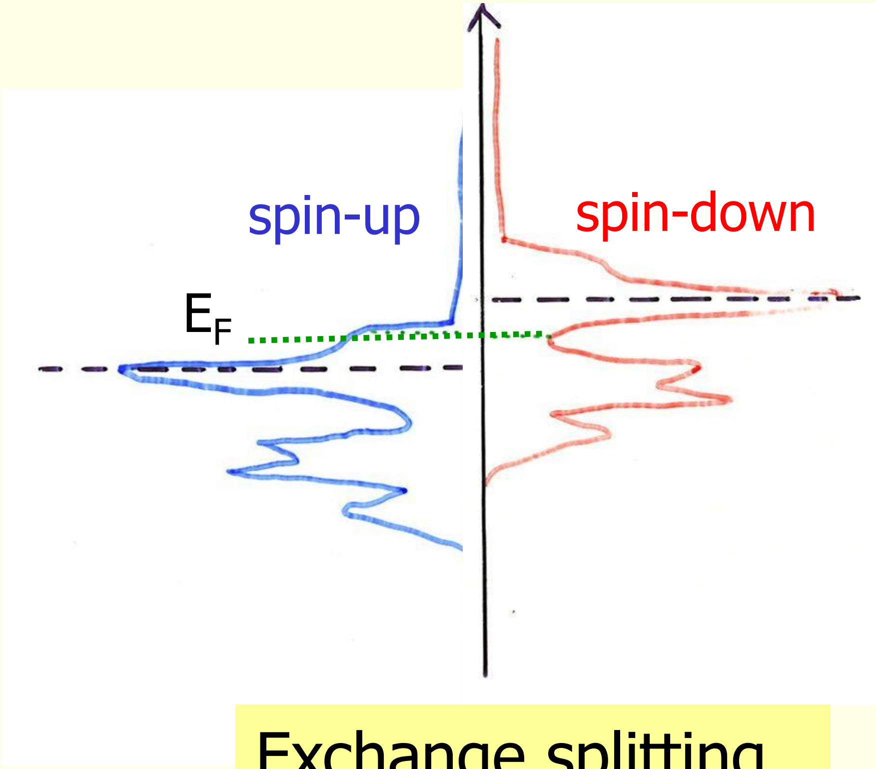
bcc Fe

- Non magnetic case



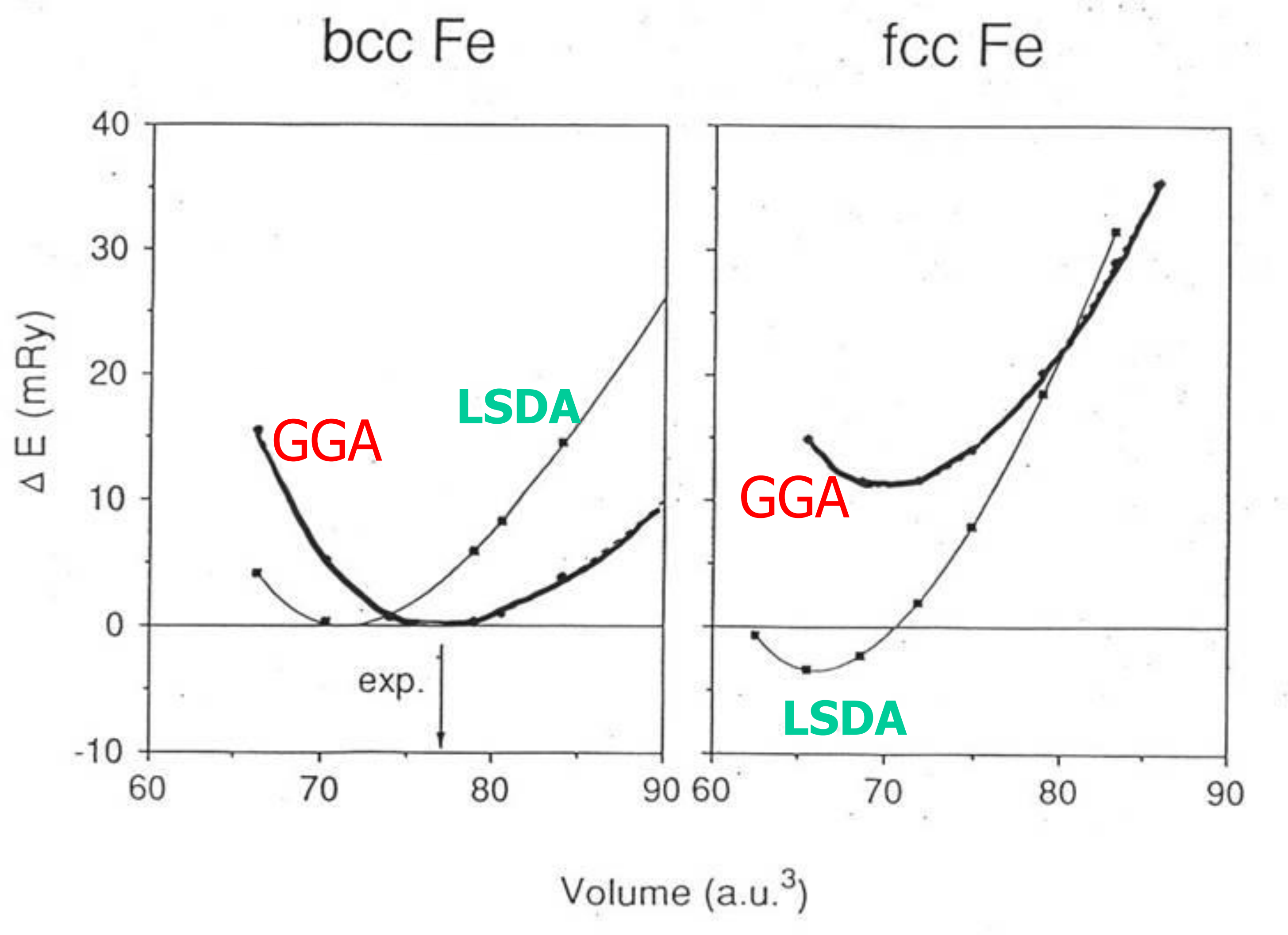
E_F at high DOS

ferromagnetic case



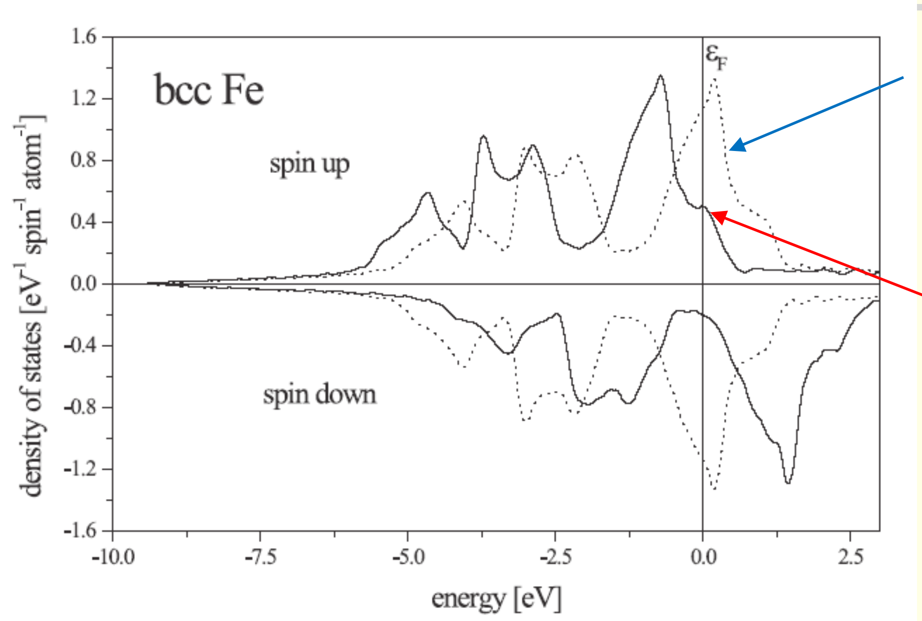
Exchange splitting

DFT ground state of iron



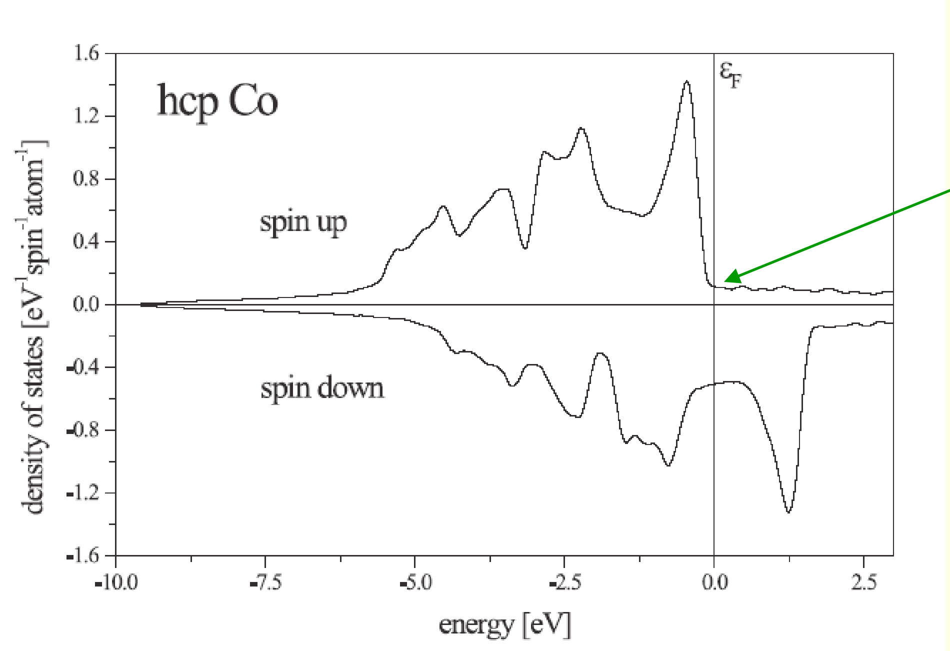
- **LSDA**
  - *NM*
  - *fcc*
  - *in contrast to experiment*
- **GGA**
  - *FM*
  - *bcc*
  - *Correct lattice constant*
- Experiment
  - *FM*
  - *bcc*

Iron and its alloys



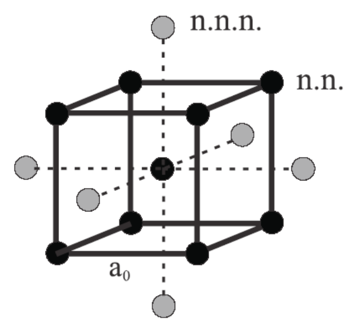
non-spin polarized

Fe:
weak ferromagnet
(almost)

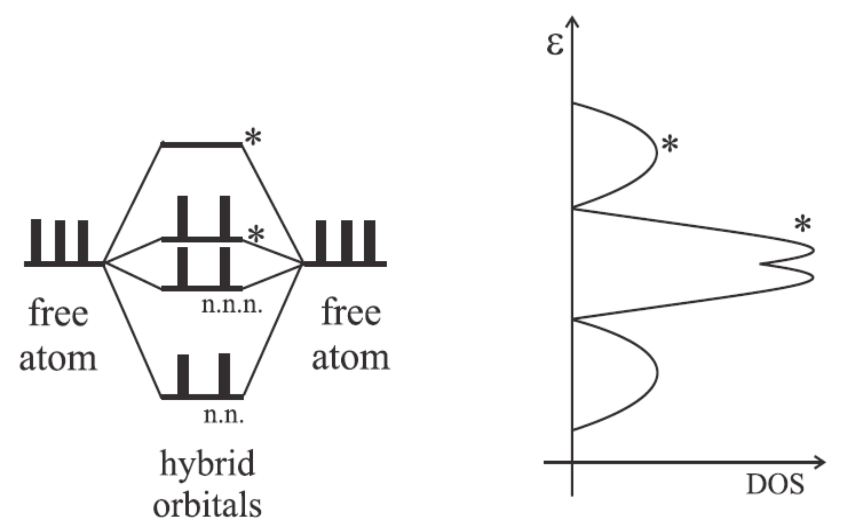


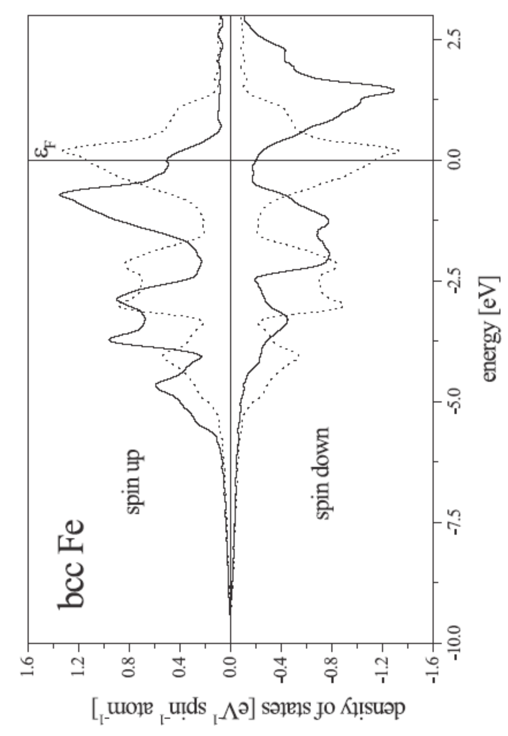
Co:
strong ferromagnet

Magnetism and crystal structure



V. Heine: „metals are systems with unsaturated covalent bonds“



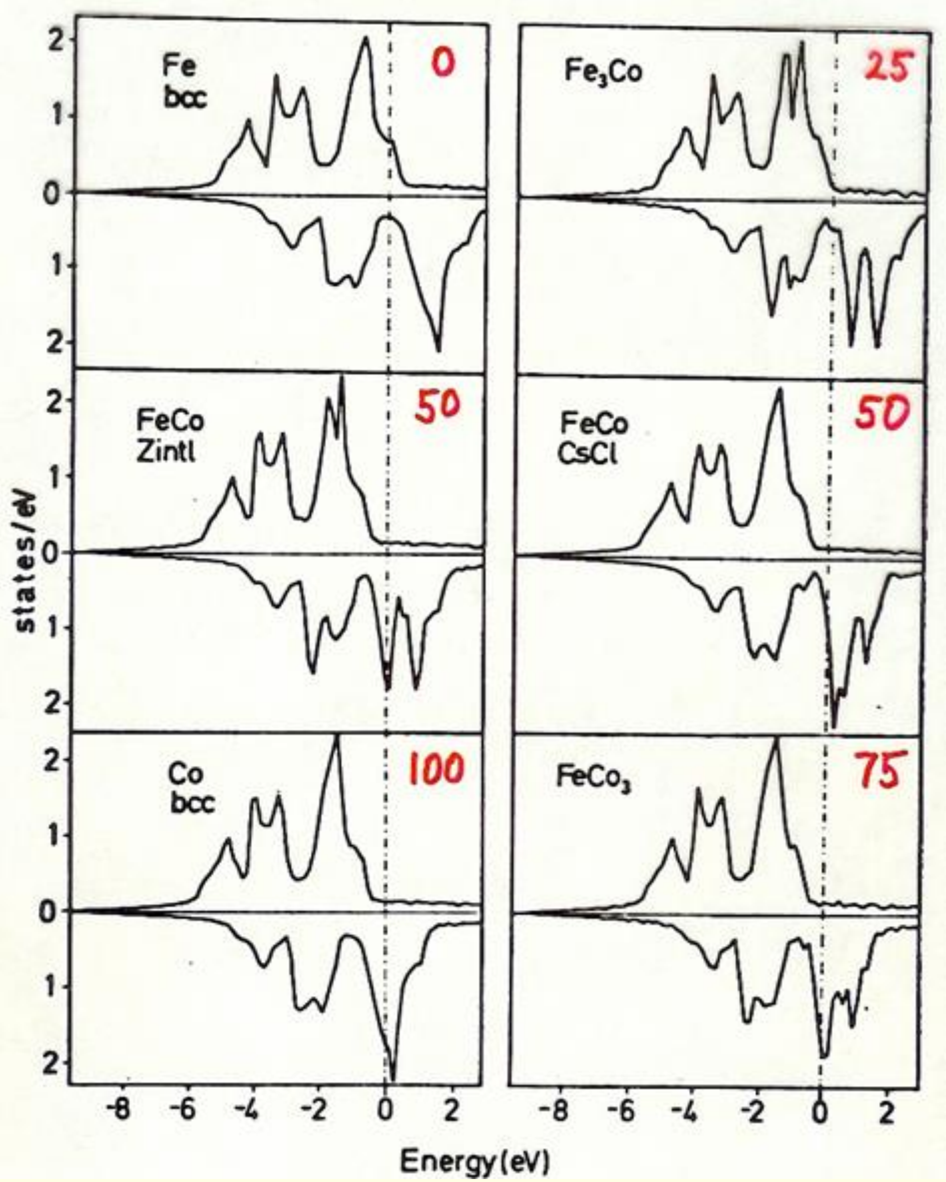


Covalent magnetism Fe-Co alloys

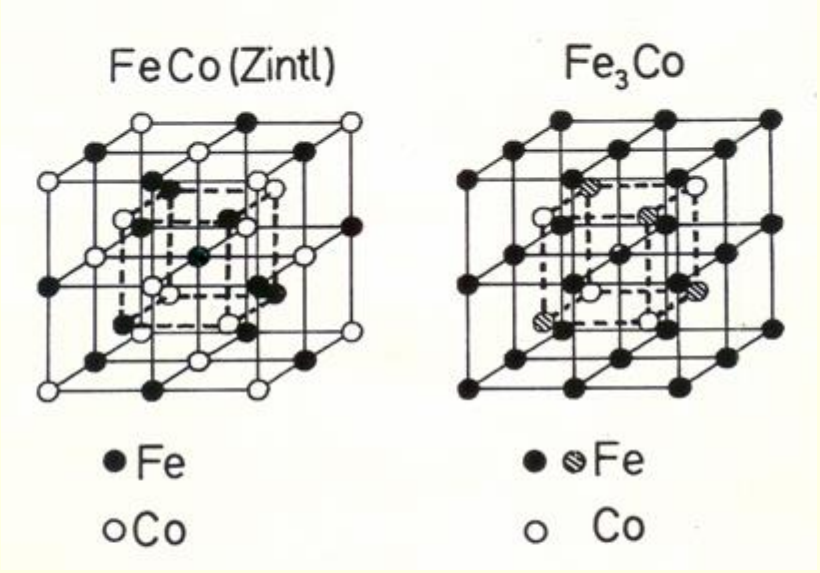
- e.g. Fe-Co alloys
- Wigner delay times

Spin projected DOS of Fe-Co alloys

% Co



- The alloy is represented by ordered structures
  - *Fe_3Co and $FeCo_3$ (Heusler)*
  - *FeCo Zintl or CsCl*
  - *Fe, Co bcc*

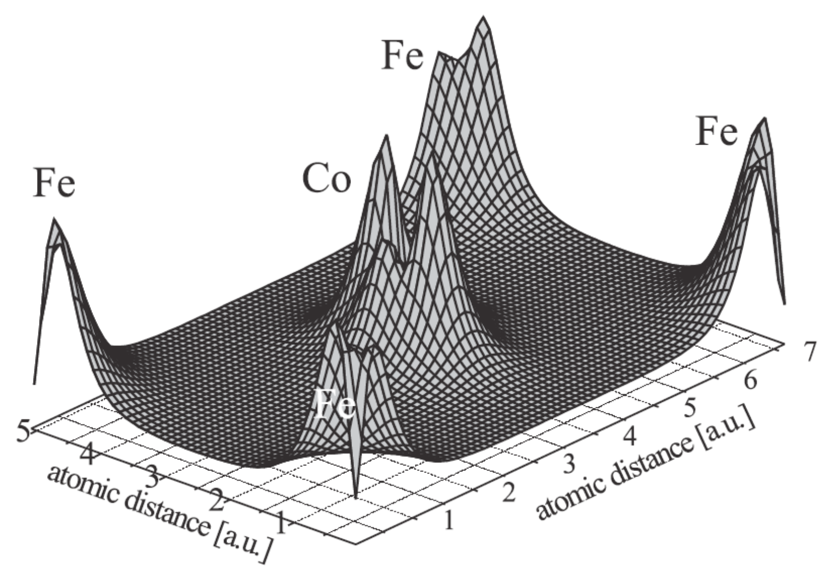


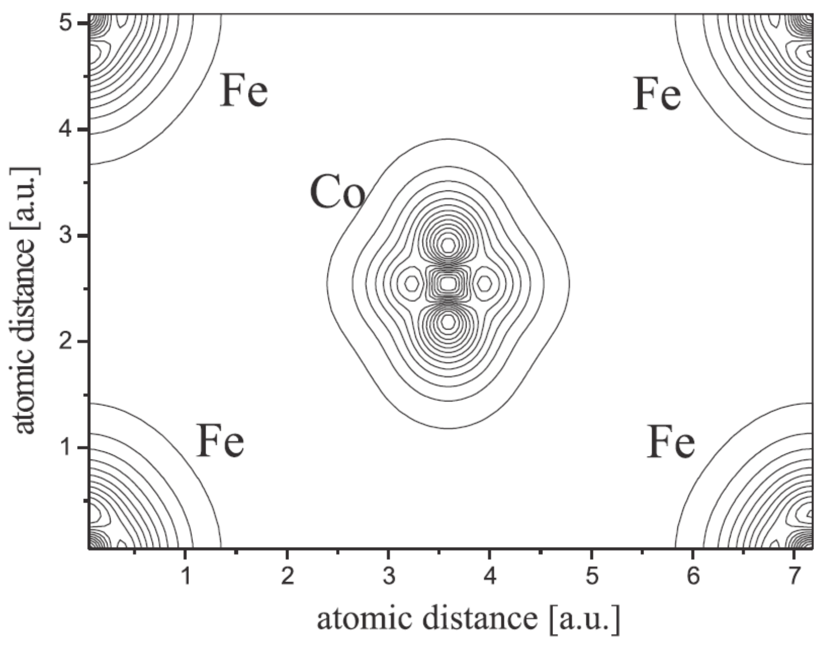
Iron and its alloys

Itinerant or localized?

- Magnetization density difference between
  - *Majoity spin*
  - *Minority spin*

$$m(r)=\rho^{\uparrow}(r)-\rho^{\downarrow}(r)$$





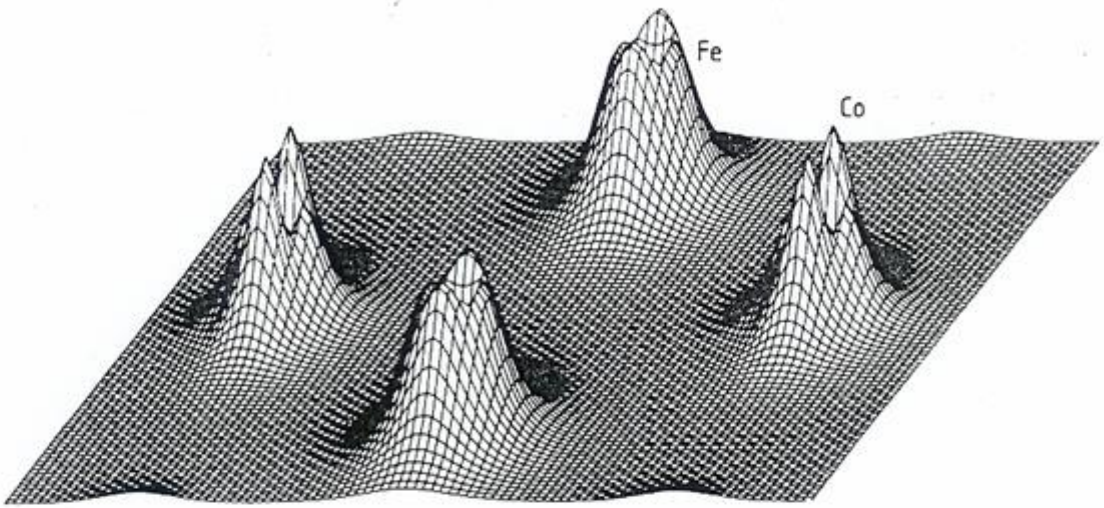
Magnetization density in FeCo

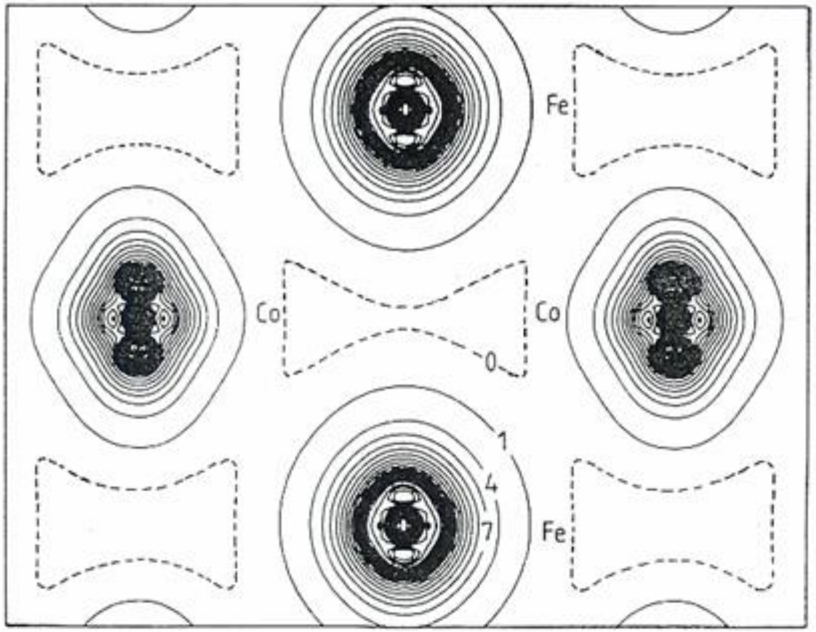
- Magnetization density difference between
  - *Majoity spin*
  - *Minority spin*

$$m(r)=\rho^{\uparrow}(r)-\rho^{\downarrow}(r)$$

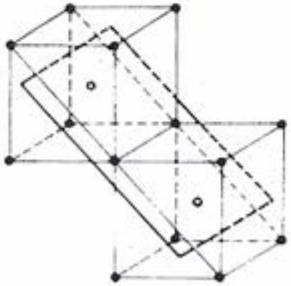
- Localized around
  - *Fe and Co*
  - *slightly negative between the atoms*
- Itinerant electrons

K.Schwarz, P.Mohn, P.Blaha, J.Kübler,
Electronic and magnetic structure of bcc Fe-Co alloys from band theory,
J.Phys.F:Met.Phys. **14**, 2659 (1984)

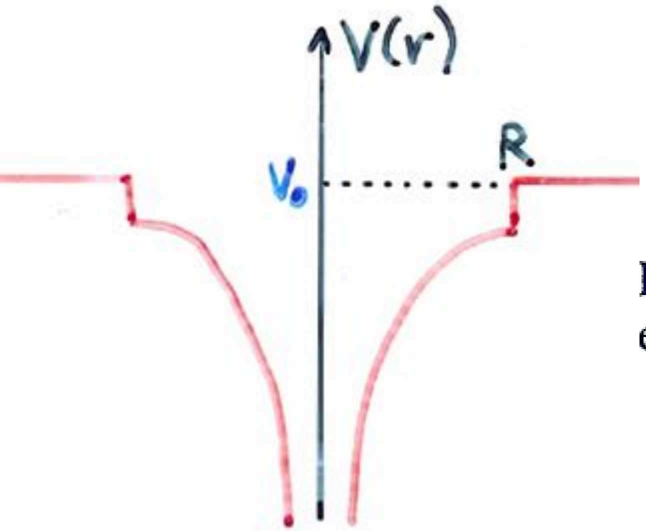




CsCl
structure



Bonding by Wigner delay time



single scatterer (Friedel)

$$V(r)=\begin{cases} V(r) & r \leqq b, \\ 0 & r > b. \end{cases} \qquad (1)$$

Inside such a sphere of radius b the radial Schrödinger equation (in Rydberg atomic units)

$$\left[-\frac{d^2}{dr^2}-\frac{2}{r}\frac{d}{dr}+\frac{l(l+1)}{r^2}+V(r)-\varepsilon\right]R_l(\varepsilon,r)=0, \qquad (2)$$

V(r)=0 solution:

$$S_l(r)=A_l[\overset{\text{Bessel}}{\overset{\downarrow}{j_l}}(kr)\cos\eta_l(\varepsilon)-\overset{\text{Neumann}}{\overset{\downarrow}{n_l}}(kr)\sin\eta_l(\varepsilon)], \qquad (3)$$

R_l joined in value and slope defines phase shift :

$$\tan\eta_l(\varepsilon)=\frac{R_l(\varepsilon,b)j_l'(kb)-j_l(kb)R_l'(\varepsilon,b)}{R_l(\varepsilon,b)n_l'(kb)-n_l(kb)R_l'(\varepsilon,b)}, \qquad (4)$$

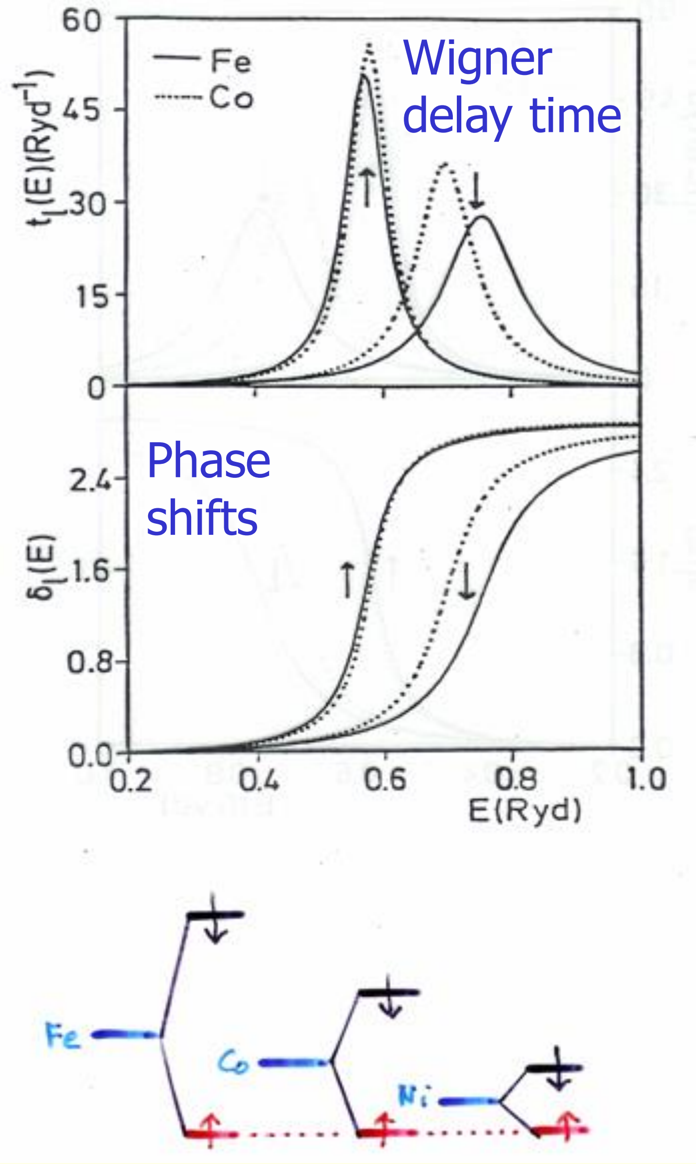
Friedel sum

$$N(\varepsilon)=\frac{2}{\pi}\sum_{l=0}^{\infty}(2l+1)\eta_l(\varepsilon),$$

Wigner delay time

$$n(\varepsilon)=\frac{dN(\varepsilon)}{d\varepsilon}=\frac{1}{\pi}\sum_{l=0}^{\infty}(2l+1)t_l^{\mathrm{D}}(\varepsilon). \qquad (6)$$

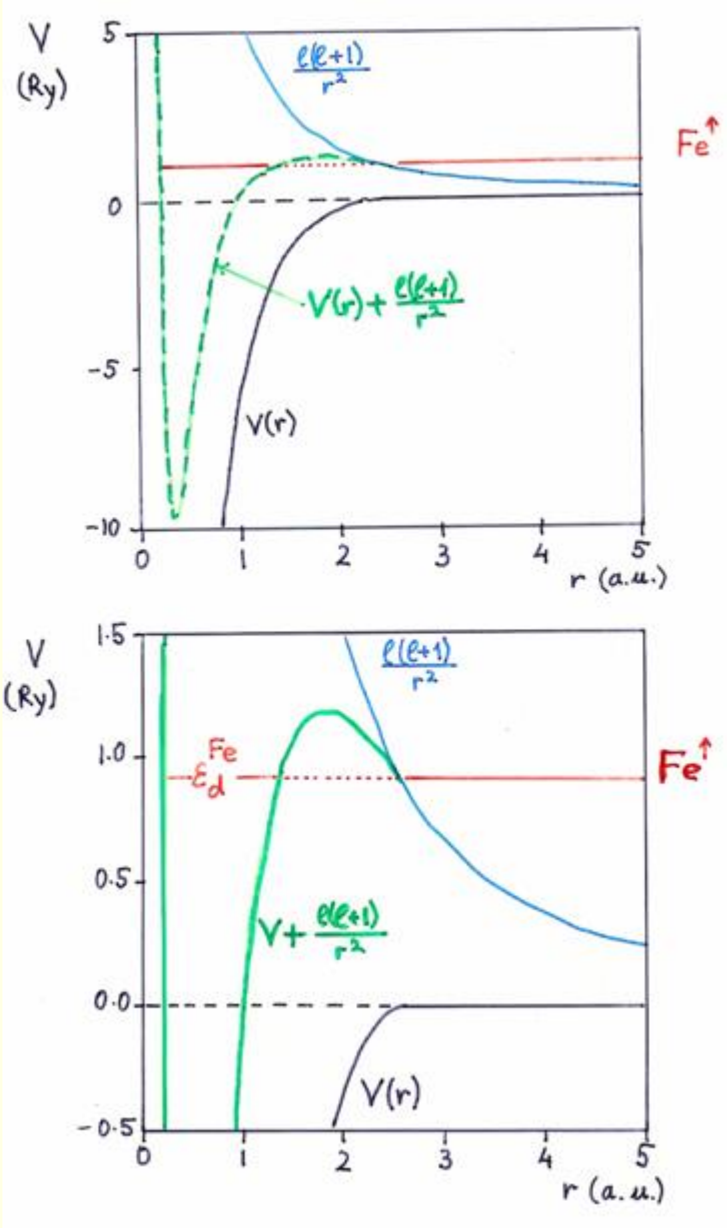
Phase shifts, Wigner delay times of Fe, Co, Ni



Wigner delay time

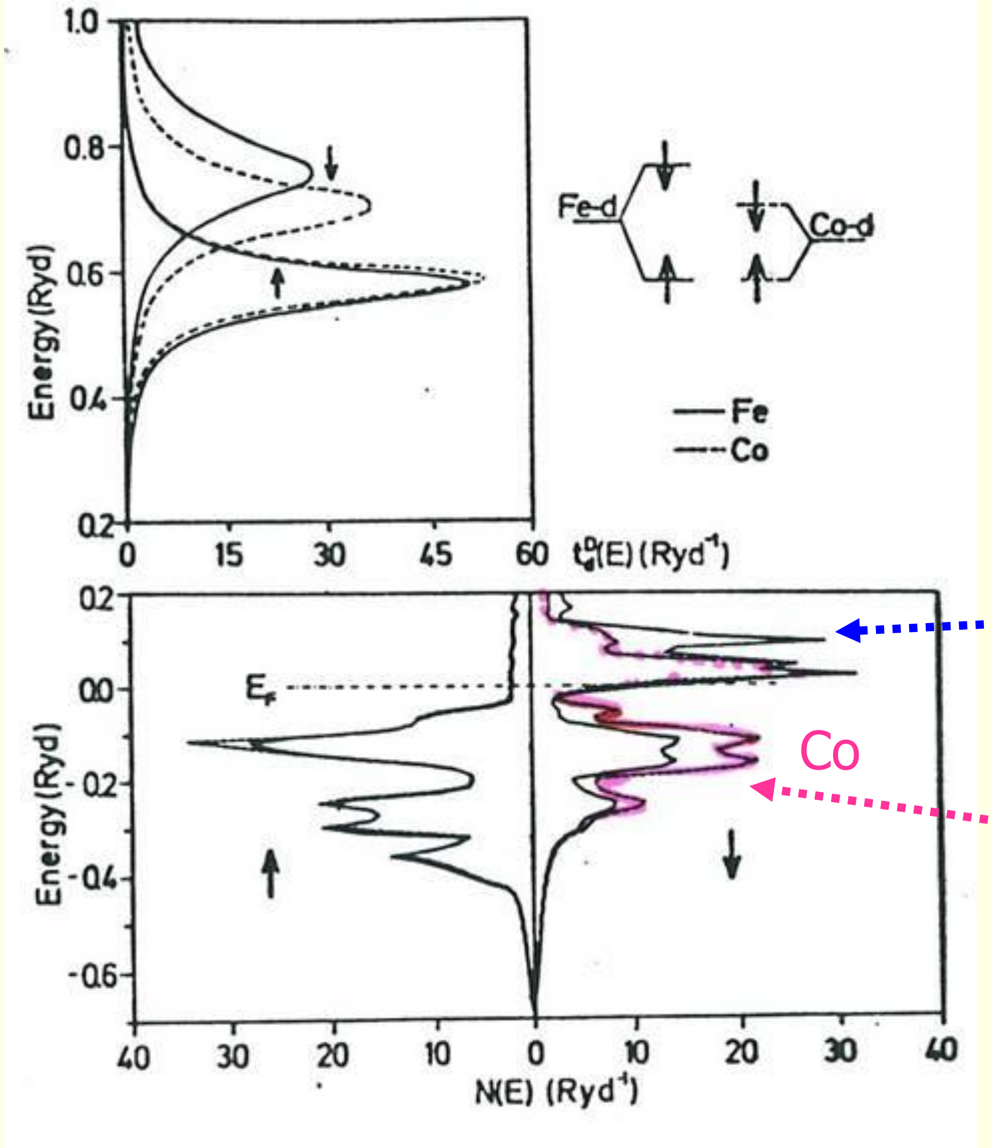
Phase shifts

resonance states



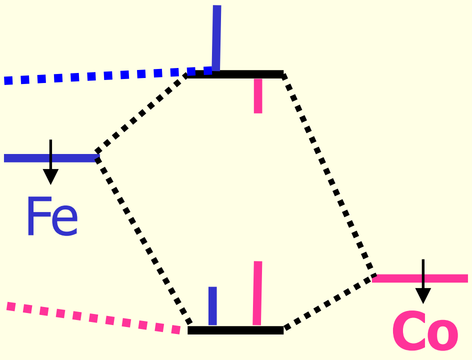
Covalent magnetism in FeCo

Wigner delay time



- For spin up
  - *Fe and Co equivalent*
  - *partial DOS similar*
  - *typical bcc DOS*
- For spin down
  - *Fe higher than Co*

antibonding

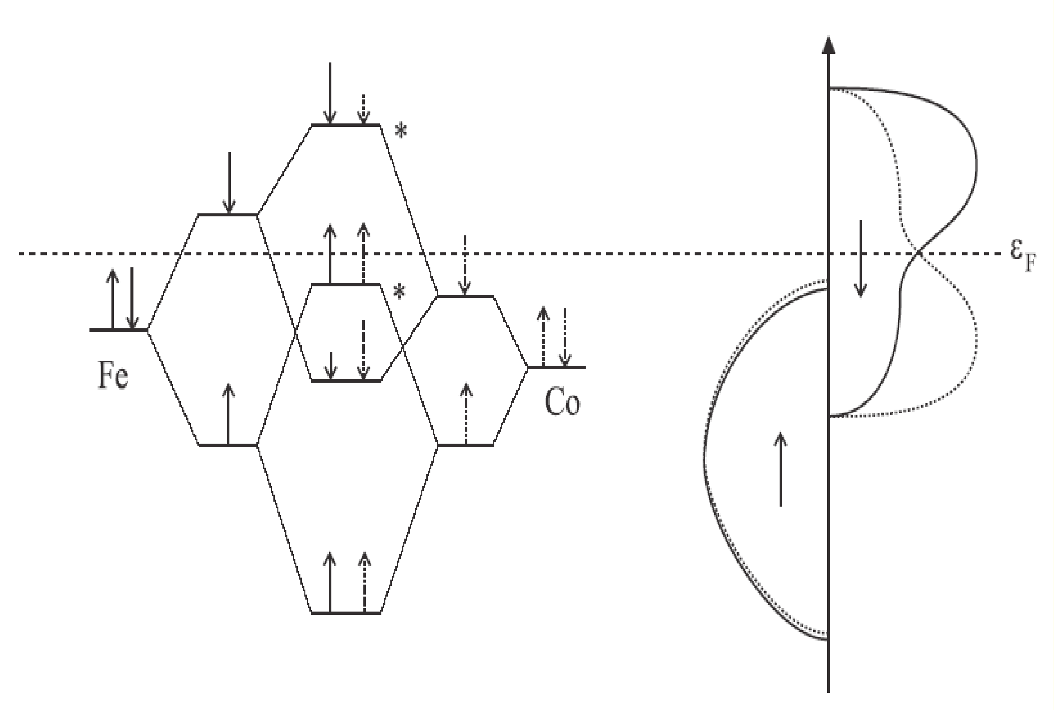


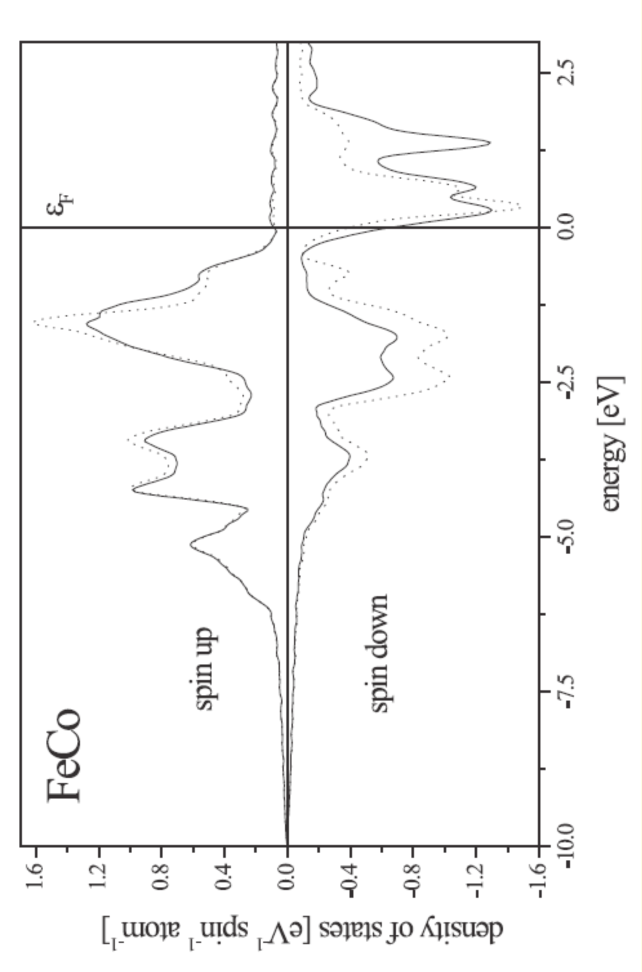
bonding

No charge transfer between Fe and Co

Magnetism and crystal structure

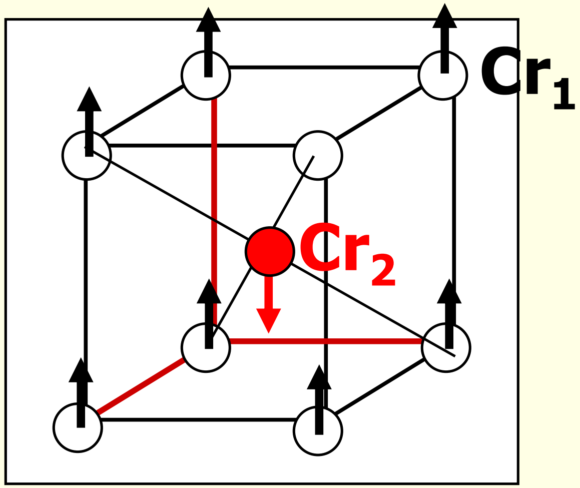
Covalent magnetism, FeCo:

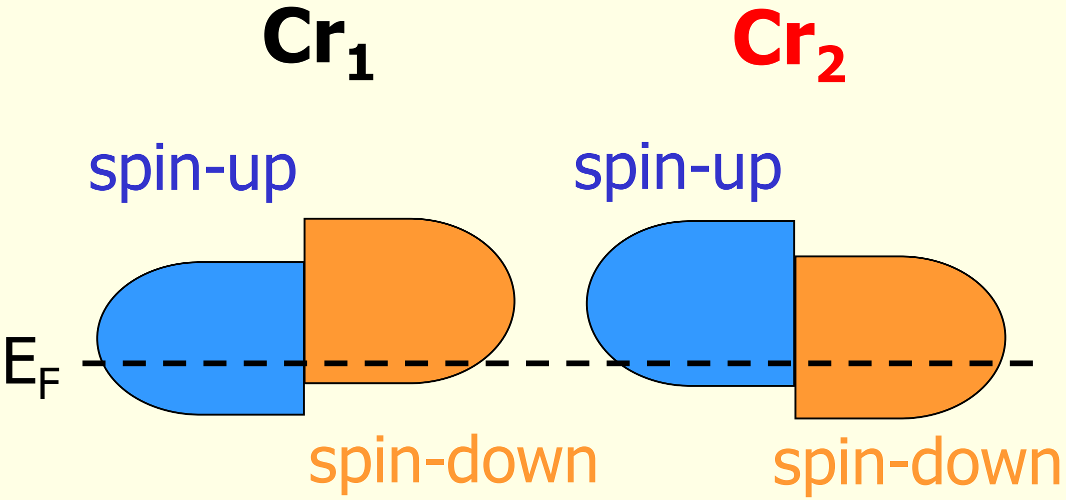




Antiferromagnetic (AFM) Cr

- Cr has AFM bcc structure





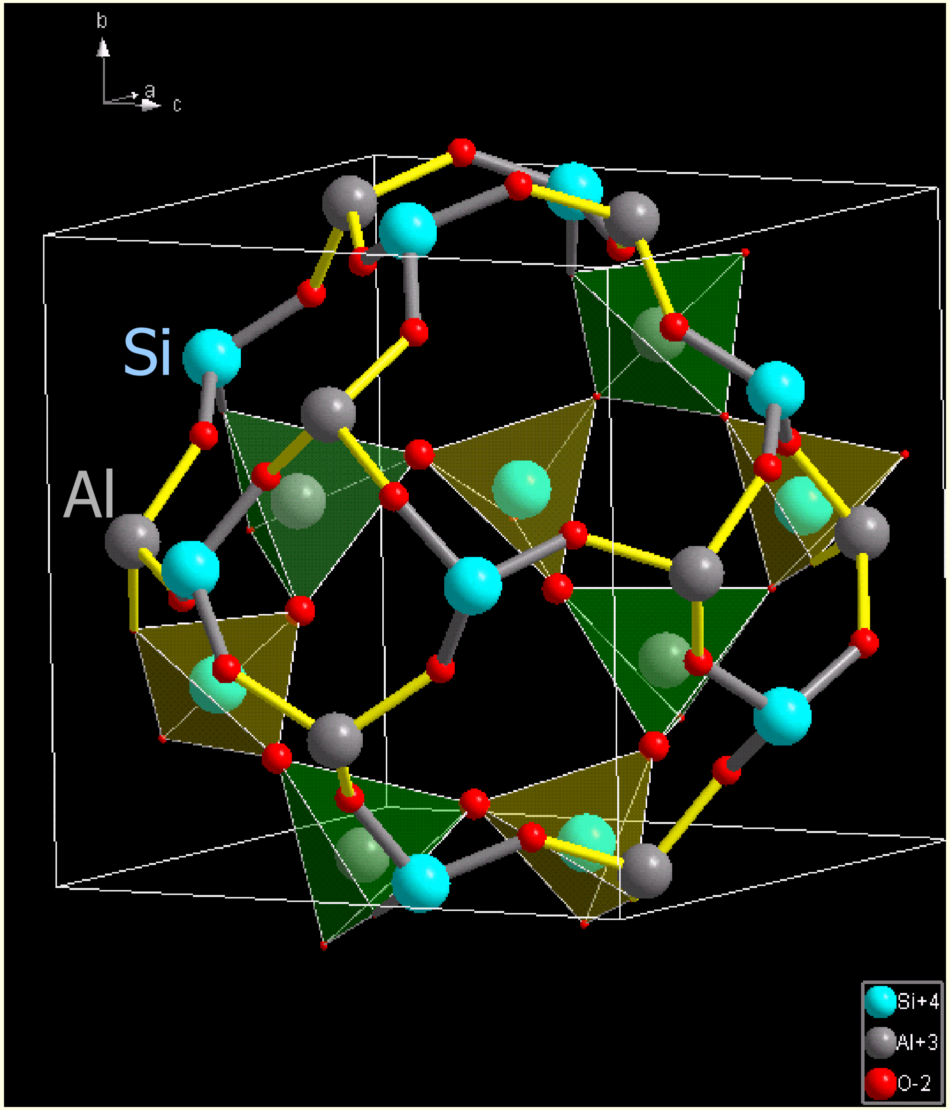
- There is a symmetry
  it is enough to do the spin-up calculation
  spin-down can be copied

$$\boxed{Cr_1^{\downarrow} = Cr_2^{\uparrow}}$$

$$\boxed{Cr_2^{\downarrow} = Cr_1^{\uparrow}}$$

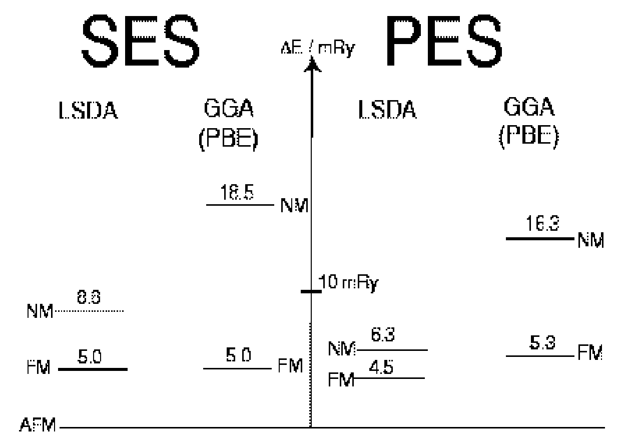
Zeolite, sodalite

- Al-silicate
- corner shared
  - *SiO_4 tetrahedra*
  - *AlO_4 tetrahedra*
- β cage
- Al / Si ratio 1
- alternating
- ordered (cubic)
- 3 e^- per cage

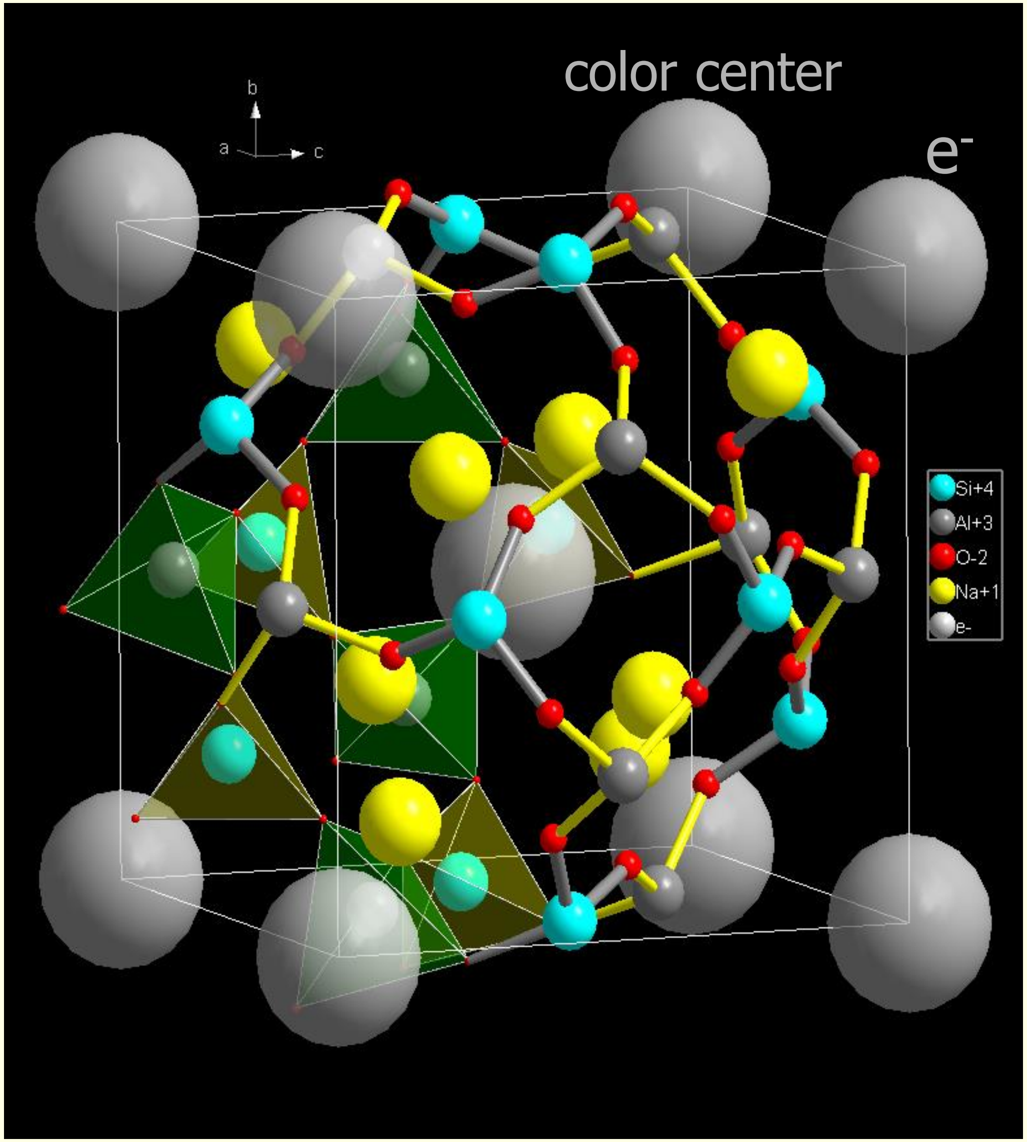


SES Sodium electro sodalite

- Si-Al zeolite (sodalite)
  - *Formed by corner-shared SiO_4 and AlO_4 tetrahedra*
- Charge compensated by *doping with*
  - *4 Na^+*
  - *one e^- (color center)*
- antiferromagnetic (AFM) order of e^-



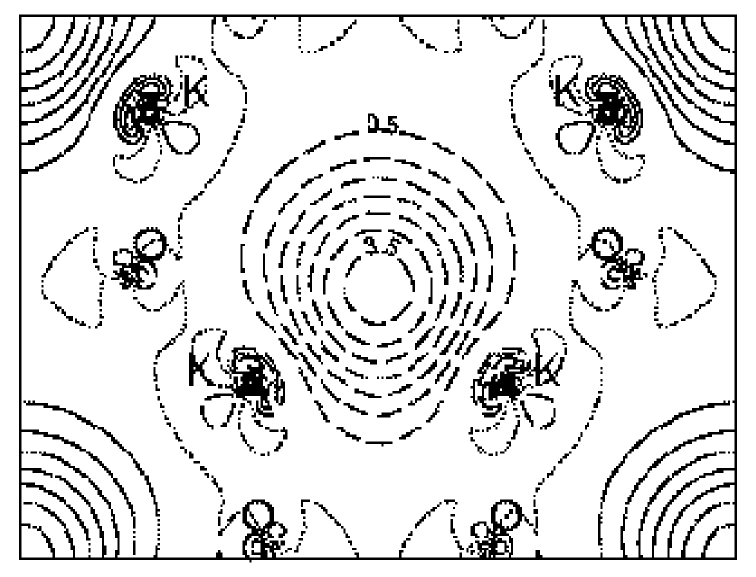
Energy (relative stability)

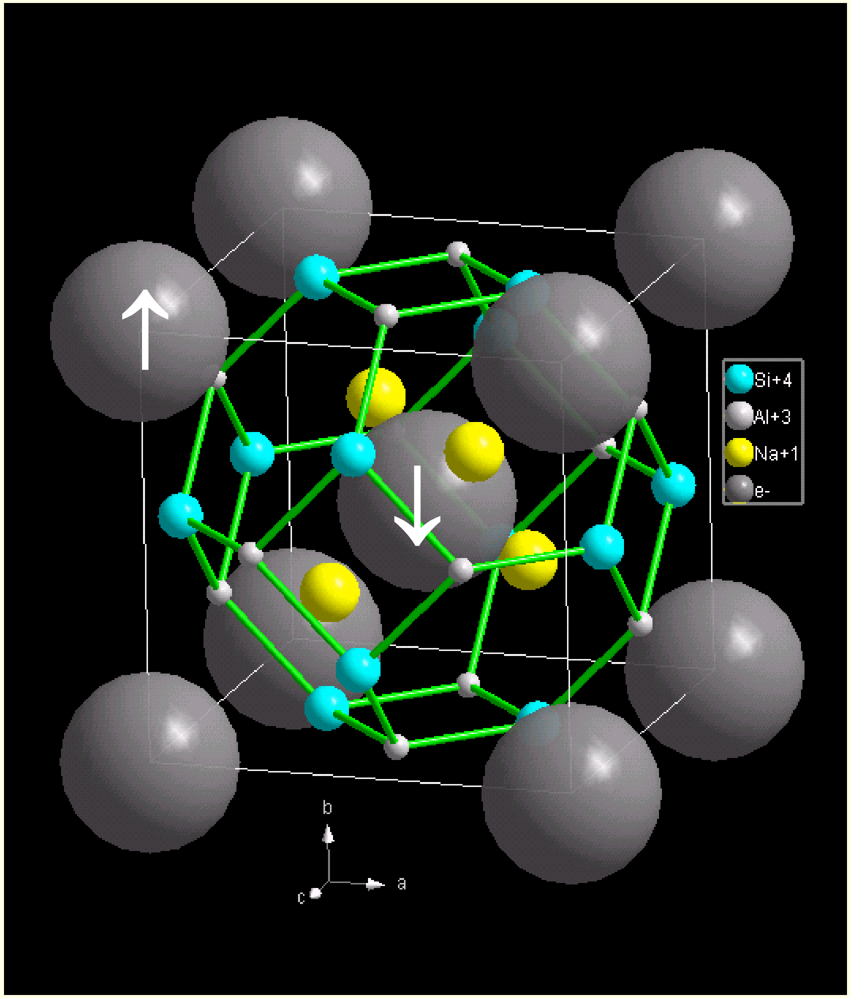


SES

AFM order between color centers (e^-)

Spin density $\rho^{\uparrow} - \rho^{\downarrow}$





G.K.H. Madsen, Bo B. Iversen, P. Blaha, K. Schwarz, Phys. Rev. B 64, 195102 (2001)

INVAR alloys (invariant)

- e.g. Fe-Ni
- Such systems essentially show no thermal expansion around room temperature

INVAR (invariant) of Fe-Ni alloys

- The thermal expansion of the Eifel tower
- Measured with a rigid Fe-Ni INVAR wire
- The length of the tower correlates with the temperature
- **$Fe_{65}Ni_{35}$** alloy has vanishing thermal expansion around room temperature

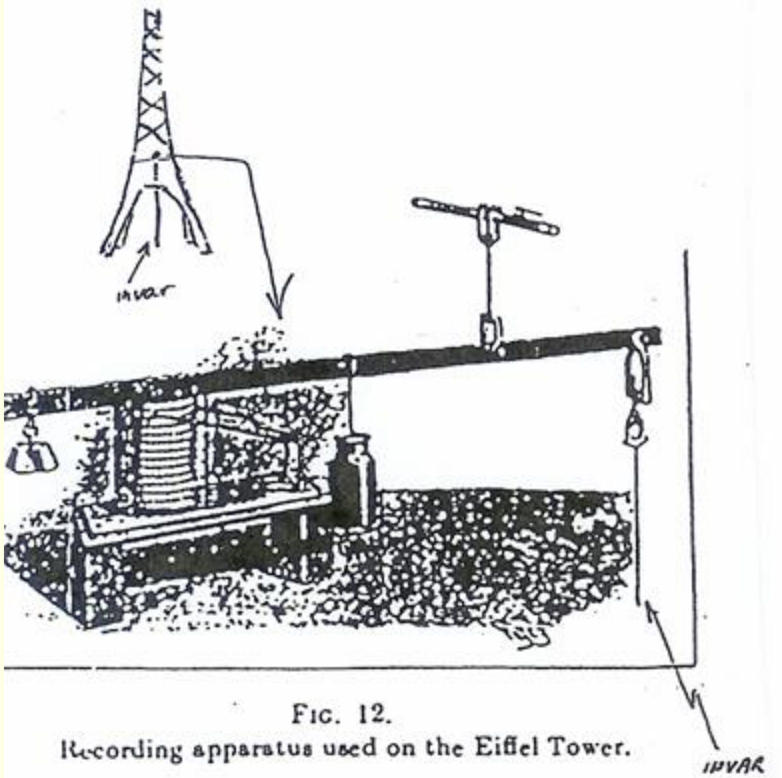
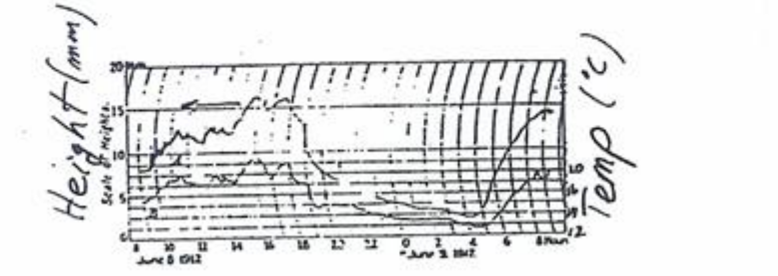
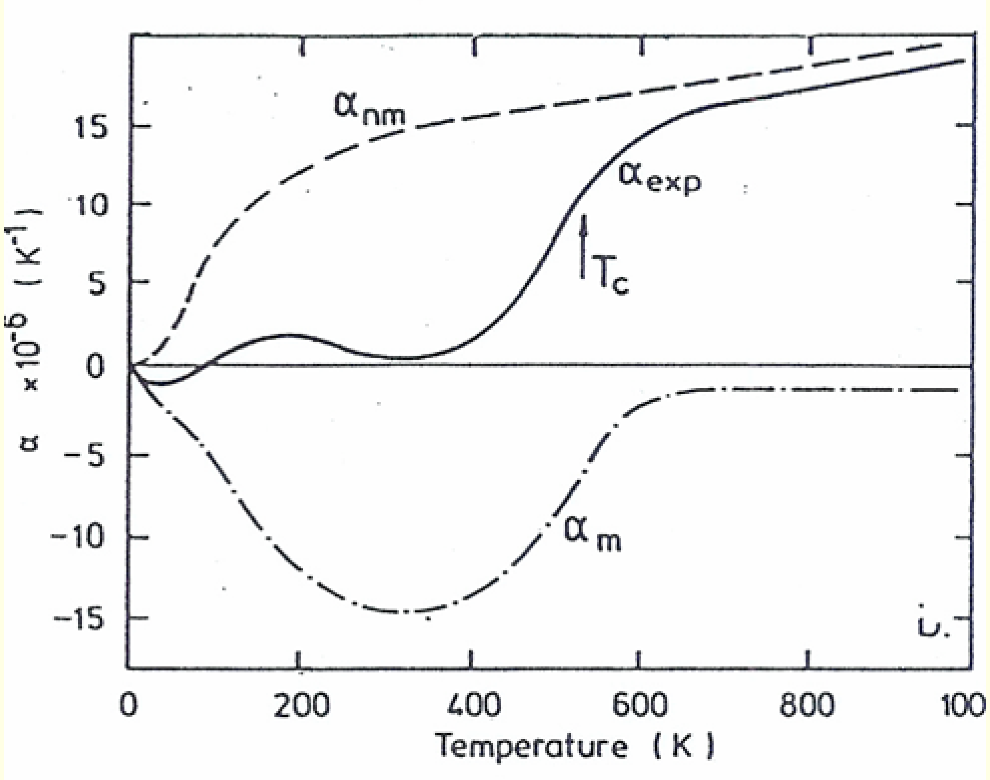


FIG. 12.
Recording apparatus used on the Eiffel Tower.



Ch.E.Guillaume (1897)

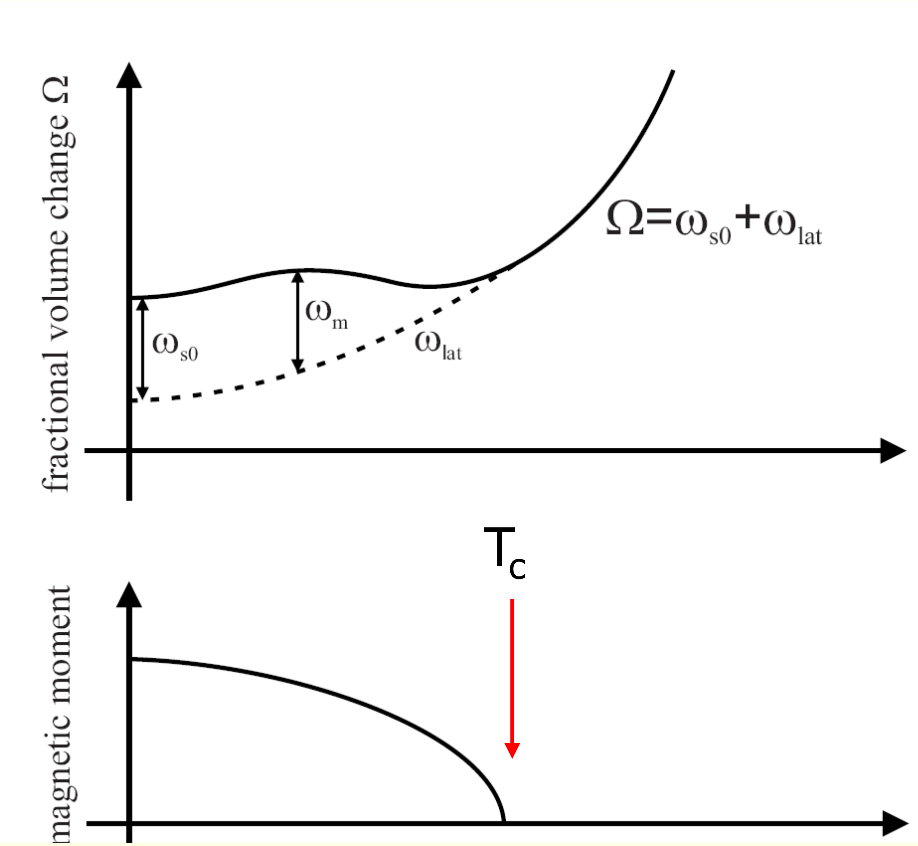


Magnetostriction and Invar behaviour

What is magnetostriction?

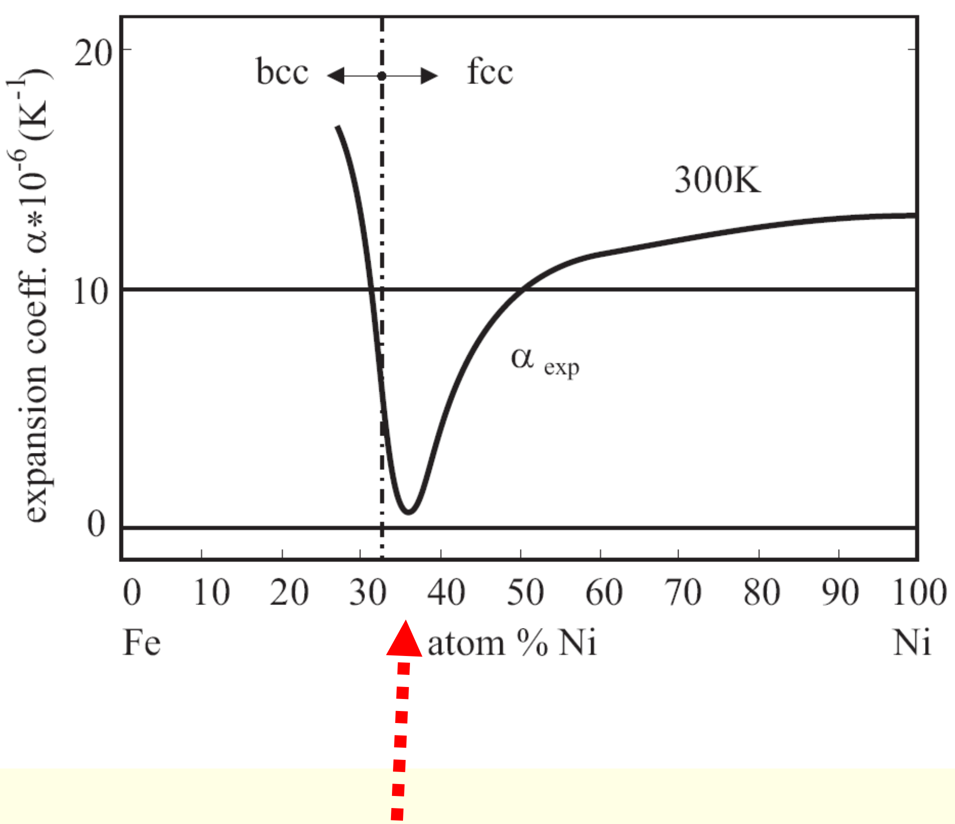
Magnetostriction ω_{s0} is the difference in volume between the volume in the magnetic ground state and the volume in a hypothetical non-magnetic state.

Above the Curie temperature the magnetic contribution ω_m vanishes.

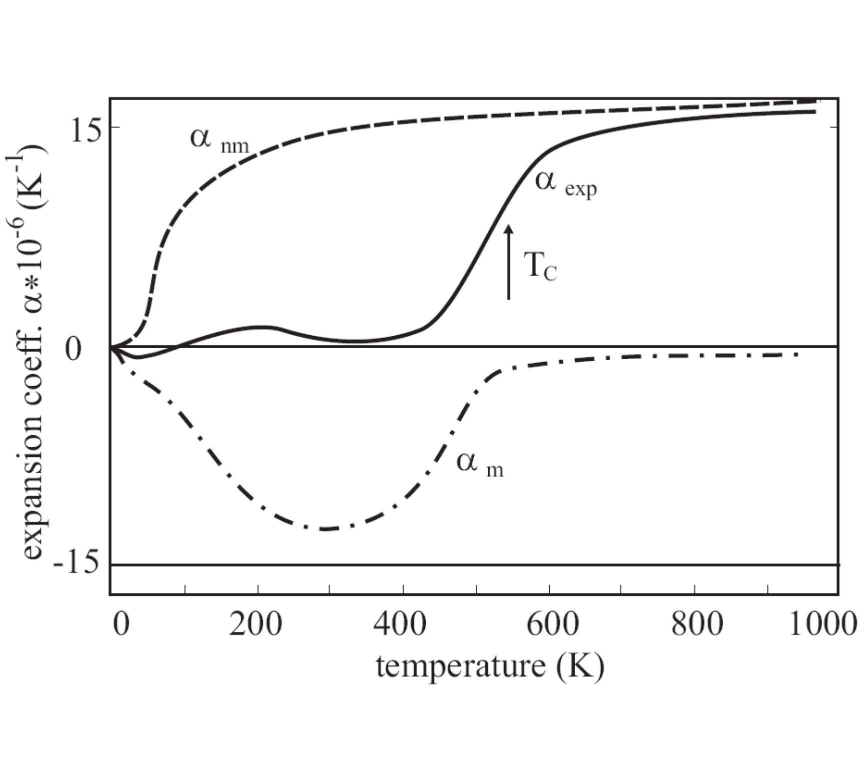


Fe-Ni Invar alloys

„classical" Fe-Ni Invar



- **$Fe_{65}Ni_{35}$** alloy has vanishing thermal expansion around room temperature

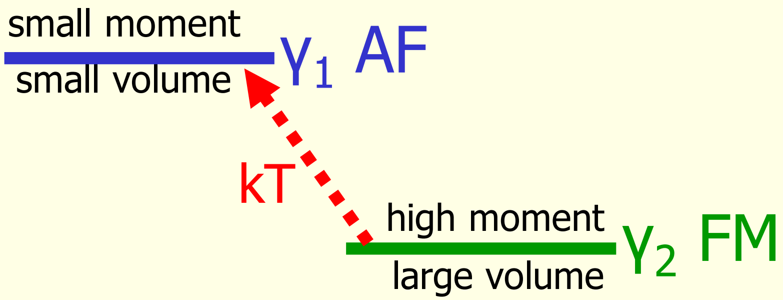


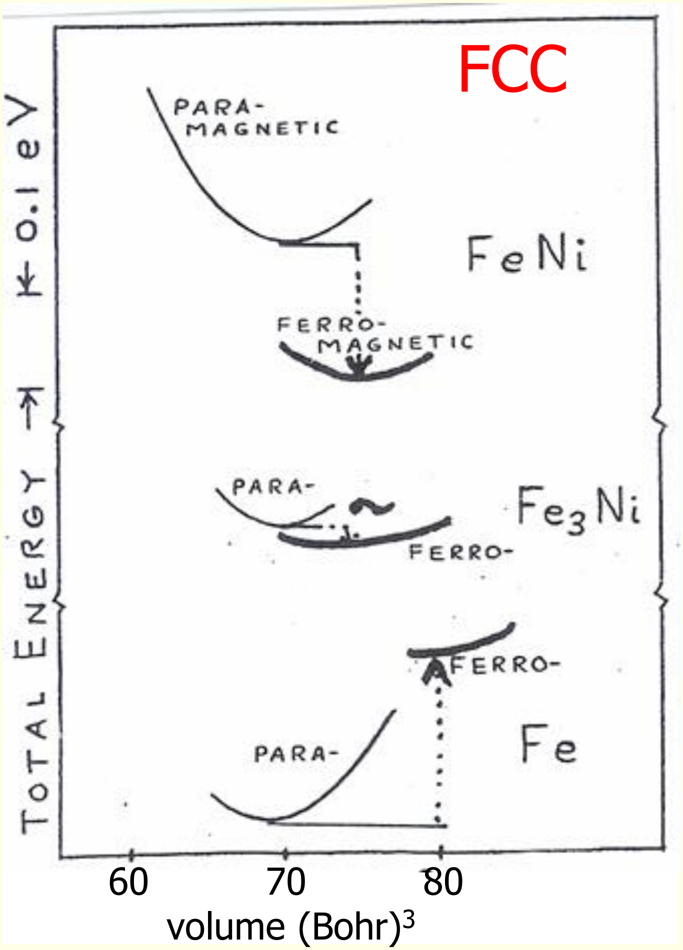
Early explanations of INVAR

R.J.Weiss
Proc.Roy.Phys.Soc (London) **32**, 281 (1963)

fcc Fe

low spin	**high spin**
m=0.5 μ_B AF	m=2.8 μ_B FM
a = 3.57 Å	a = 3.64 Å





50% Fe

75% Fe

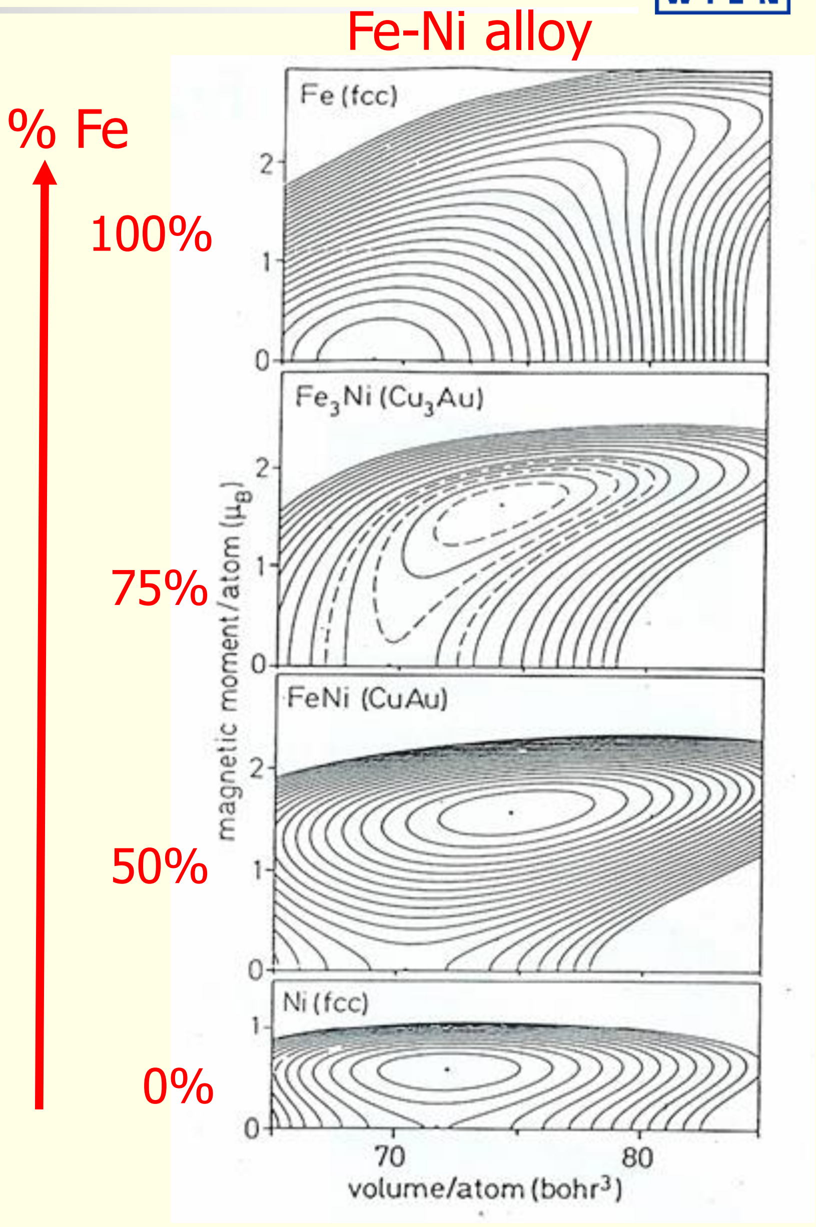
100% Fe

A.R.Williams, V.L.Moruzzi, G.D.Gelatt Jr., J.Kübler, K.Schwarz,
Aspects of transition metal magnetism,
J.Appl.Phys. **53**, 2019 (1982)

Energy surfaces of Fe-Ni alloys

- This fcc structure
  - *from non magnetic Fe (fcc)*
  - *to ferromagnetic Ni*

  - *as the composition changes*
- At the INVAR composition
  - *There is a flat energy surface*
    - as function of volume and moment



Fe-Ni alloy

% Fe

100%

75%

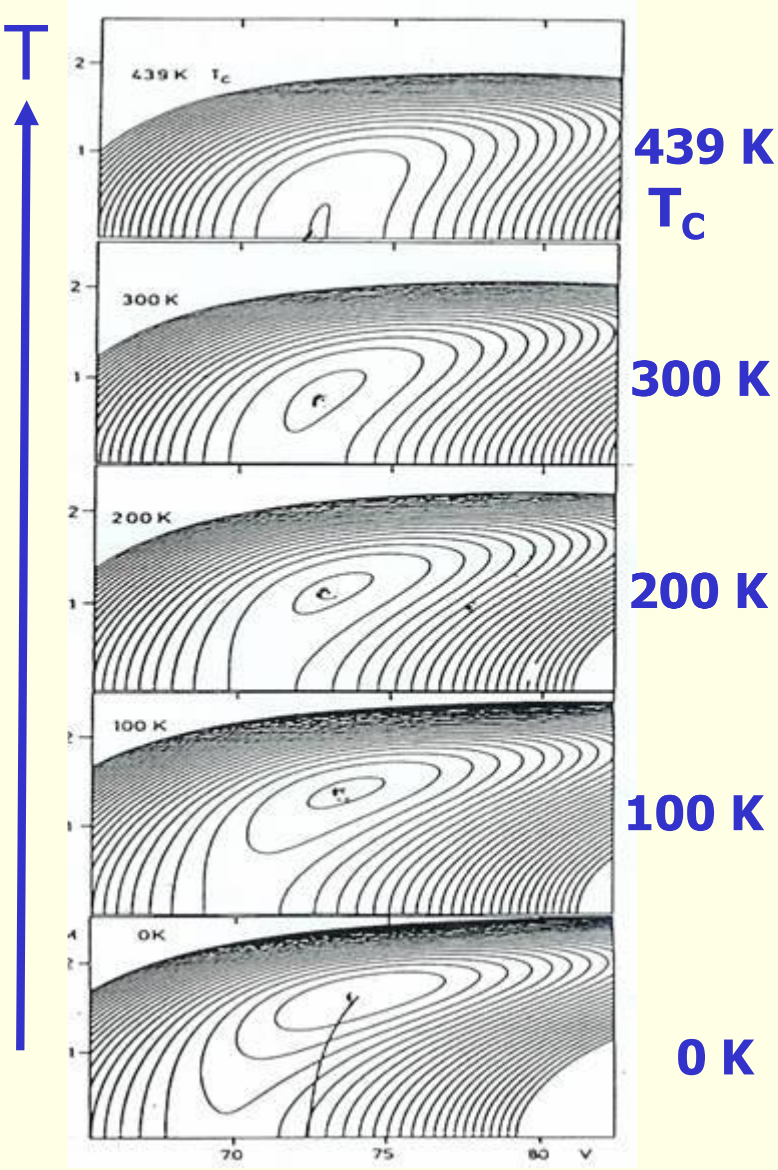
50%

0%

Finite temperature

- Energy surface at T=0 (DFT)
  - *as a function of volume and moment*
  - *using fixed spin moment (FSM) calculations*
- Finite temperature
  - *Spin and volume fluctuations*
  - *Ginzburg-Landau model*

$$H = V^{-1} \int d^3r \; (E(M + \underline{m(r)}), V + \underline{v(r)}) + \frac{C}{2} \sum_{ij} \underline{(\nabla_j m_i)^2} + \frac{D}{2} (\nabla \underline{v(r)})^2)$$



FSM calculations

- fixed spin moment (FSM)
  e.g. Fe-Ni alloy

- allows to explore energy surface $E(V,M)$
  as function of
  - *volume* ***V***
  - *magnetic moment* ***M***

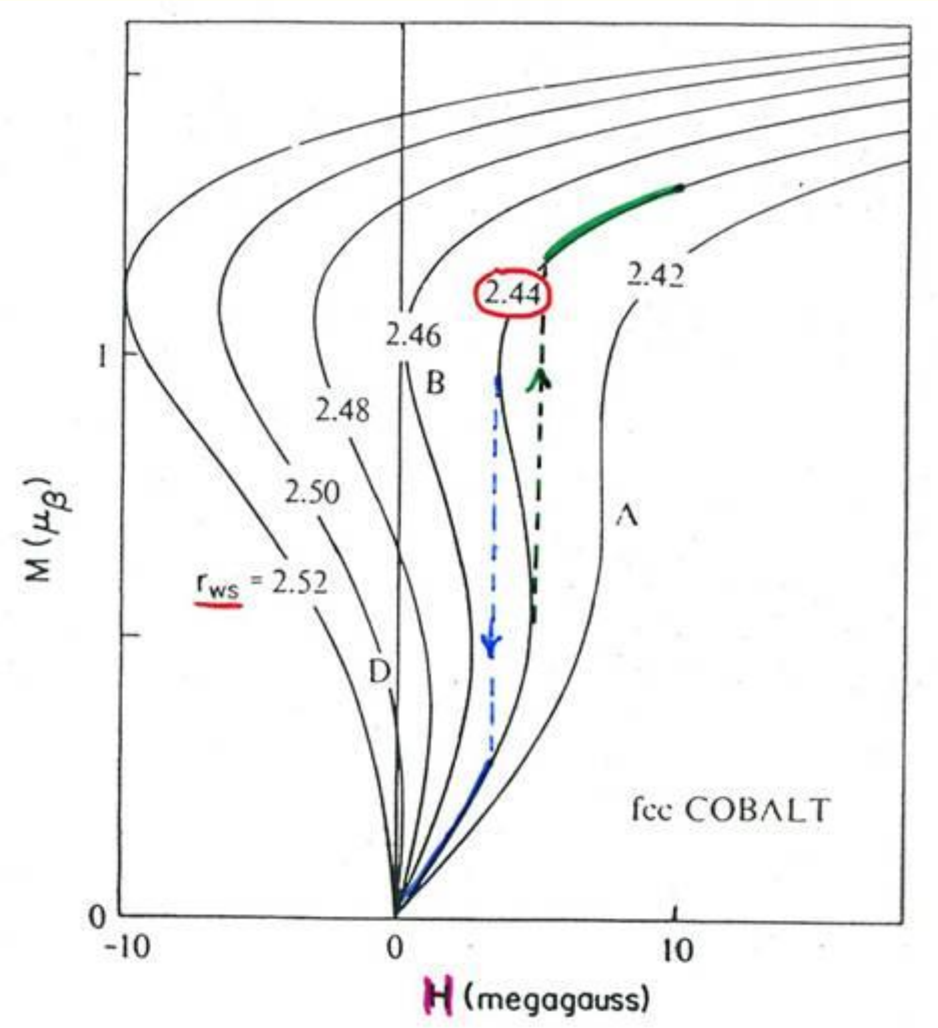
Fixed spin moment (FSM) method

- There are systems (e.g. like fcc Fe or fcc Co), for which the magnetization shows a hysteresis, when a magnetic field is applied (at a volume V).
- The volume of the unit cell defines the Wigner-Seitz radius ***r_{ws}***

$$V = \frac{4\pi r_{ws}^3}{3}$$

- The hysteresis causes numerical difficulties, since there are several solutions (in the present case 3 for a certain field H).
- In order to solve this problem the FSM method was invented

Hysteresis



Fixed spin moment (FSM) method

- Conventional scheme

$$E_F^{\uparrow} = E_F^{\downarrow}$$

$$Z_v = N^{\uparrow} + N^{\downarrow}$$

output $\boxed{M = N^{\uparrow} - N^{\downarrow}}$

constrained (FSM) method

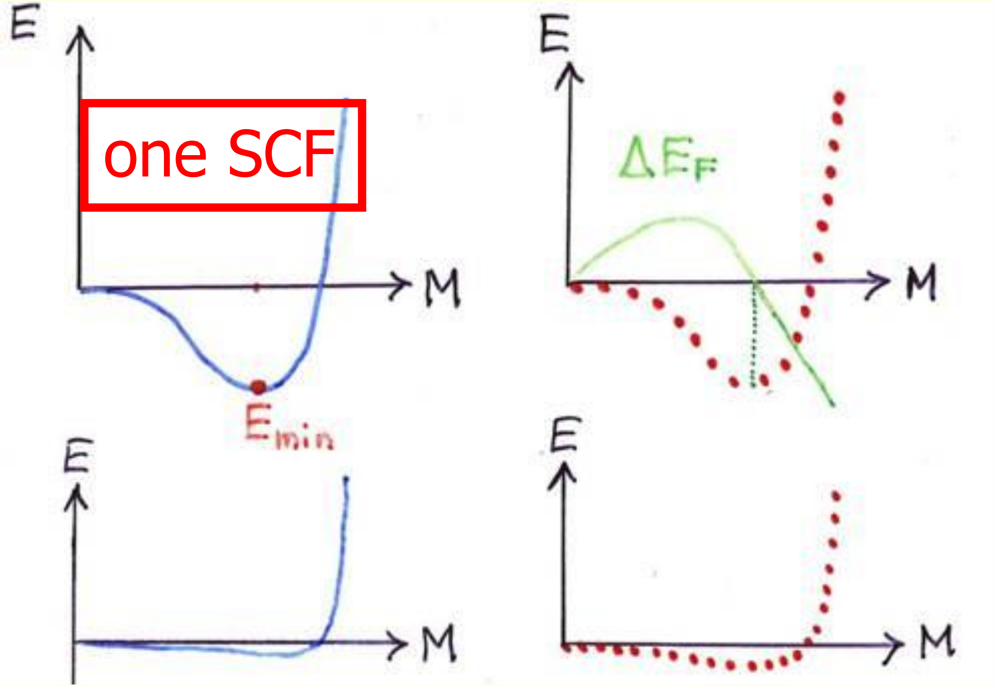
$$E_F^{\uparrow} \neq E_F^{\downarrow}$$ output

$$Z_v = N^{\uparrow} + N^{\downarrow}$$

$\boxed{M = N^{\uparrow} - N^{\downarrow}}$ input

Simple case:
bcc Fe

difficult case:
Fe$_3$Ni



one SCF

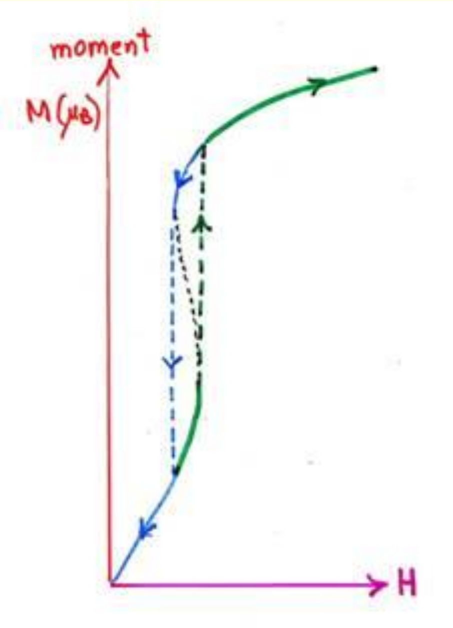
many calculations

poor convergence

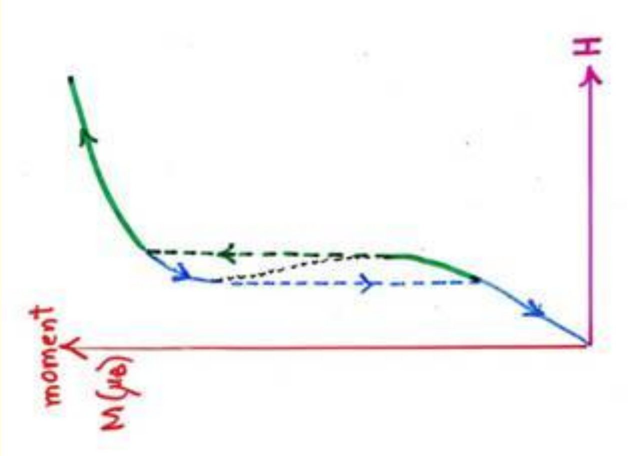
good convergence

FSM

- Physical situation:
  - *One applies a field H and obtains M*
  - *but this functions can be multivalued*



- Computational trick (unphysical):
  - *One interchanges the dependent and independent variable*
  - *this function is single valued (unique)*
  - *i.e. one chooses M and calculates H afterwards*



FSM key references

A.R.Williams, V.L.Moruzzi, J.Kübler, K.Schwarz,
Bull.Am.Phys.Soc. **29**, 278 (1984)

K.Schwarz, P.Mohn
J.Phys.F **14**, L129 (1984)

P.H.Dederichs, S.Blügel, R.Zoller, H.Akai,
Phys. Rev, Lett. **53**,2512 (1984)

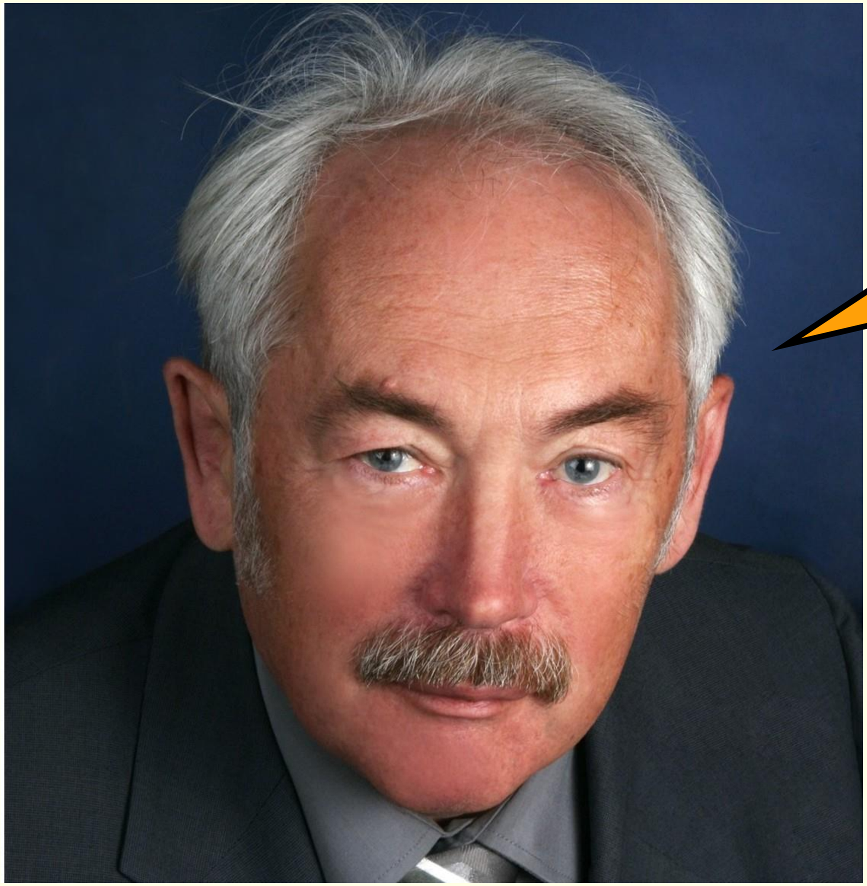
Unusual magnetic systems

- GMR (Giant Magneto Resistance)
- half-metallic systems

  e.g. CrO_2
- important for spintronics

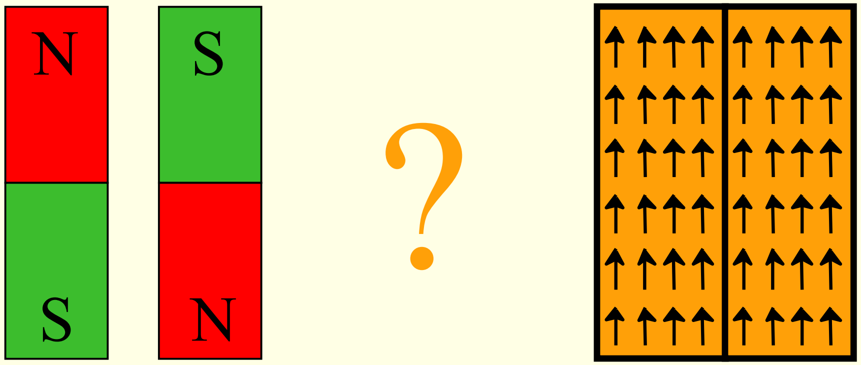
Once upon a time, …

Once upon a time, in the early 1980’s …



Peter Grünberg

“What happens if
I bring two ferromagnets close
–I mean *really* close–
together?”



Giant magnetoresistance (GMR)

Ferromagnet
Metal
Ferromagnet

Electrical resistance: R_P <(>) R_{AP}

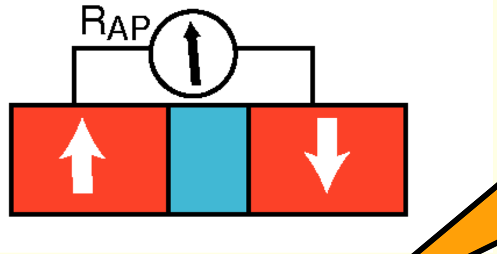
The electrical resistance depends on the relative magnetic alignment of the ferromagnetic layers

$$\text{GMR} = \frac{R_{AP} - R_P}{R_P}$$

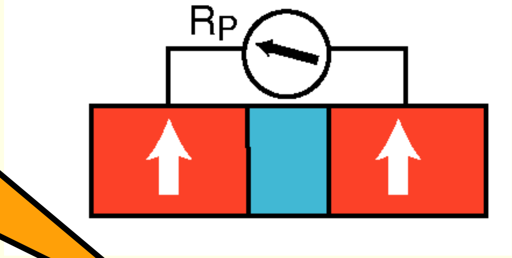
19% for trilayers @RT
80% for multilayers @ RT

GMR is much larger than the anisotropic magnetoresistance (AMR)

1988: … simultaneously, but independent …

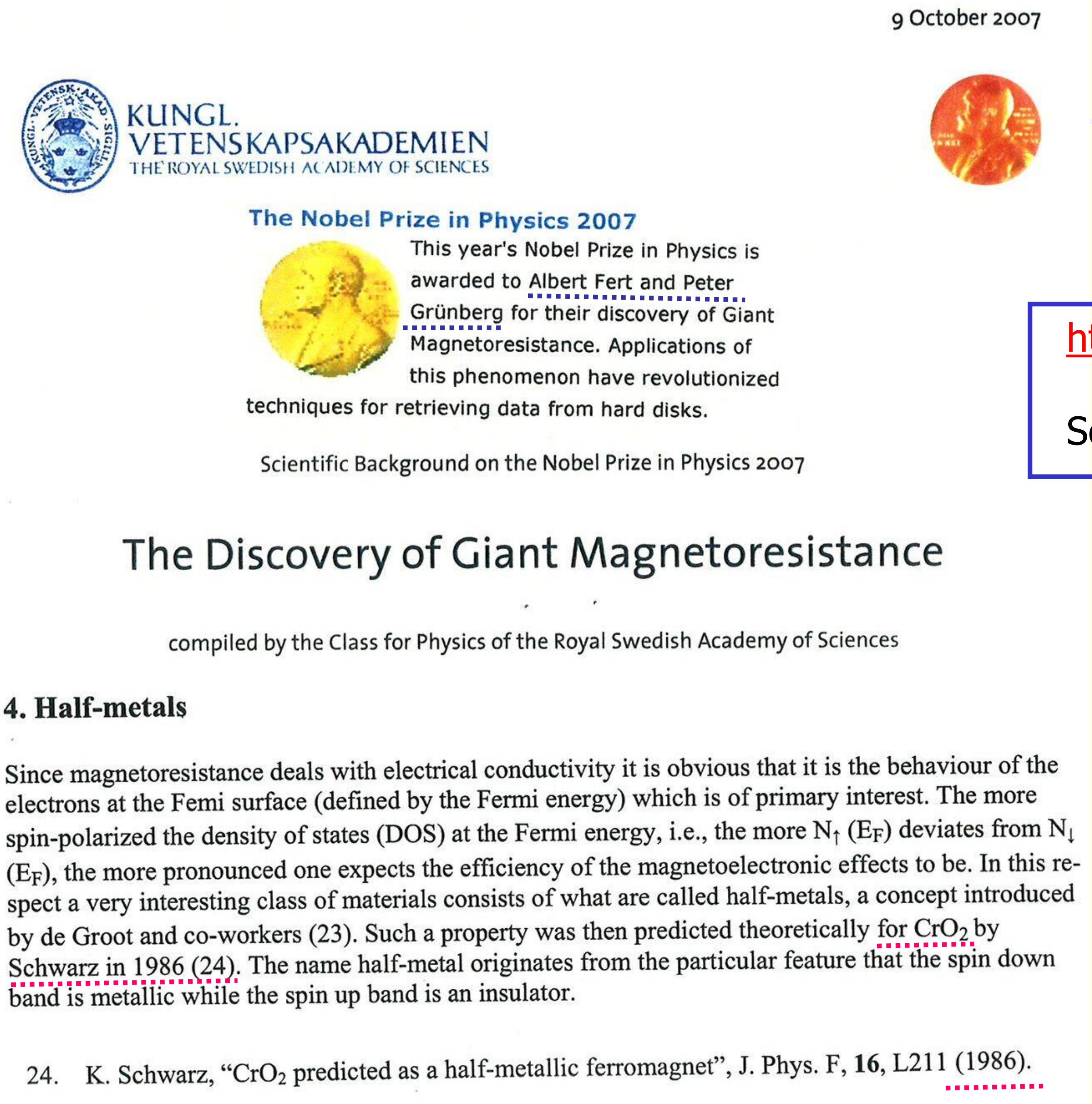


“Does the electrical resistance depend on the magnetization alignment?”



Albert Fert

Peter Grünberg



9 October 2007

KUNGL.
VETENSKAPSAKADEMIEN
THE ROYAL SWEDISH ACADEMY OF SCIENCES

The Nobel Prize in Physics 2007

This year's Nobel Prize in Physics is awarded to Albert Fert and Peter Grünberg for their discovery of Giant Magnetoresistance. Applications of this phenomenon have revolutionized techniques for retrieving data from hard disks.

Scientific Background on the Nobel Prize in Physics 2007

The Discovery of Giant Magnetoresistance

compiled by the Class for Physics of the Royal Swedish Academy of Sciences

4. Half-metals

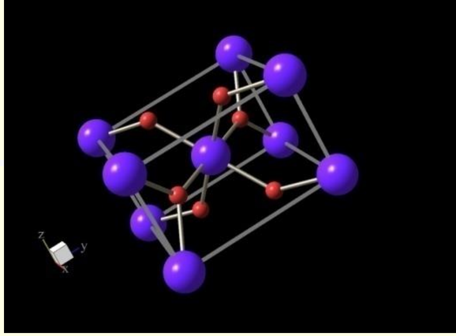
Since magnetoresistance deals with electrical conductivity it is obvious that it is the behaviour of the electrons at the Femi surface (defined by the Fermi energy) which is of primary interest. The more spin-polarized the density of states (DOS) at the Fermi energy, i.e., the more $N_\uparrow$ (E_F) deviates from $N_\downarrow$ (E_F), the more pronounced one expects the efficiency of the magnetoelectronic effects to be. In this respect a very interesting class of materials consists of what are called half-metals, a concept introduced by de Groot and co-workers (23). Such a property was then predicted theoretically for CrO_2 by Schwarz in 1986 (24). The name half-metal originates from the particular feature that the spin down band is metallic while the spin up band is an insulator.

24. K. Schwarz, "CrO_2 predicted as a half-metallic ferromagnet", J. Phys. F, **16**, L211 (1986).

http://www.kva.se/

Scientific background

CrO_2 half-metallic ferromagnet



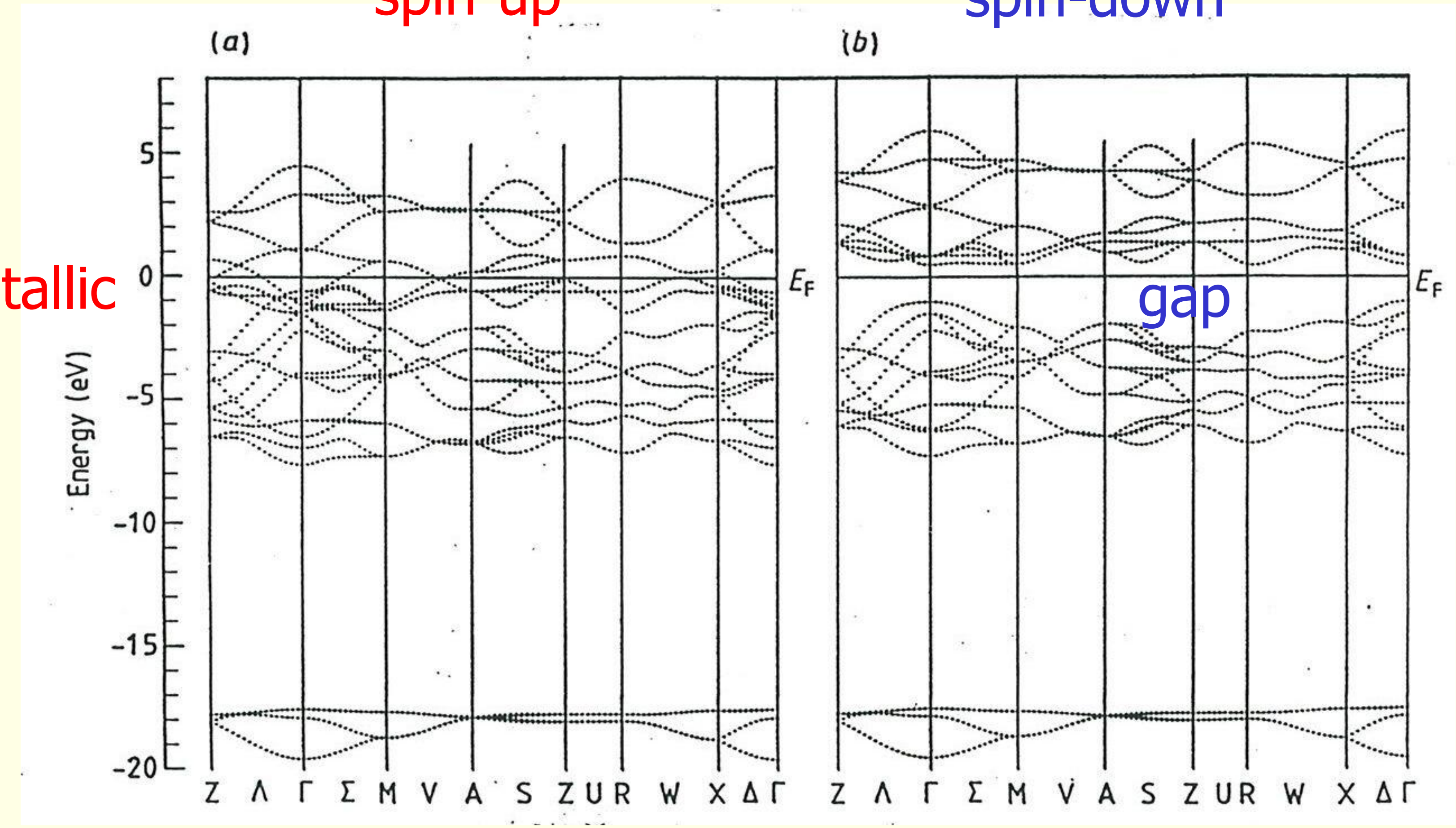
- CrO_2 (rutile structure)

spin-up

spin-down

metallic

gap



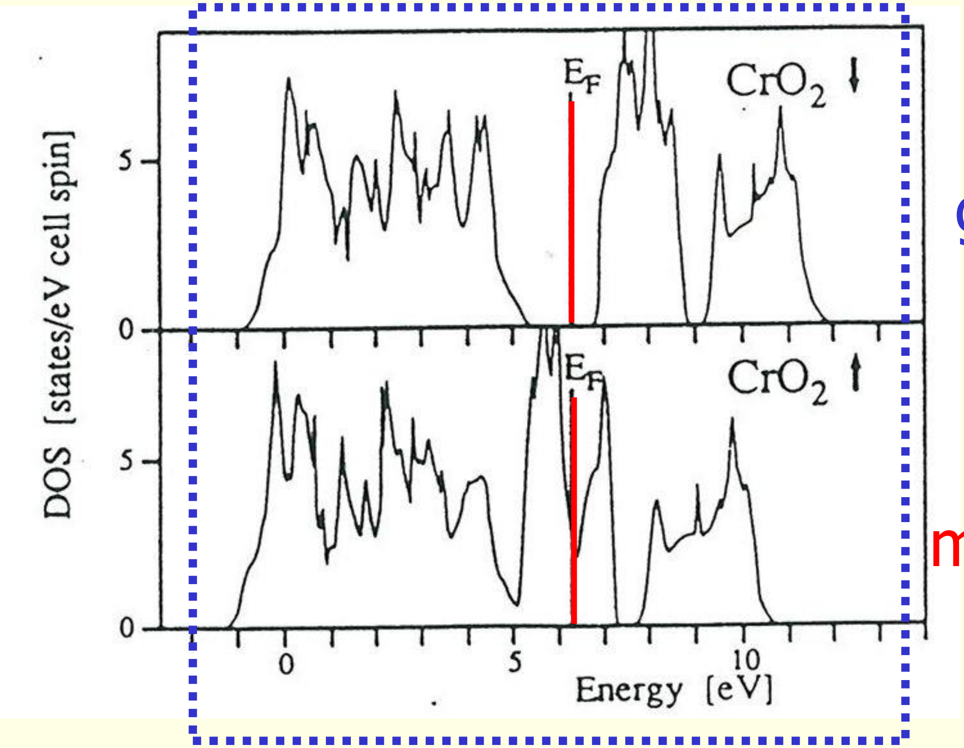
important for spintronics

CrO_2 DOS

K.Schwarz,
CrO_2 predicted as a
half-metallic ferromagnet,
J.Phys.F:Met.Phys. **16**, L211 (1986)

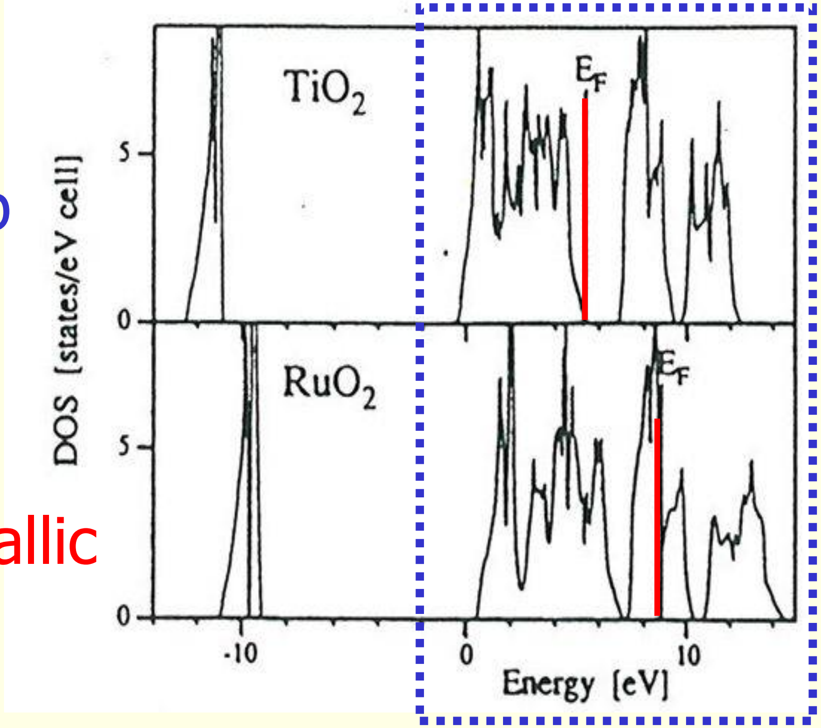
- The DOS features of CrO_2 are qualitatively like
  - *TiO_2 (for spin-down)*
  - *RuO_2 (for spin-up)*

	4	5	6	7	8
spin ↓	**Ti**	**V**	**Cr**	**Mn**	**Fe**
↑	**Zr**	**Nb**	**Mo**	**Tc**	**Ru**



gap

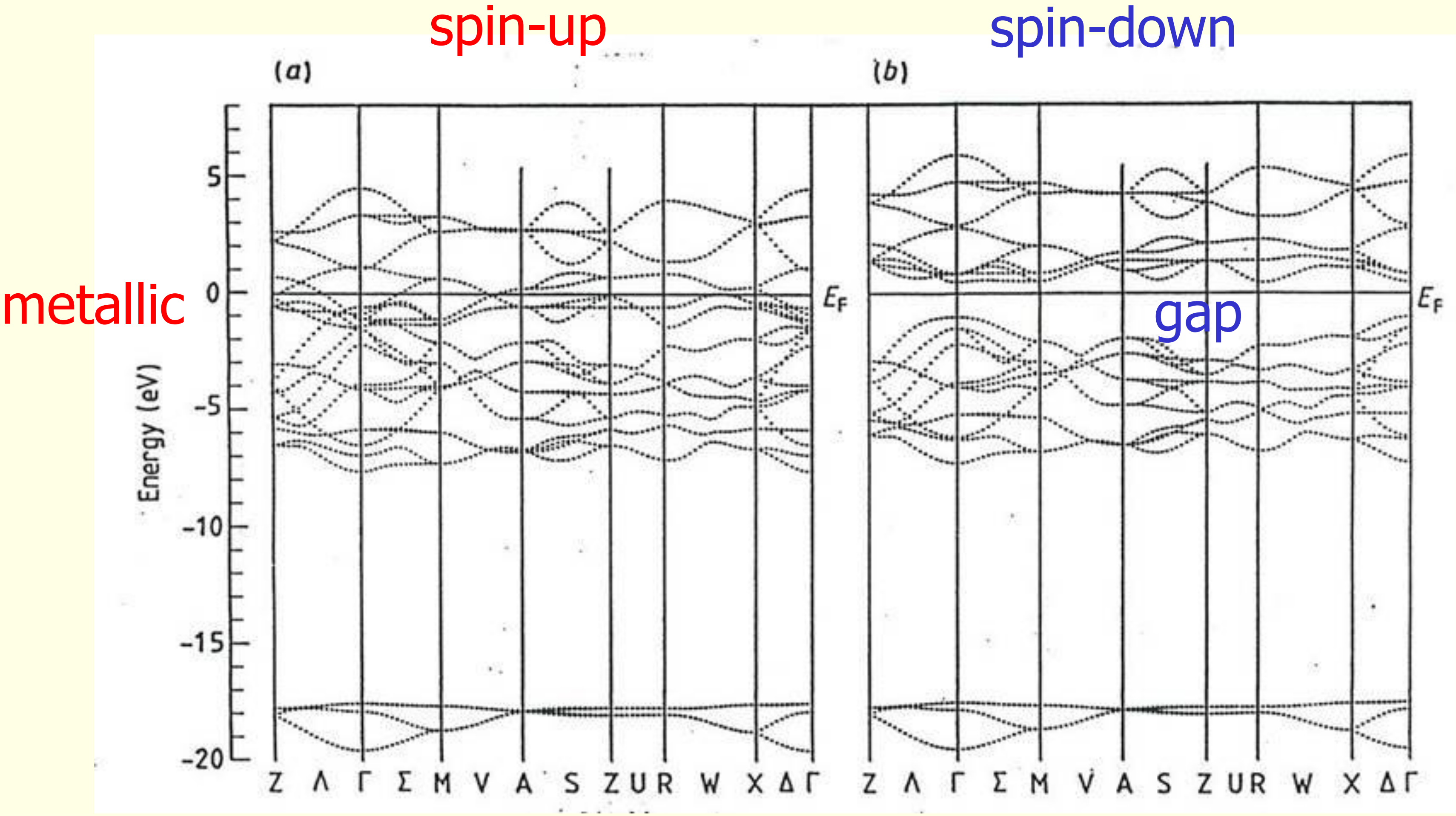
metallic



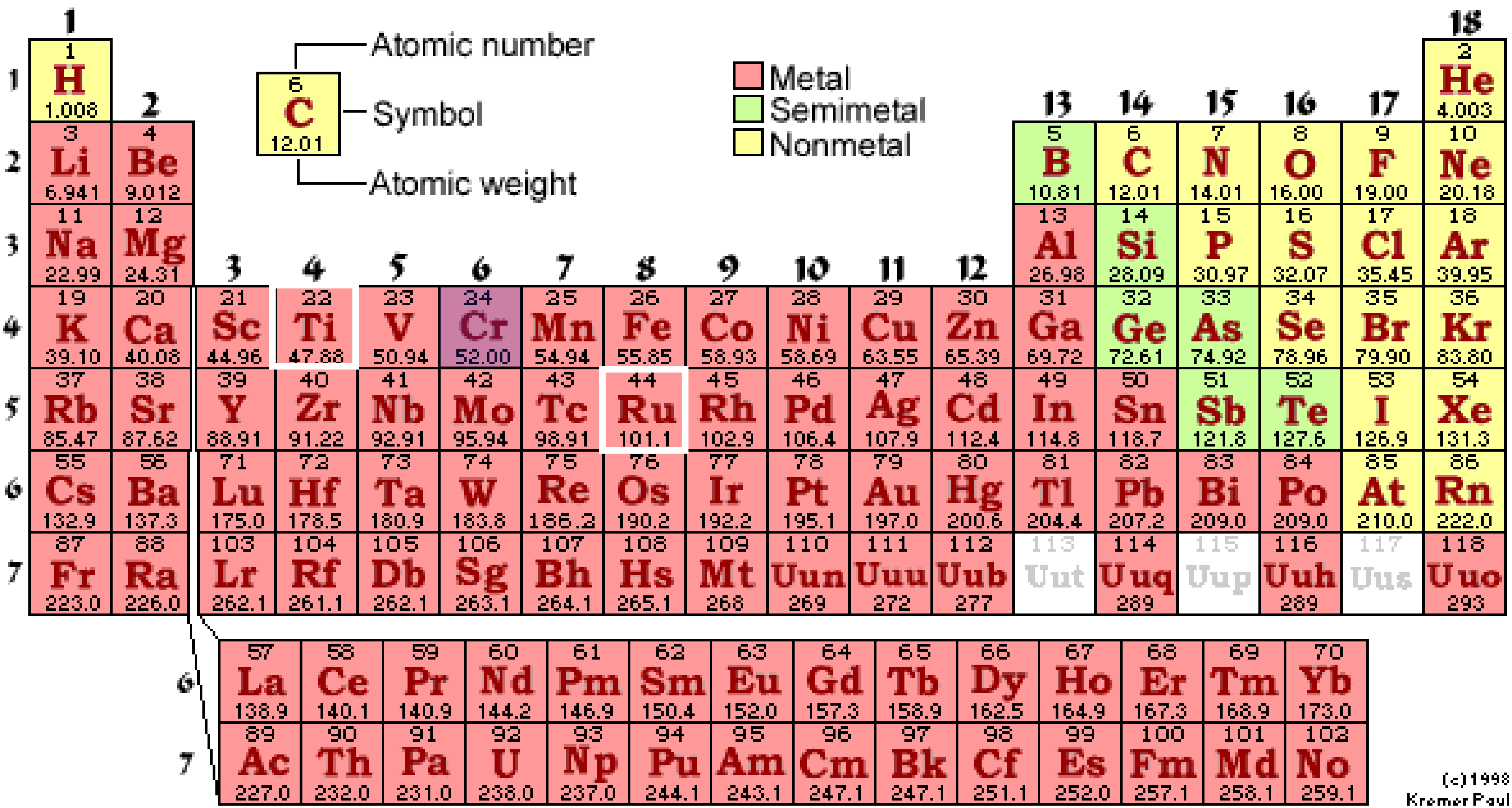
all three compound crystallize in the rutile structure

Half-metallic ferromagnet

- CrO_2 (rutile structure)



CrO_2 spin-down (TiO_2) spin-up (RuO_2)



Atomic number
Symbol
Atomic weight

6 C 12.01

🟥 Metal
🟩 Semimetal
🟨 Nonmetal

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 **H** 1.008																	2 **He** 4.003
2	3 **Li** 6.941	4 **Be** 9.012											5 **B** 10.81	6 **C** 12.01	7 **N** 14.01	8 **O** 16.00	9 **F** 19.00	10 **Ne** 20.18
3	11 **Na** 22.99	12 **Mg** 24.31											13 **Al** 26.98	14 **Si** 28.09	15 **P** 30.97	16 **S** 32.07	17 **Cl** 35.45	18 **Ar** 39.95
4	19 **K** 39.10	20 **Ca** 40.08	21 **Sc** 44.96	22 **Ti** 47.88	23 **V** 50.94	24 **Cr** 52.00	25 **Mn** 54.94	26 **Fe** 55.85	27 **Co** 58.93	28 **Ni** 58.69	29 **Cu** 63.55	30 **Zn** 65.39	31 **Ga** 69.72	32 **Ge** 72.61	33 **As** 74.92	34 **Se** 78.96	35 **Br** 79.90	36 **Kr** 83.80
5	37 **Rb** 85.47	38 **Sr** 87.62	39 **Y** 88.91	40 **Zr** 91.22	41 **Nb** 92.91	42 **Mo** 95.94	43 **Tc** 98.91	44 **Ru** 101.1	45 **Rh** 102.9	46 **Pd** 106.4	47 **Ag** 107.9	48 **Cd** 112.4	49 **In** 114.8	50 **Sn** 118.7	51 **Sb** 121.8	52 **Te** 127.6	53 **I** 126.9	54 **Xe** 131.3
6	55 **Cs** 132.9	56 **Ba** 137.3	71 **Lu** 175.0	72 **Hf** 178.5	73 **Ta** 180.9	74 **W** 183.8	75 **Re** 186.2	76 **Os** 190.2	77 **Ir** 192.2	78 **Pt** 195.1	79 **Au** 197.0	80 **Hg** 200.6	81 **Tl** 204.4	82 **Pb** 207.2	83 **Bi** 209.0	84 **Po** 209.0	85 **At** 210.0	86 **Rn** 222.0
7	87 **Fr** 223.0	88 **Ra** 226.0	103 **Lr** 262.1	104 **Rf** 261.1	105 **Db** 262.1	106 **Sg** 263.1	107 **Bh** 264.1	108 **Hs** 265.1	109 **Mt** 268	110 **Uun** 269	111 **Uuu** 272	112 **Uub** 277	113 **Uut**	114 **Uuq** 289	115 **Uup**	116 **Uuh** 289	117 **Uus**	118 **Uuo** 293

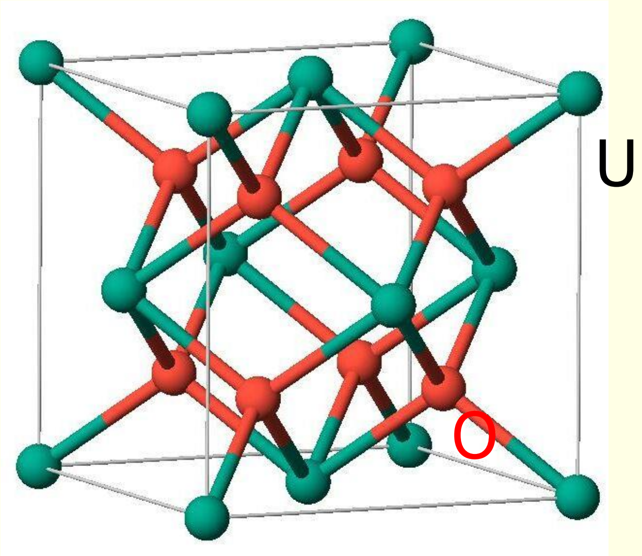
6	57 **La** 138.9	58 **Ce** 140.1	59 **Pr** 140.9	60 **Nd** 144.2	61 **Pm** 146.9	62 **Sm** 150.4	63 **Eu** 152.0	64 **Gd** 157.3	65 **Tb** 158.9	66 **Dy** 162.5	67 **Ho** 164.9	68 **Er** 167.3	69 **Tm** 168.9	70 **Yb** 173.0
7	89 **Ac** 227.0	90 **Th** 232.0	91 **Pa** 231.0	92 **U** 238.0	93 **Np** 237.0	94 **Pu** 244.1	95 **Am** 243.1	96 **Cm** 247.1	97 **Bk** 247.1	98 **Cf** 251.1	99 **Es** 252.0	100 **Fm** 257.1	101 **Md** 258.1	102 **No** 259.1

(c)1998
Kremer Paul

Magnetic structure of uranium dioxide UO_2

- R.Laskowski
- G.K.H.Madsen
- P.Blaha
- K.Schwarz

- topics
  - *non-collinear magnetism*
  - *spin-orbit coupling*
  - *LDA+U (correlation of U-5f electrons)*
  - *Structure relaxations*
  - *electric field gradient (EFG)*



R.Laskowski, G.K.H.Madsen, P.Blaha, K.Schwarz:
Magnetic structure and electric-field gradients of uranium dioxide: An ab initio study
Phys.Rev.B **69**, 140408-1-4 (2004)

Atomic configuration of uranium (Z=92)

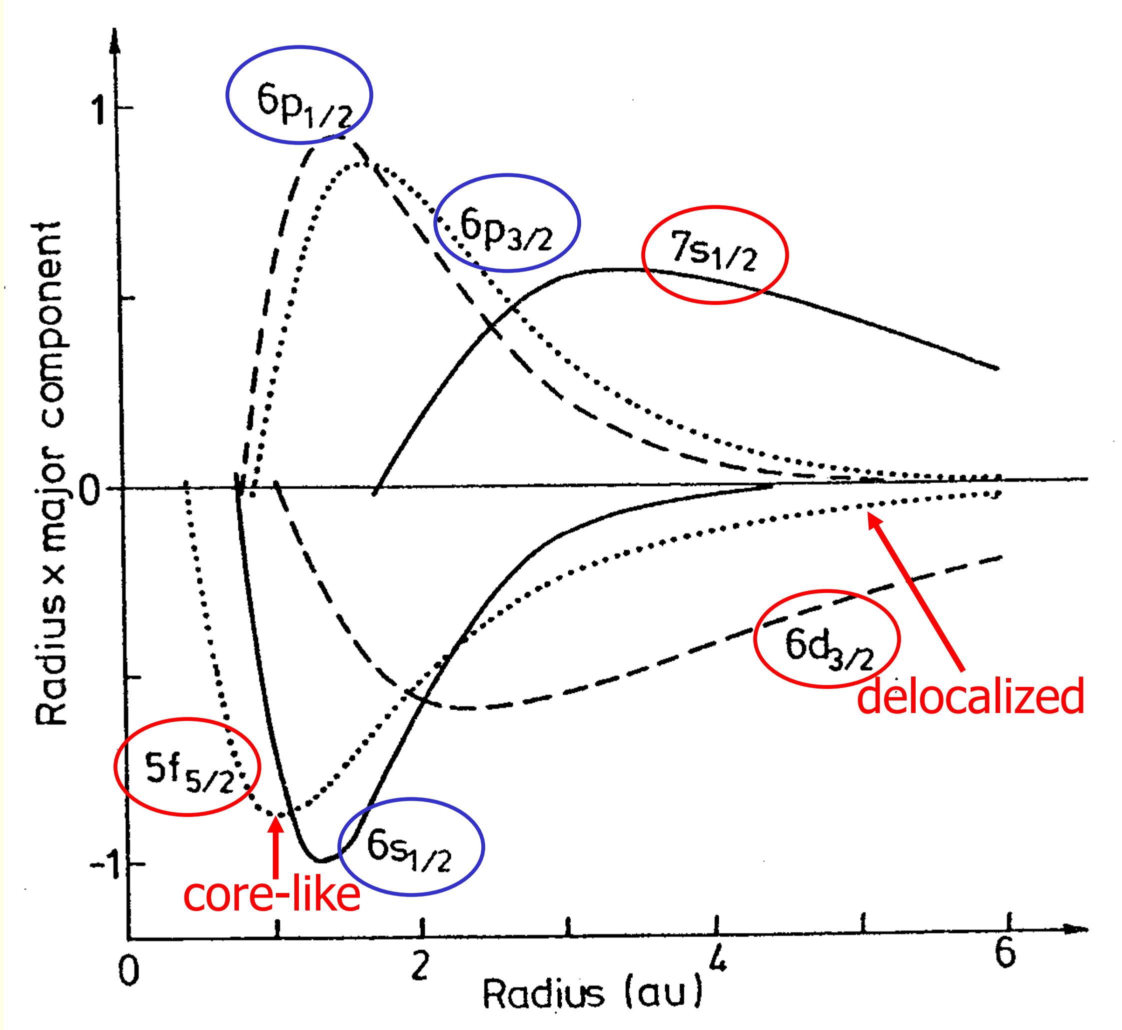
[Rn]

U [Xe] $4f^{14}$ $5d^{10}$ $6s^2$ $6p^6$ $5f^3$ $6d^1$ $7s^2$

core **semi-core** **valence**

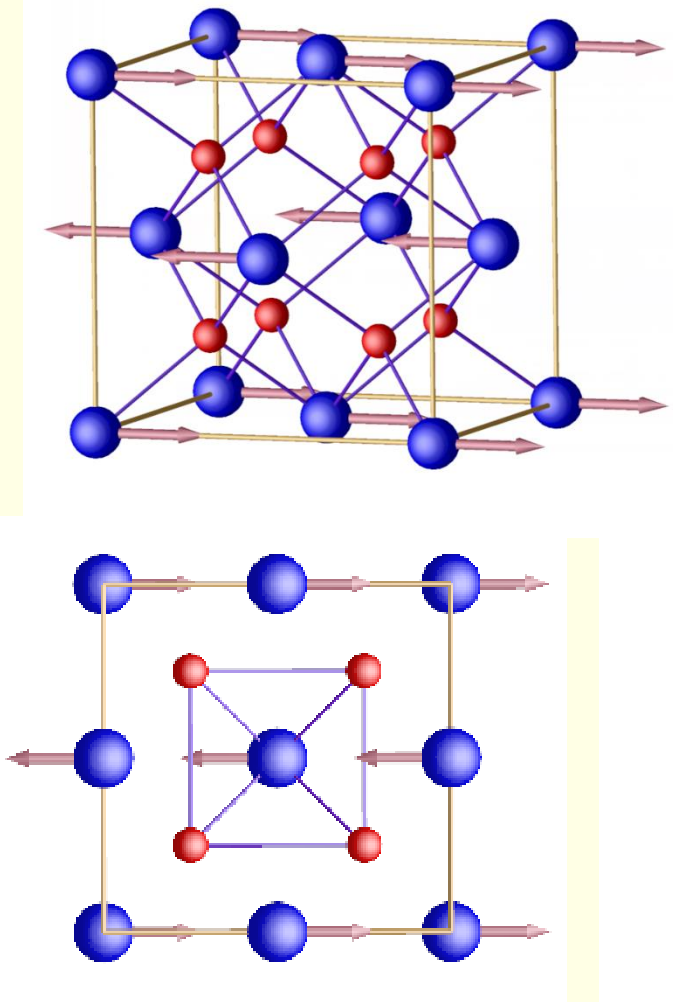
E_j (Ryd)

nrel	**j** (relativ.)	
n ℓ	**ℓ-s**	**ℓ+s**
7s		-0.25
6d	-0.29	-0.25
5f	-0.17	-0.11
6p	-1.46	-2.10
6s		-3.40
5d	-7.48	-6.89
5p	-18.05	-14.06
5s		-22.57
4f	-27.58	-26.77
…		
1s		-8513.38

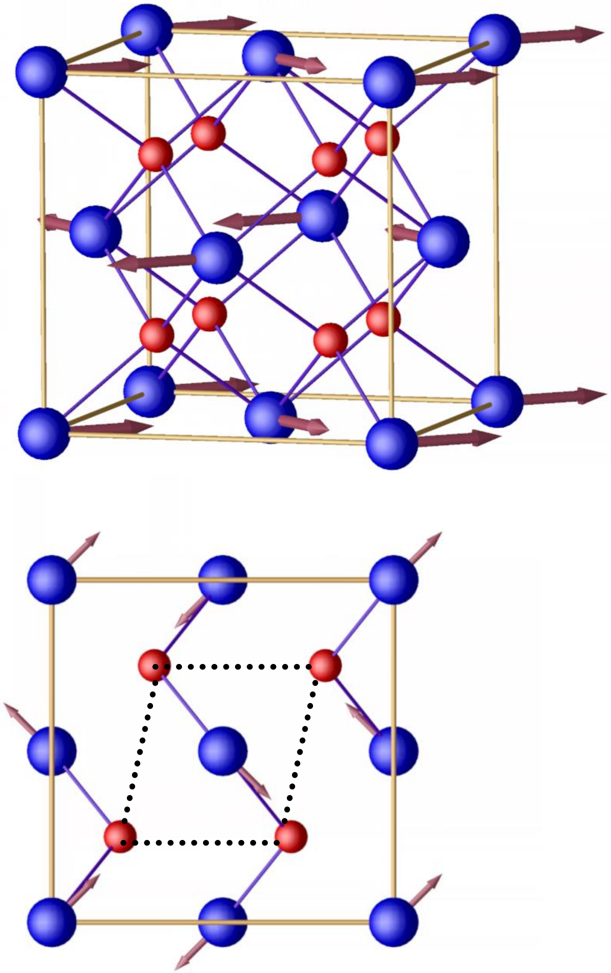


non-collinear magnetism in UO_2

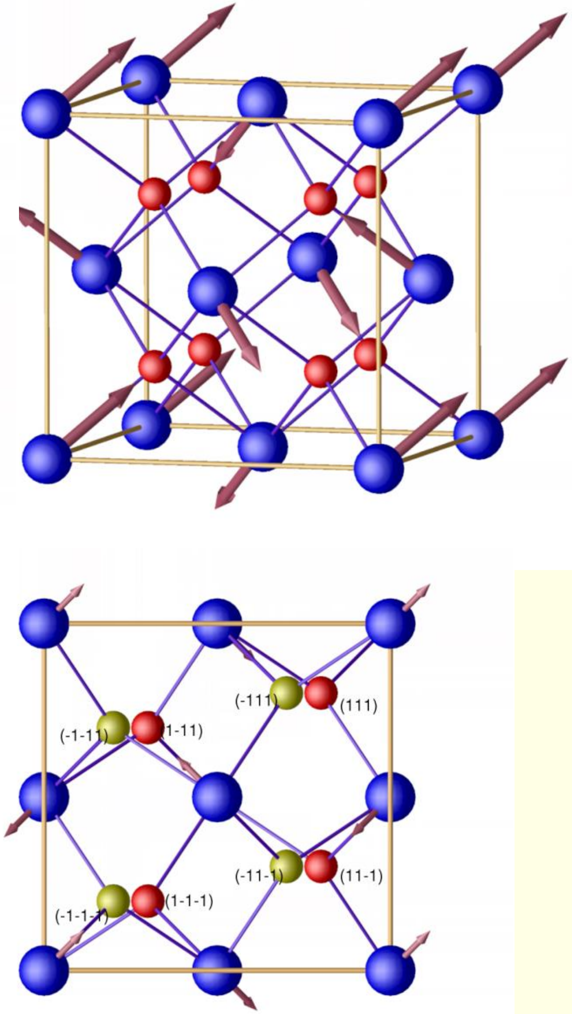
collinear 1k-



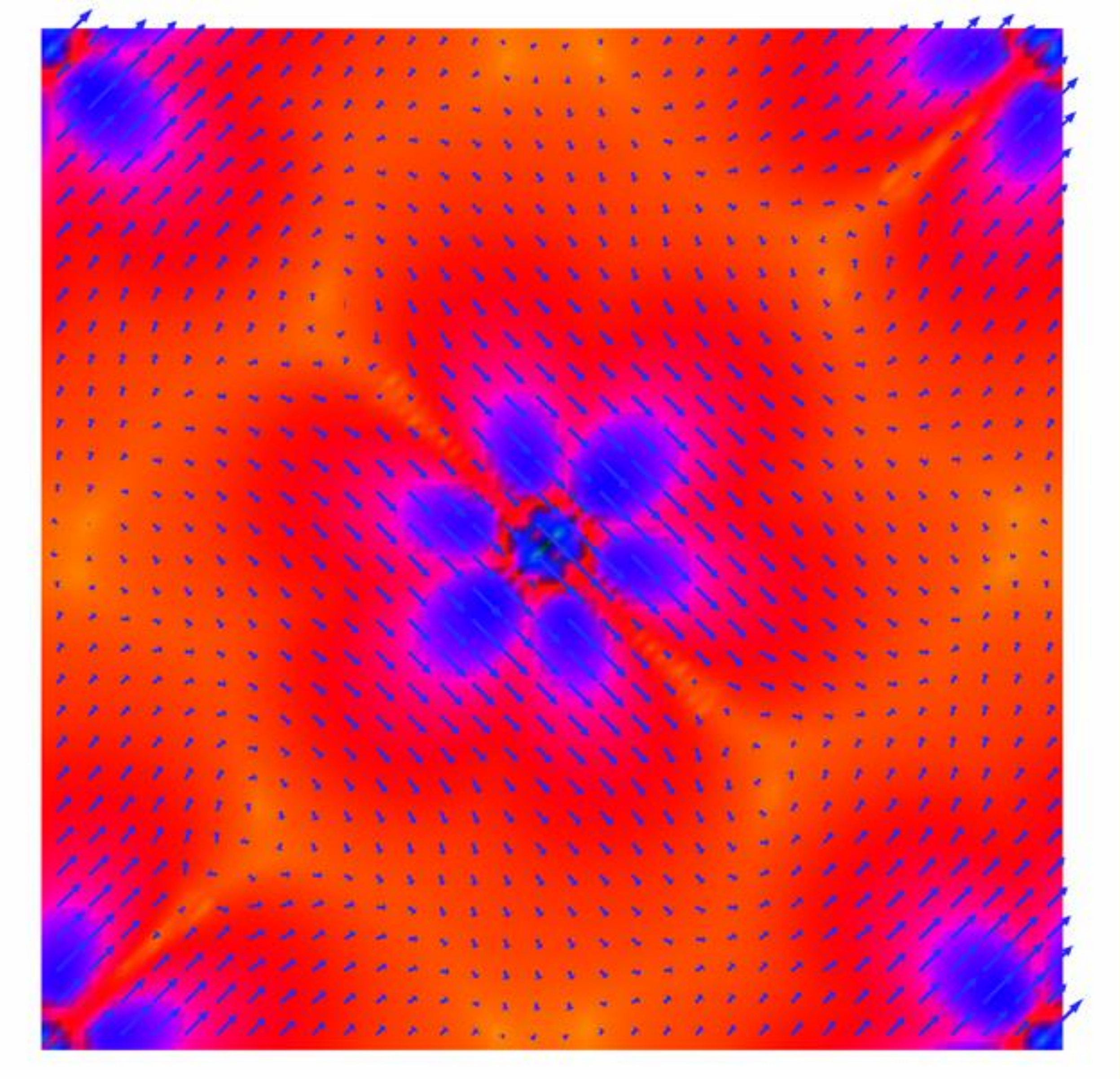
non-collinear 2k-



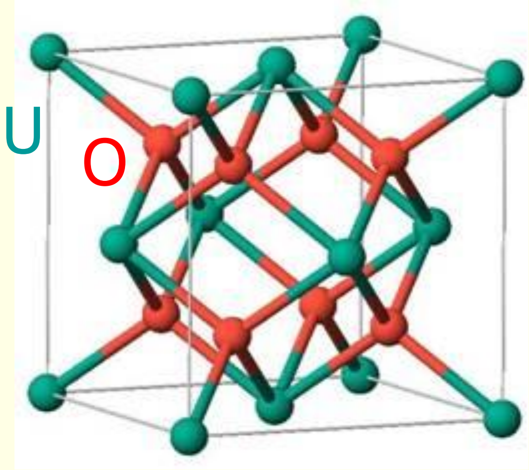
or 3k-structure



UO_2 2k structure, LDA+SO+U



- Magnetisation direction perpenticular at the two U sites (arrows)
- Magnetisation density (color)

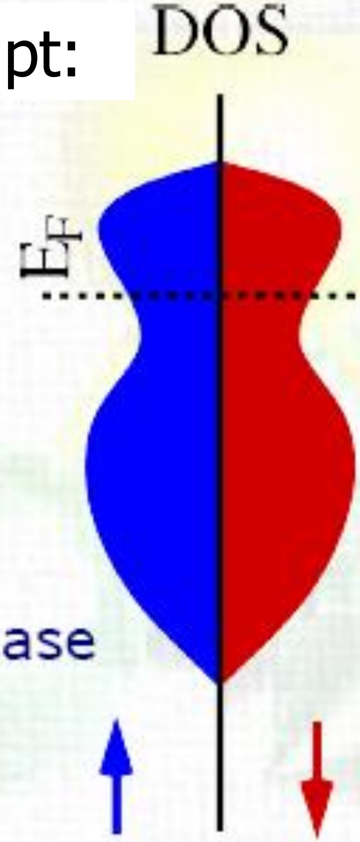


Magnetism with WIEN2k

- Wien2k can only handle collinear or non-magnetic cases

run_lapw script:

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

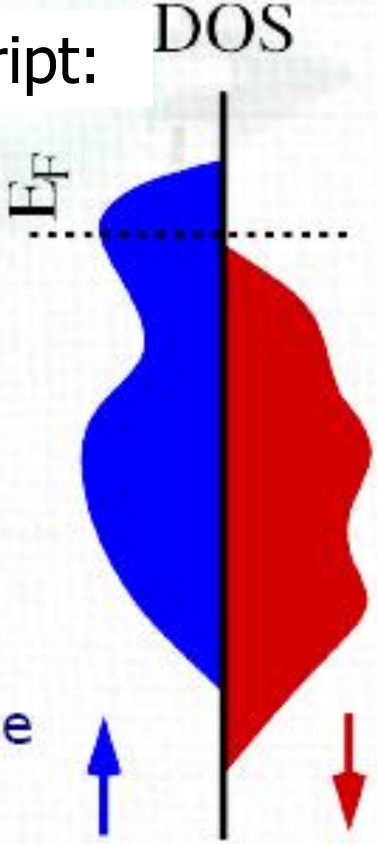


non-magnetic case

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

runsp_lapw script:

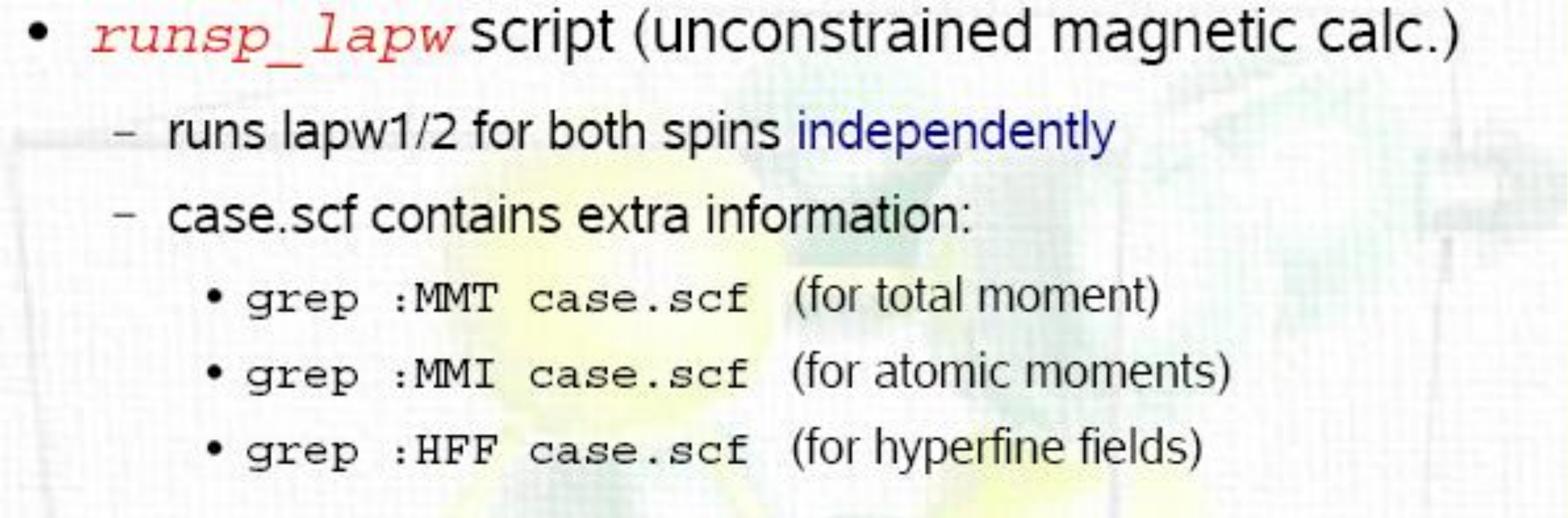
```
x lapw0
x lapw1 -up
x lapw1 -dn
x lapw2 -up
x lapw2 -dn
x lcore -up
x lcore -dn
x mixer
```



magnetic case

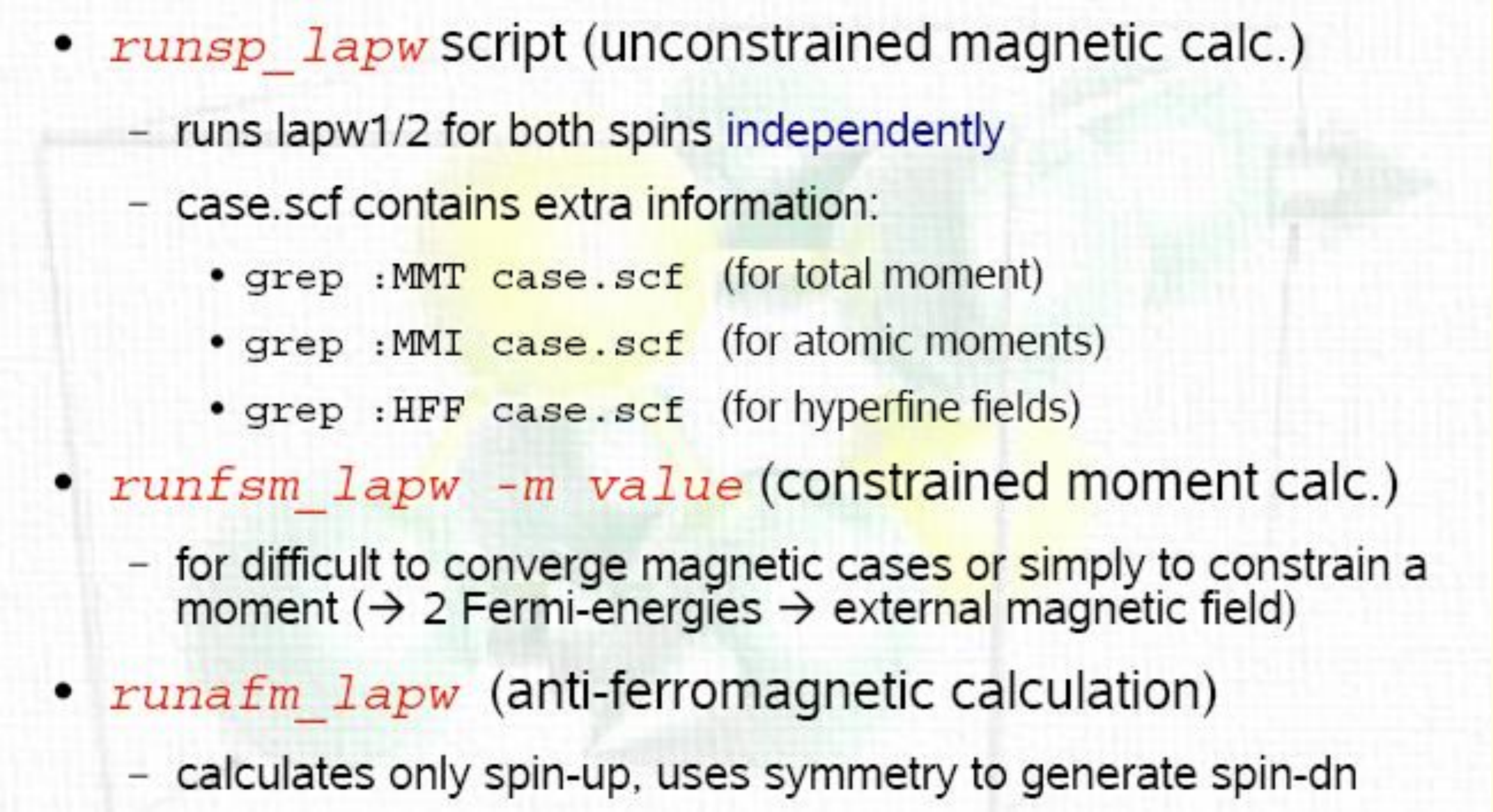
$m = n_\uparrow - n_\downarrow \neq 0$

Spin polarized calculations



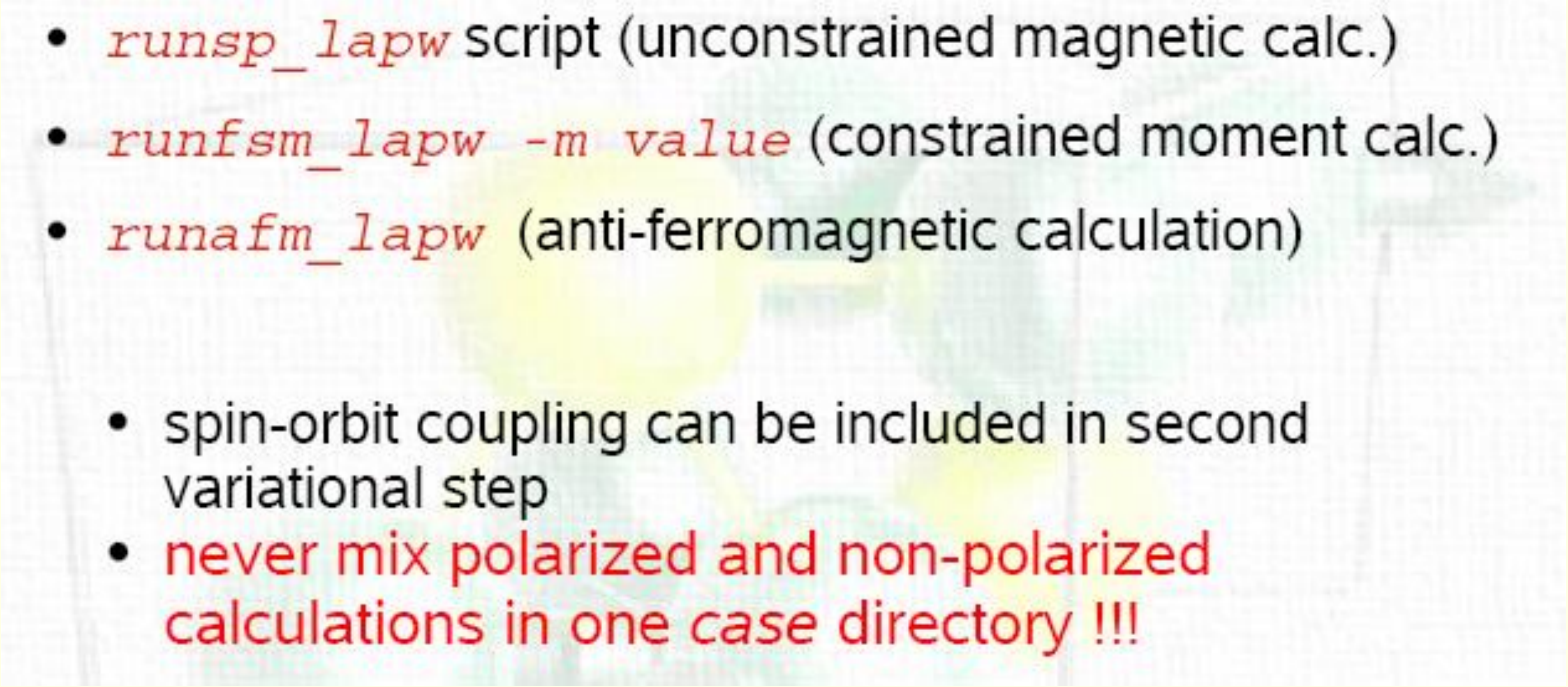
- *runsp_lapw* script (unconstrained magnetic calc.)
  - runs lapw1/2 for both spins independently
  - case.scf contains extra information:
    - `grep :MMT case.scf` (for total moment)
    - `grep :MMI case.scf` (for atomic moments)
    - `grep :HFF case.scf` (for hyperfine fields)

Run spin-polarized, FSM or AFM calculations



- *runsp_lapw* script (unconstrained magnetic calc.)
  - runs lapw1/2 for both spins independently
  - case.scf contains extra information:
    - `grep :MMT case.scf` (for total moment)
    - `grep :MMI case.scf` (for atomic moments)
    - `grep :HFF case.scf` (for hyperfine fields)
- *runfsm_lapw -m value* (constrained moment calc.)
  - for difficult to converge magnetic cases or simply to constrain a moment (→ 2 Fermi-energies → external magnetic field)
- *runafm_lapw* (anti-ferromagnetic calculation)
  - calculates only spin-up, uses symmetry to generate spin-dn

Various magnetism cases



- `runsp_lapw` script (unconstrained magnetic calc.)
- `runfsm_lapw -m value` (constrained moment calc.)
- `runafm_lapw` (anti-ferromagnetic calculation)

  - spin-orbit coupling can be included in second variational step
  - never mix polarized and non-polarized calculations in one *case* directory !!!

Thank you for your attention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