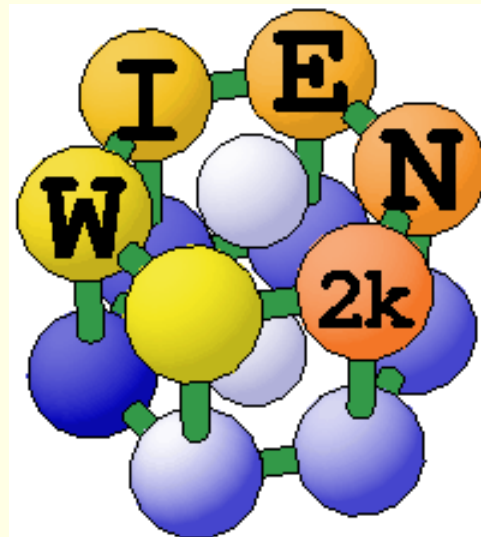


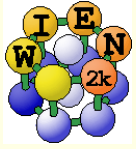
# Magnetism (FM, AFM, FSM)

**Karlheinz Schwarz**

Institute of Materials Chemistry

TU Wien

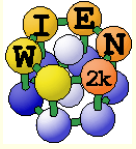




# Localized vs. itinerant systems

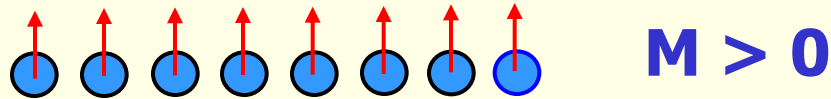


- In **localized** systems (e.g. some rare earth) the magnetism is mainly governed by the atom (Hund's rule)
- In **itinerant (delocalized)** systems (many transition metals) magnetism comes from partial occupation of states, which differ between spin-up and spin-down.
- **Boarderline** cases (some f-electron systems)  
details of the structure (e.g. lattice spacing) determine whether or not some electrons are localized or itinerant.

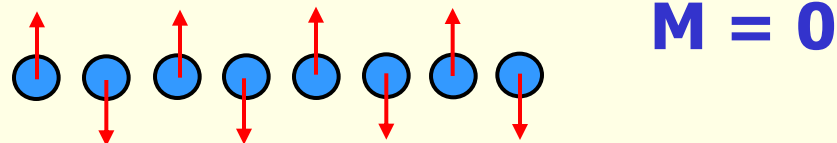


# Ferro-, antiferro-, or ferri-magnetic

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

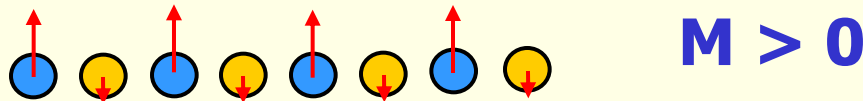


- **Antiferromagnetic (AFM)** (e.g. Cr)



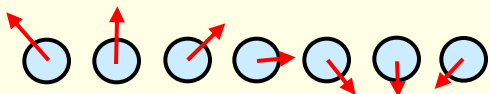
- **Ferrimagnetic** cases

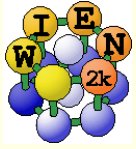
the moments at different atoms are antiparallel but of different magnitude



- **Non-collinear magnetism (NCM)**

the magnetic moments are not lined up parallel.





## Experimental facts:

	$\sigma$ [emu/g]	$\sigma$ [ $\mu_B$ ]	$T_c$ [K]	$\rho$ at 298K [ $\text{g/cm}^3$ ]
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

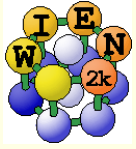


Curie  
temperature



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

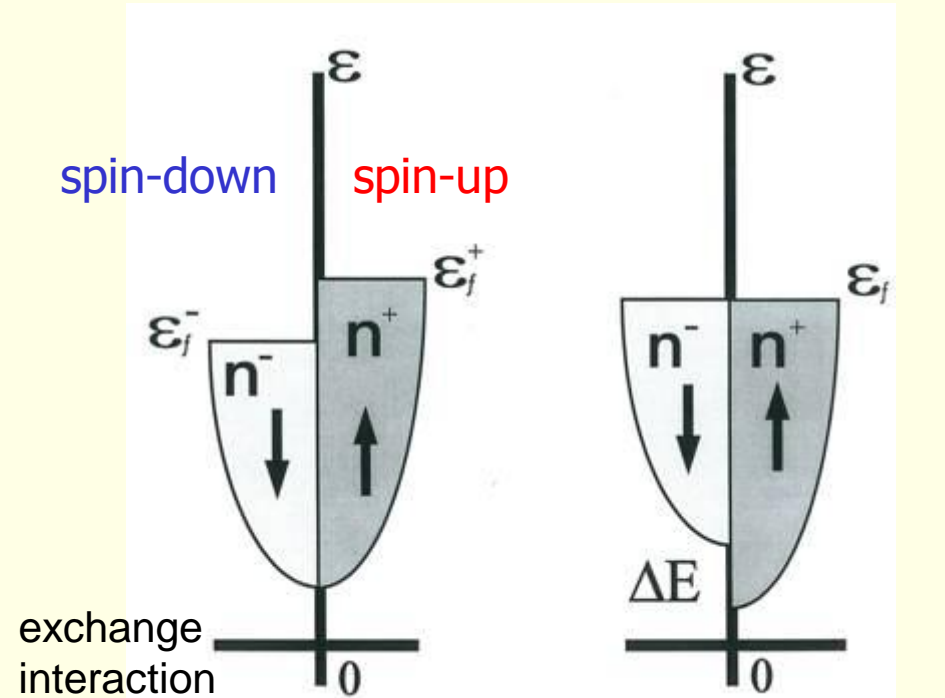


# Stoner model for itinerant electrons

In a

- **non magnetic (NM) case**  
 $\mathbf{N}_\uparrow = \mathbf{N}_\downarrow$  (spin-up and spin-down)
- **ferromagnetic (FM) case**  
 $\mathbf{N}_\uparrow > \mathbf{N}_\downarrow$  (majority and minority spin)  
 the moments at all sites are parallel (collinear)
- **the (spin) magnetic moment  $\mathbf{m}$** 
  - $\mathbf{m} = \mathbf{N}_\uparrow - \mathbf{N}_\downarrow$
  - 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

## Exchange splitting

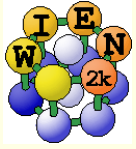


$$E_b = \int_0^{\epsilon_F} \epsilon \mathcal{N}(\epsilon) d\epsilon - \int_{\epsilon^-}^{\epsilon_F} \epsilon \mathcal{N}(\epsilon) d\epsilon + \int_0^{\epsilon_F} \epsilon \mathcal{N}(\epsilon) d\epsilon + \int_{\epsilon_F}^{\epsilon^+} \epsilon \mathcal{N}(\epsilon) d\epsilon - \frac{I_s M^2}{2}$$

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

**Stoner criterion**

$$2\mu_B^2 I_s \mathcal{N}(\epsilon_F) > 1$$



# Stoner model for itinerant electrons

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

- **Stoner criterion**

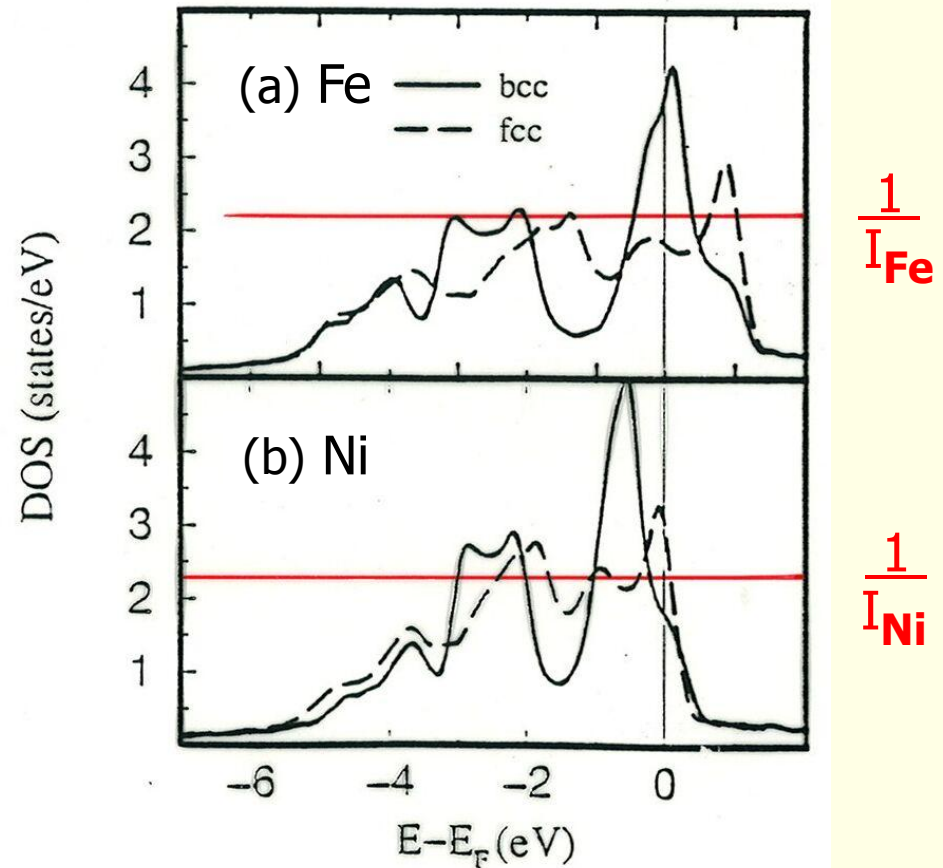
$$I \cdot N(E_F) > 1$$

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

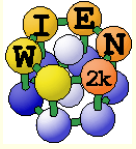
$I$  Stoner parameter

$\sim$  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)

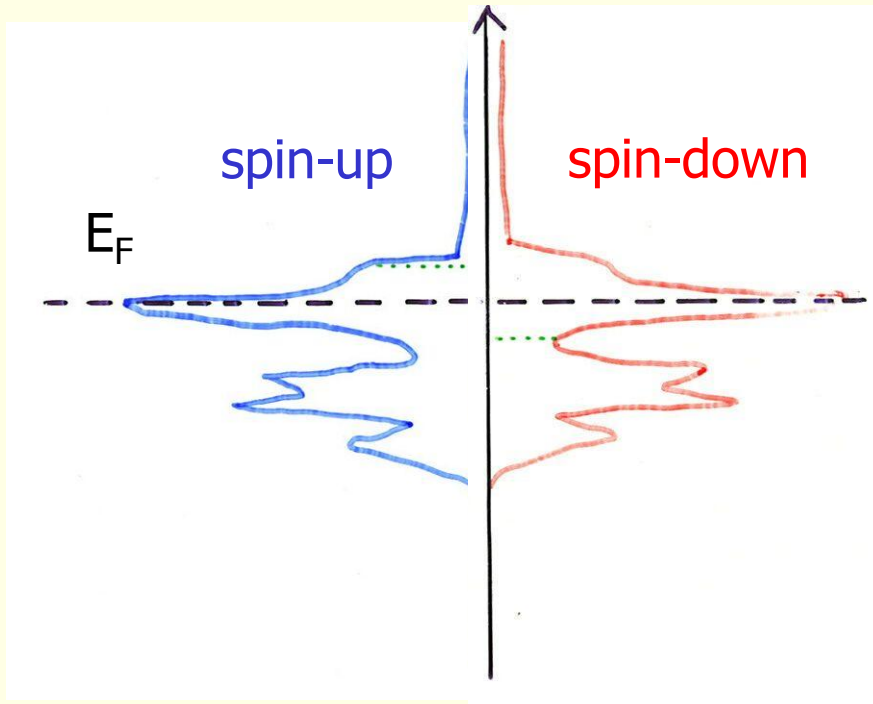


bcc Fe

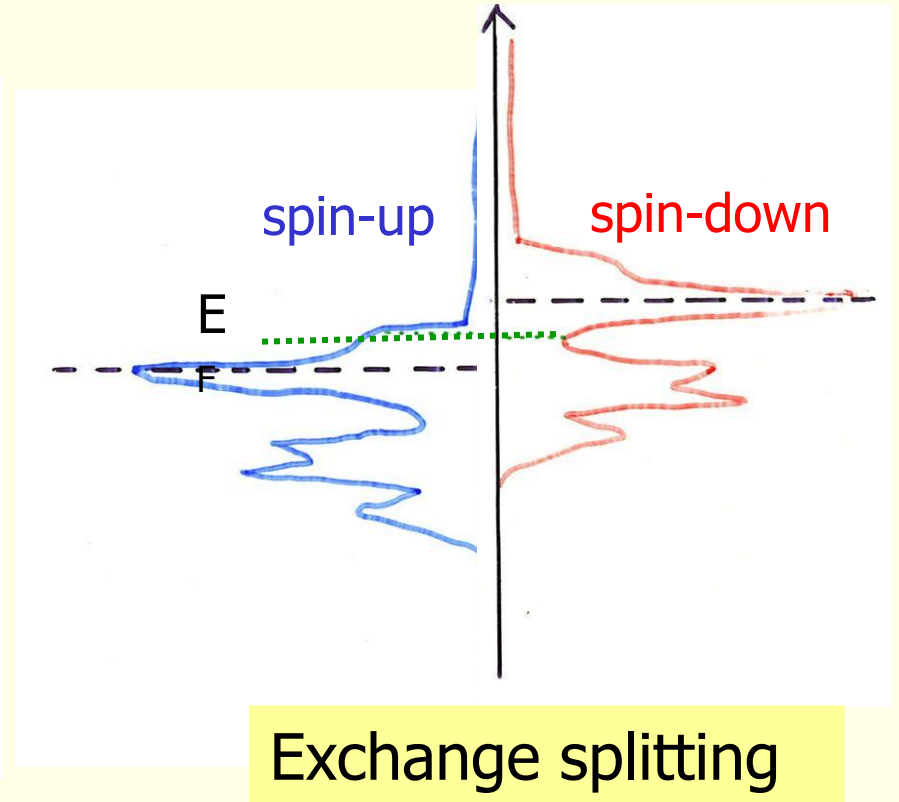


ferromagnetic case

■ Non magnetic case



$E_F$  at high DOS

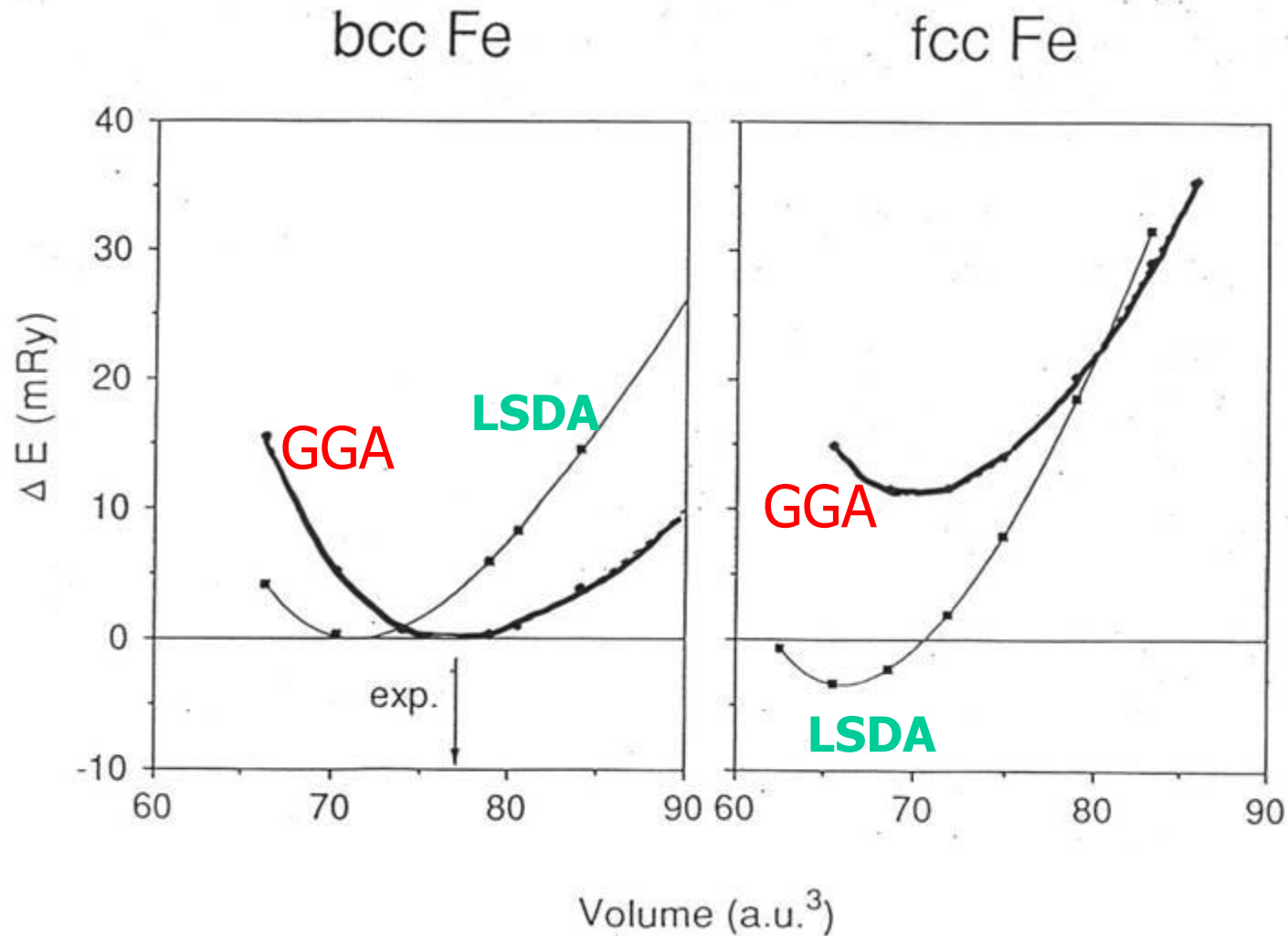


Exchange splitting

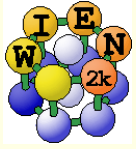




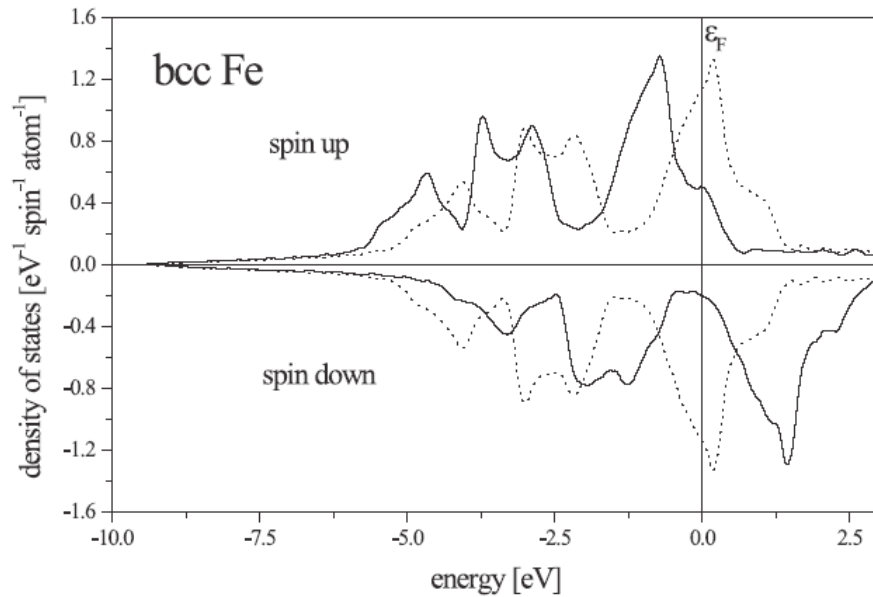
# DFT ground state of iron



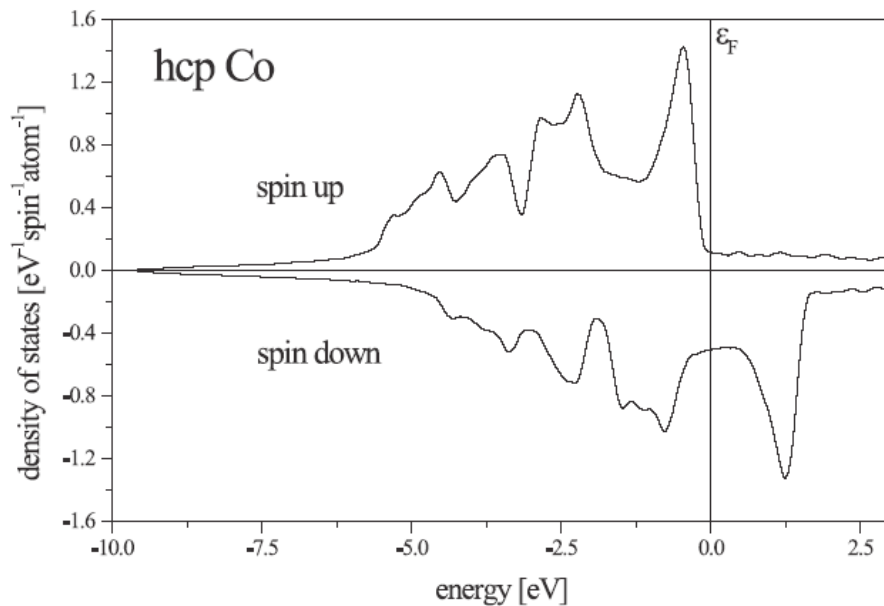
- **LSDA**
  - *NM*
  - *fcc*
  - *in contrast to experiment*
- **GGA**
  - *FM*
  - *bcc*
  - *Correct lattice constant*
- **Experiment**
  - *FM*
  - *bcc*



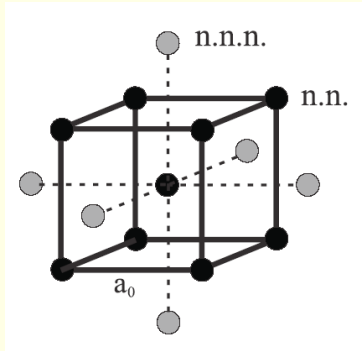
# Iron and its alloys



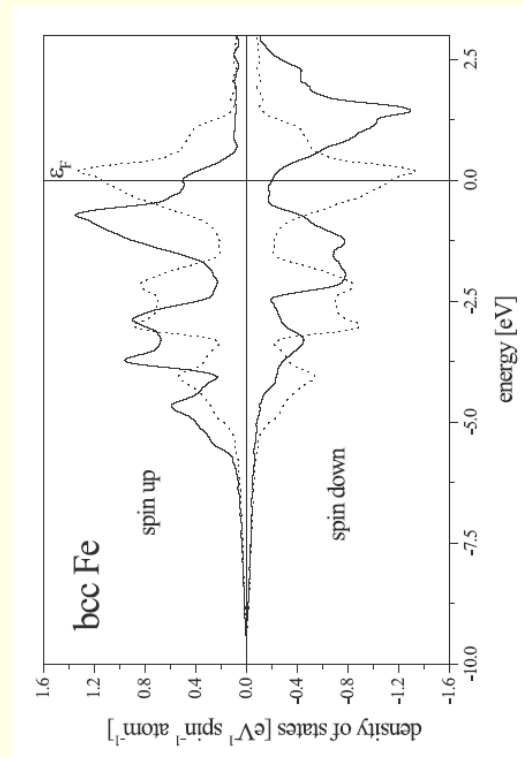
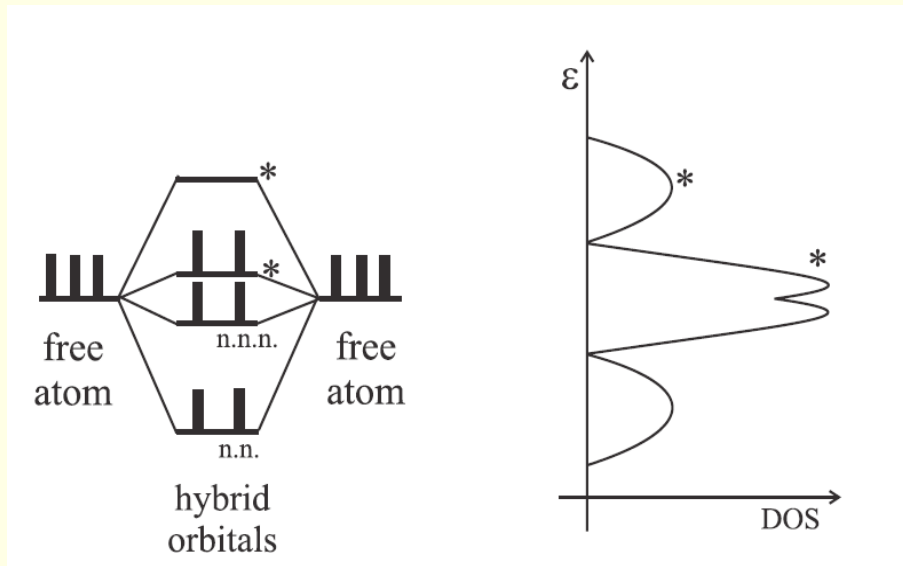
Fe: weak ferromagnet  
(almost)

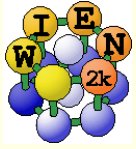


Co: strong ferromagnet



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



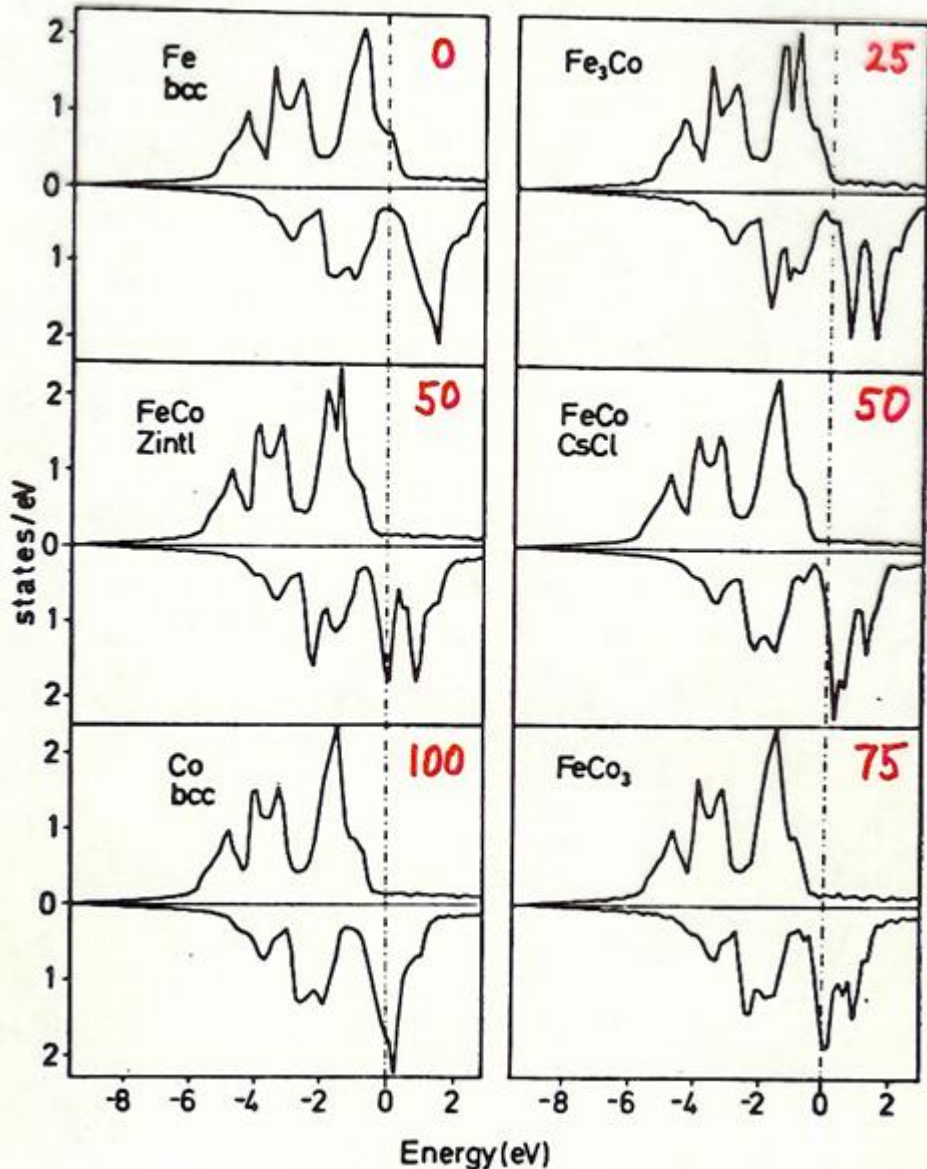


# Covalent magnetism Fe-Co alloys

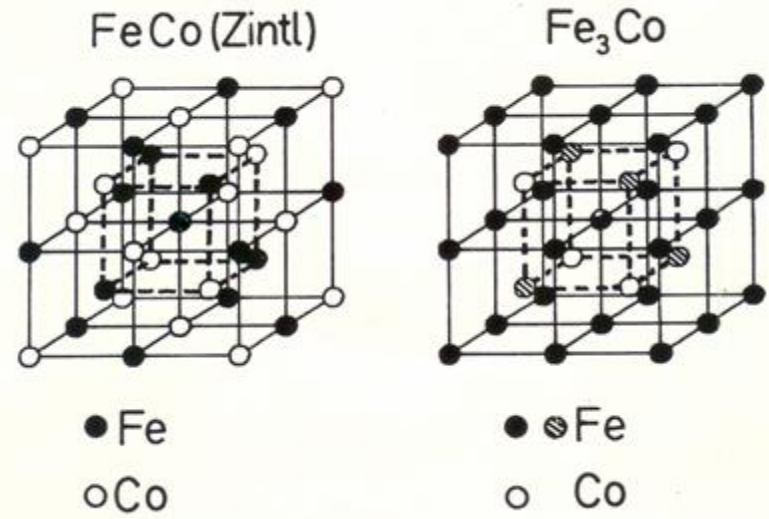


- e.g. Fe-Co alloys
- Wigner delay times

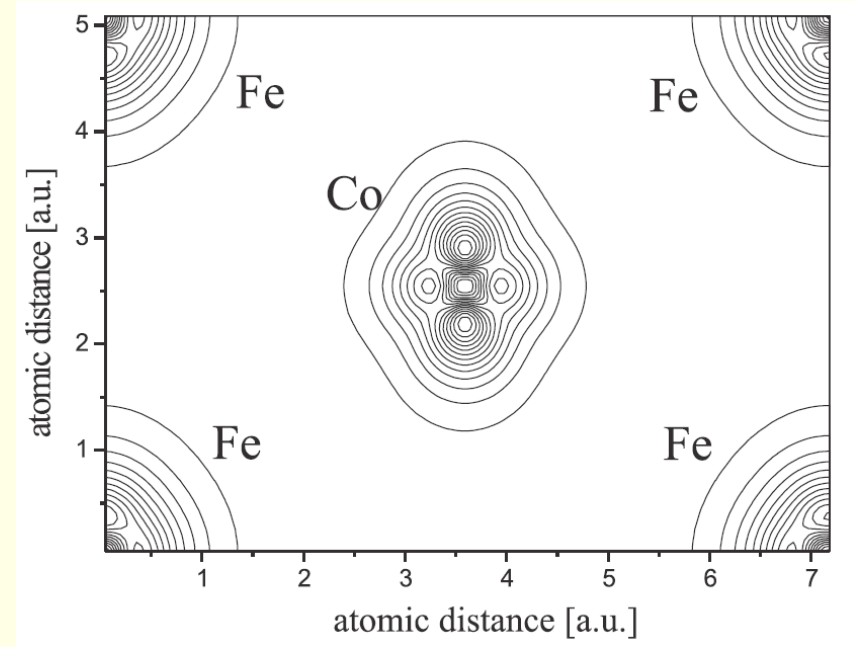
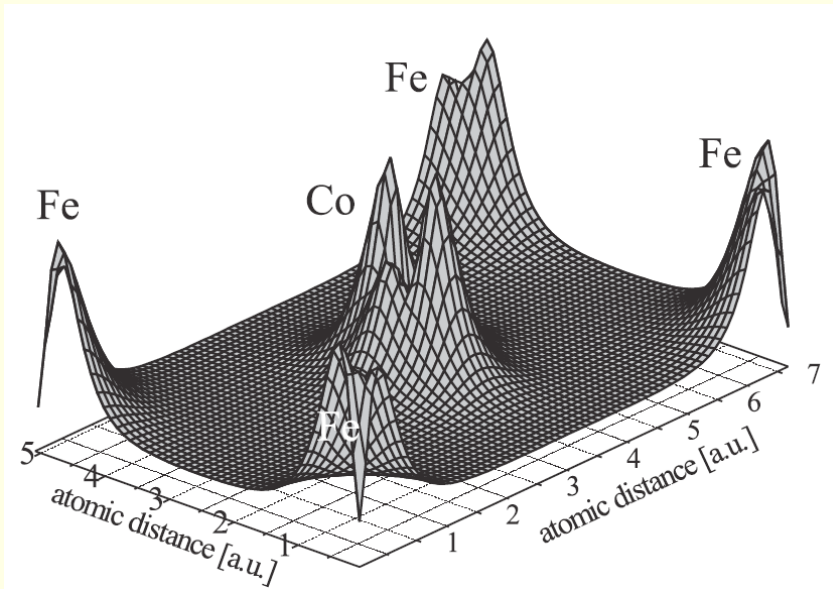
**% Co**



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



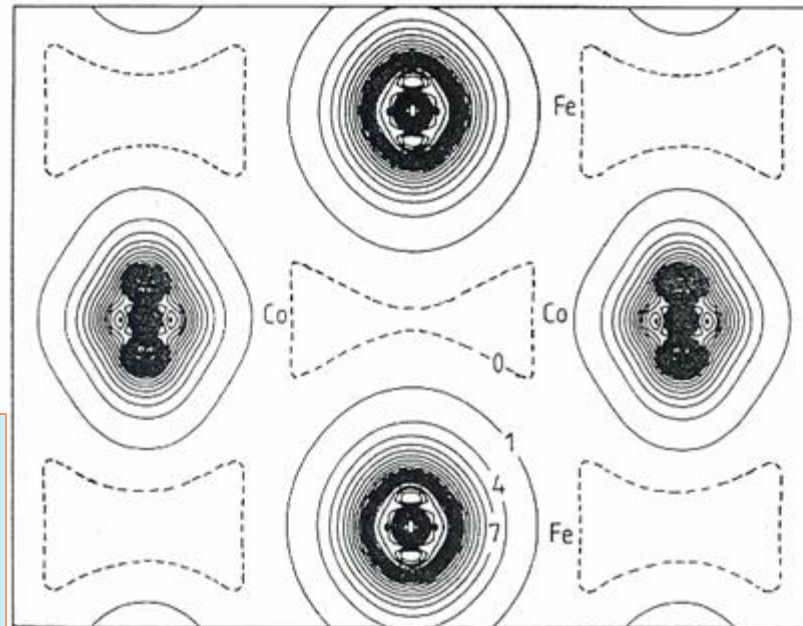
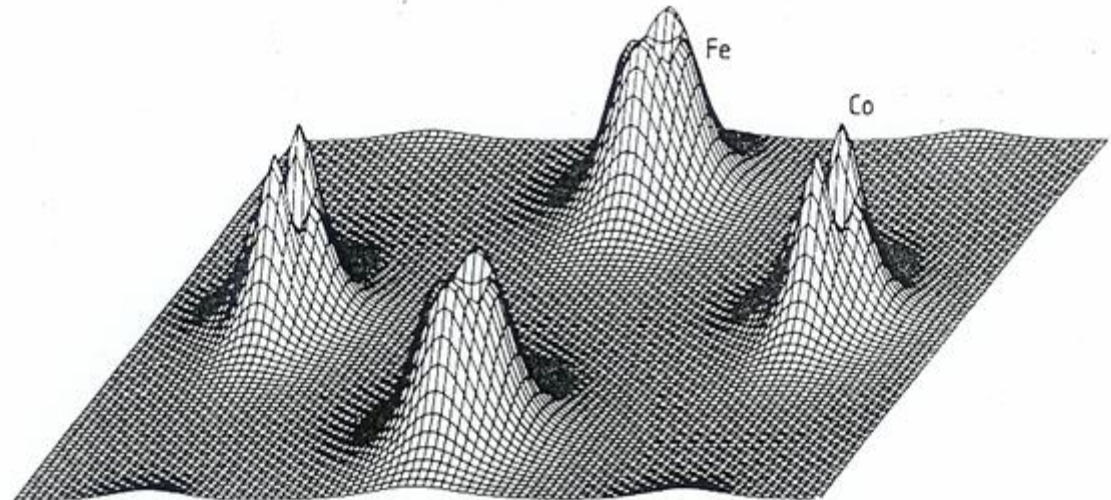
## Itinerant or localized?



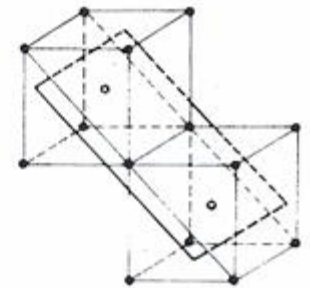
- Magnetization density difference between
  - Majority spin
  - Minority spin

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

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



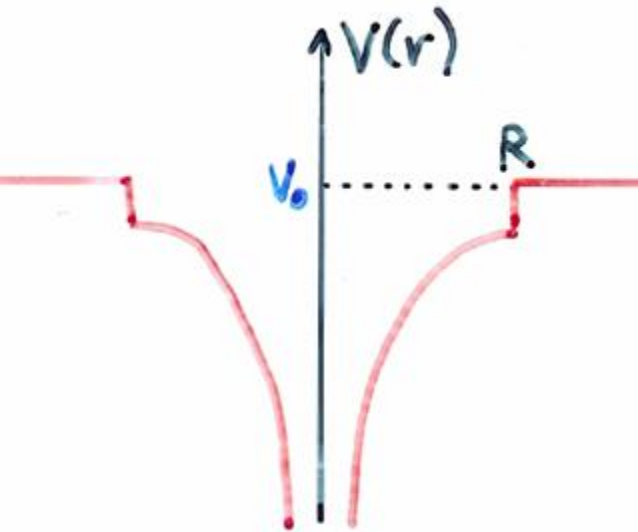
CsCl structure



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)



# Bonding by Wigner delay time



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

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

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

single scatterer (Friedel)

$V(r)=0$  solution:

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

$R_l$  joined in value and slope defines phase shift :

$$\tan \eta_l(\varepsilon) = \frac{R_l(\varepsilon, b) j'_l(kb) - j_l(kb) R'_l(\varepsilon, b)}{R_l(\varepsilon, b) n'_l(kb) - n_l(kb) R'_l(\varepsilon, b)}, \quad (4)$$

Friedel sum

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

Wigner delay time

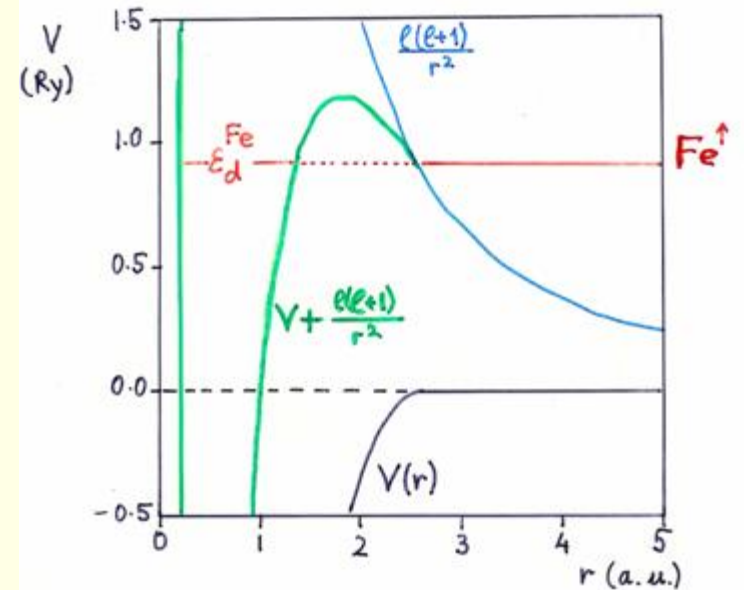
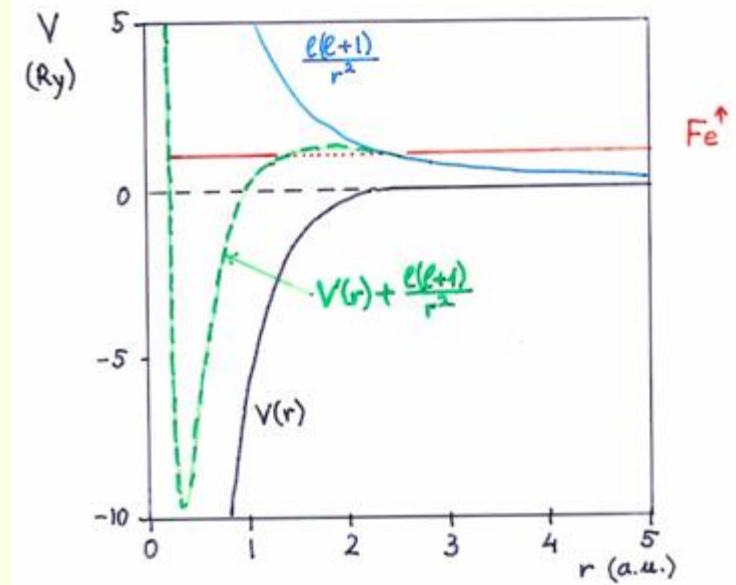
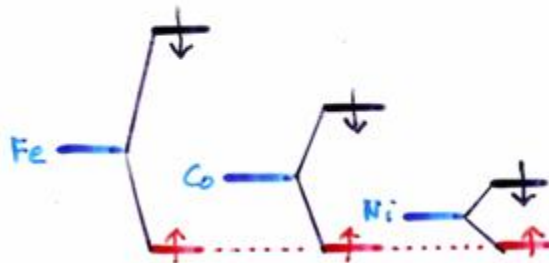
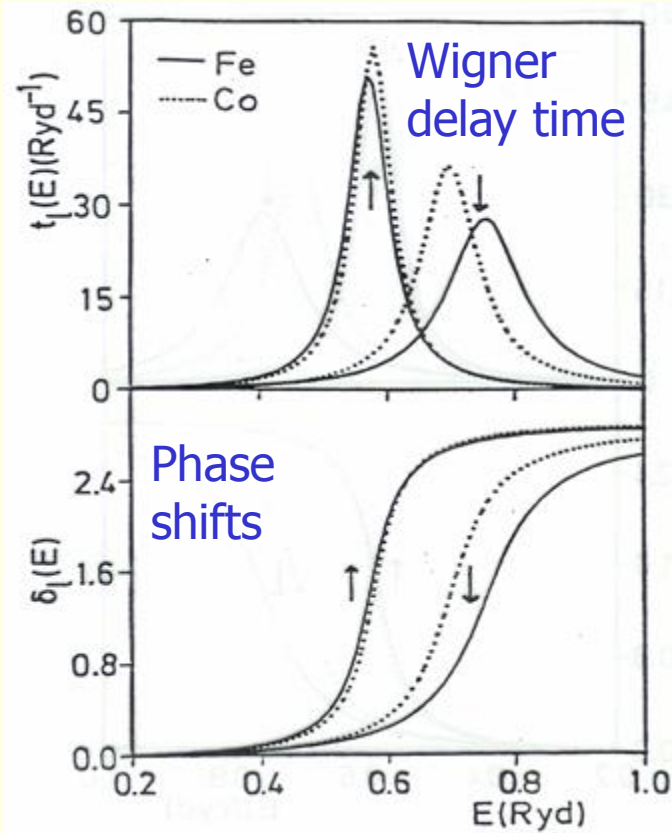
$$n(\varepsilon) = \frac{dN(\varepsilon)}{d\varepsilon} = \frac{1}{\pi} \sum_{l=0}^{\infty} (2l+1) t_l^D(\varepsilon). \quad (6)$$





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

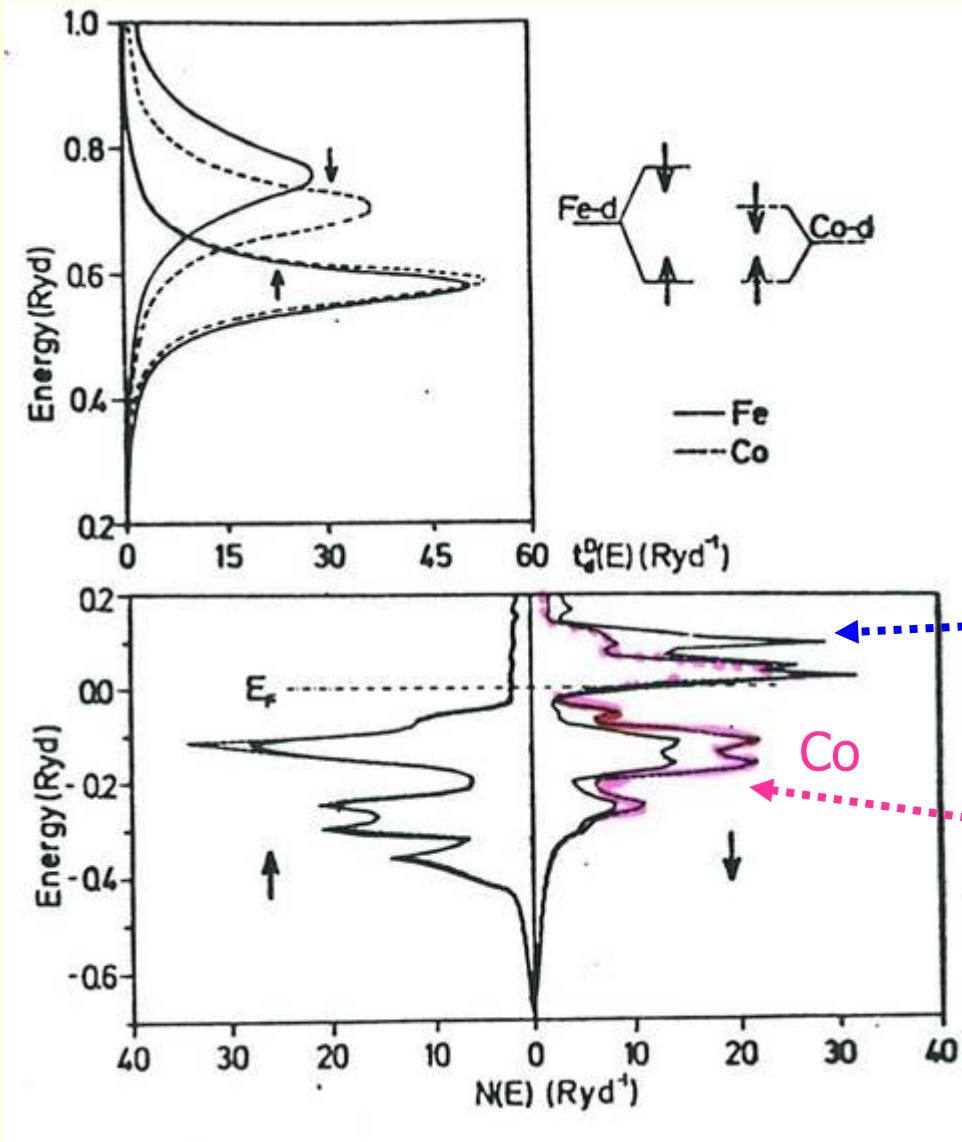
resonance states





# Covalent magnetism in FeCo

## Wigner delay time



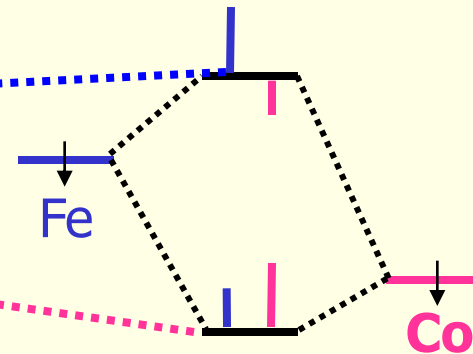
### ■ For spin up

- *Fe and Co equivalent*
- *partial DOS similar*
- *typical bcc DOS*

### ■ For spin down

- *Fe higher than Co*

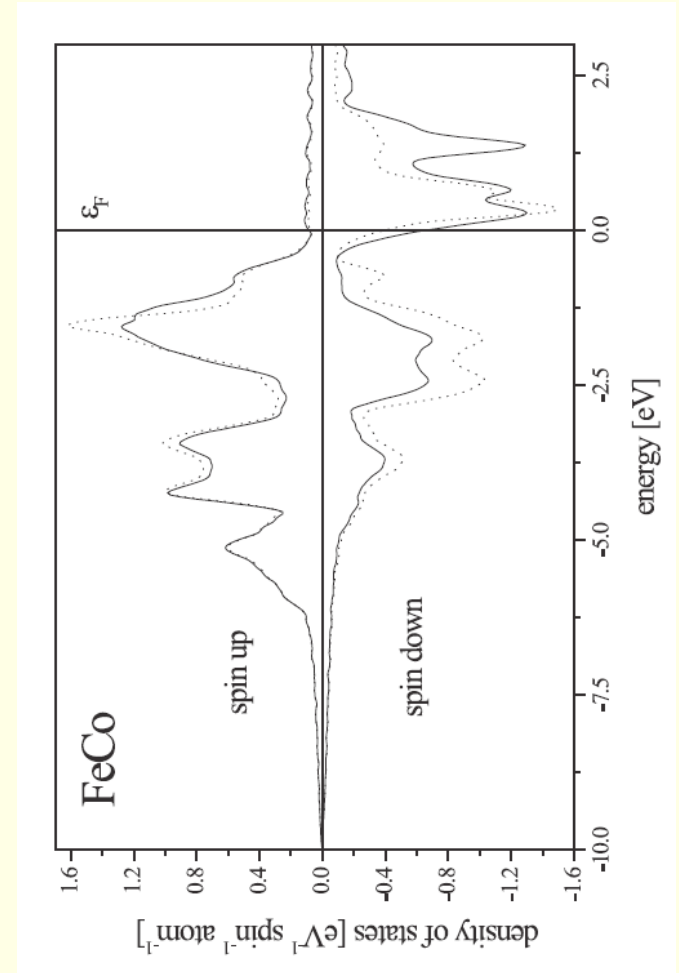
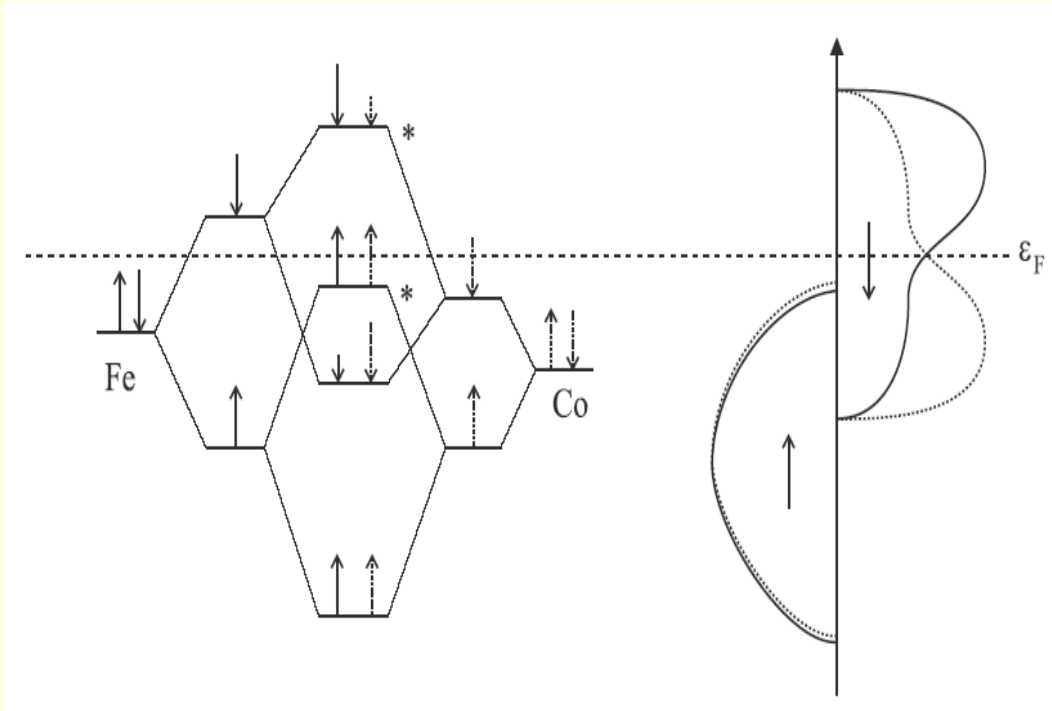
antibonding



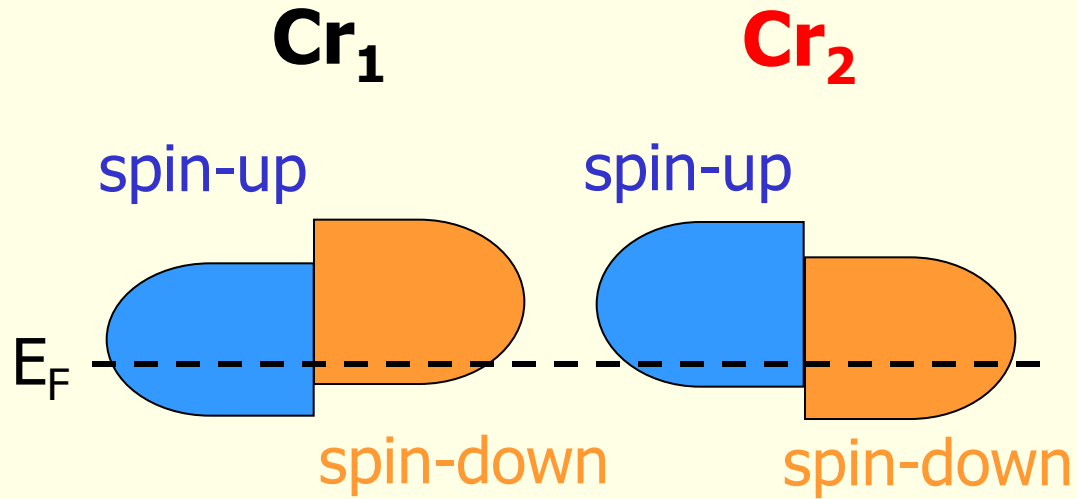
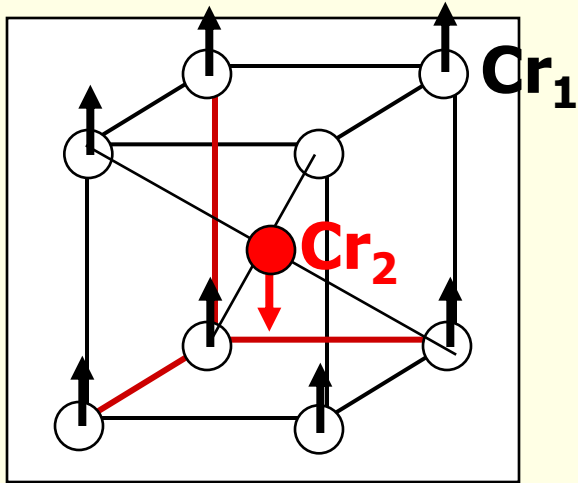
bonding

No charge transfer between Fe and Co

## Covalent magnetism, FeCo:



- Cr has AFM bcc structure

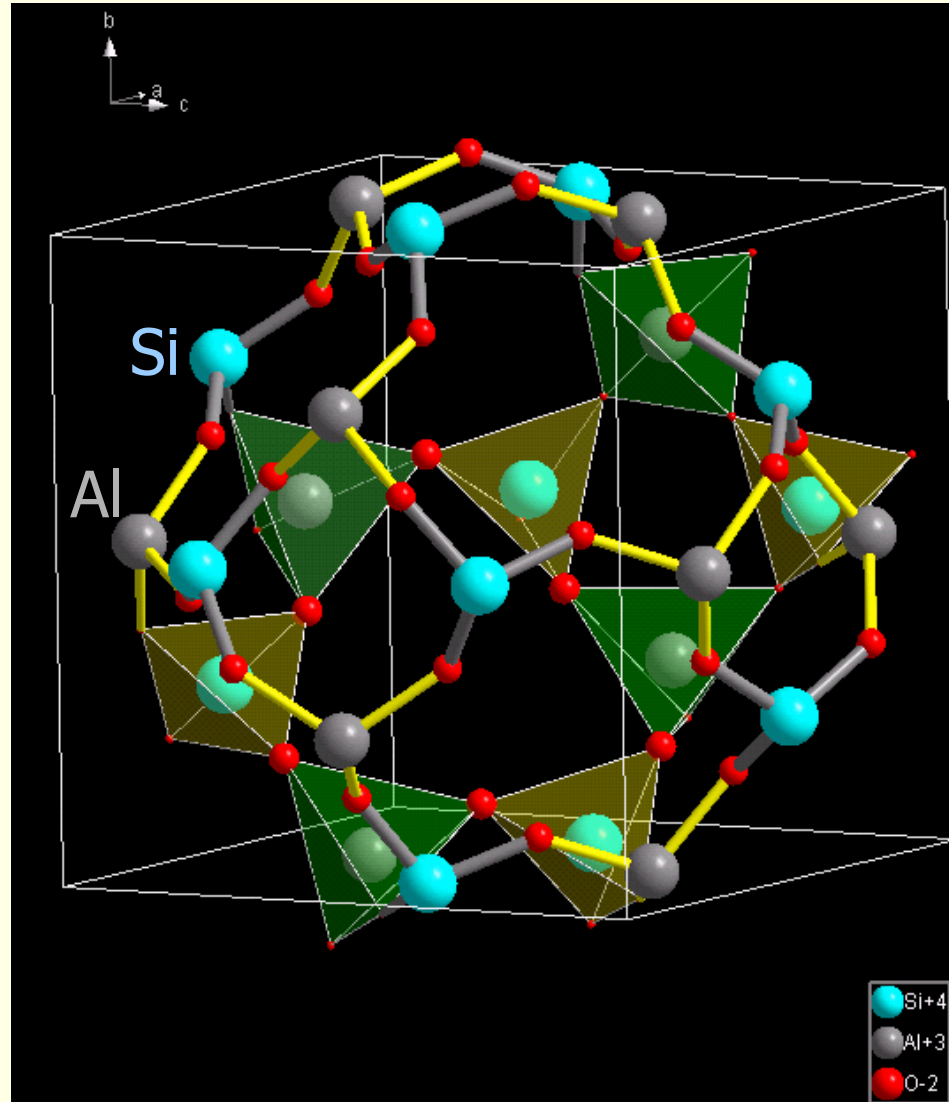


- There is a symmetry  
it is enough to do the spin-up  
calculation  
spin-down can be copied

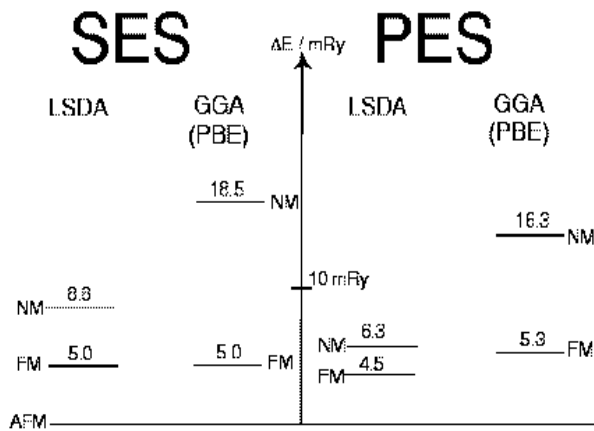
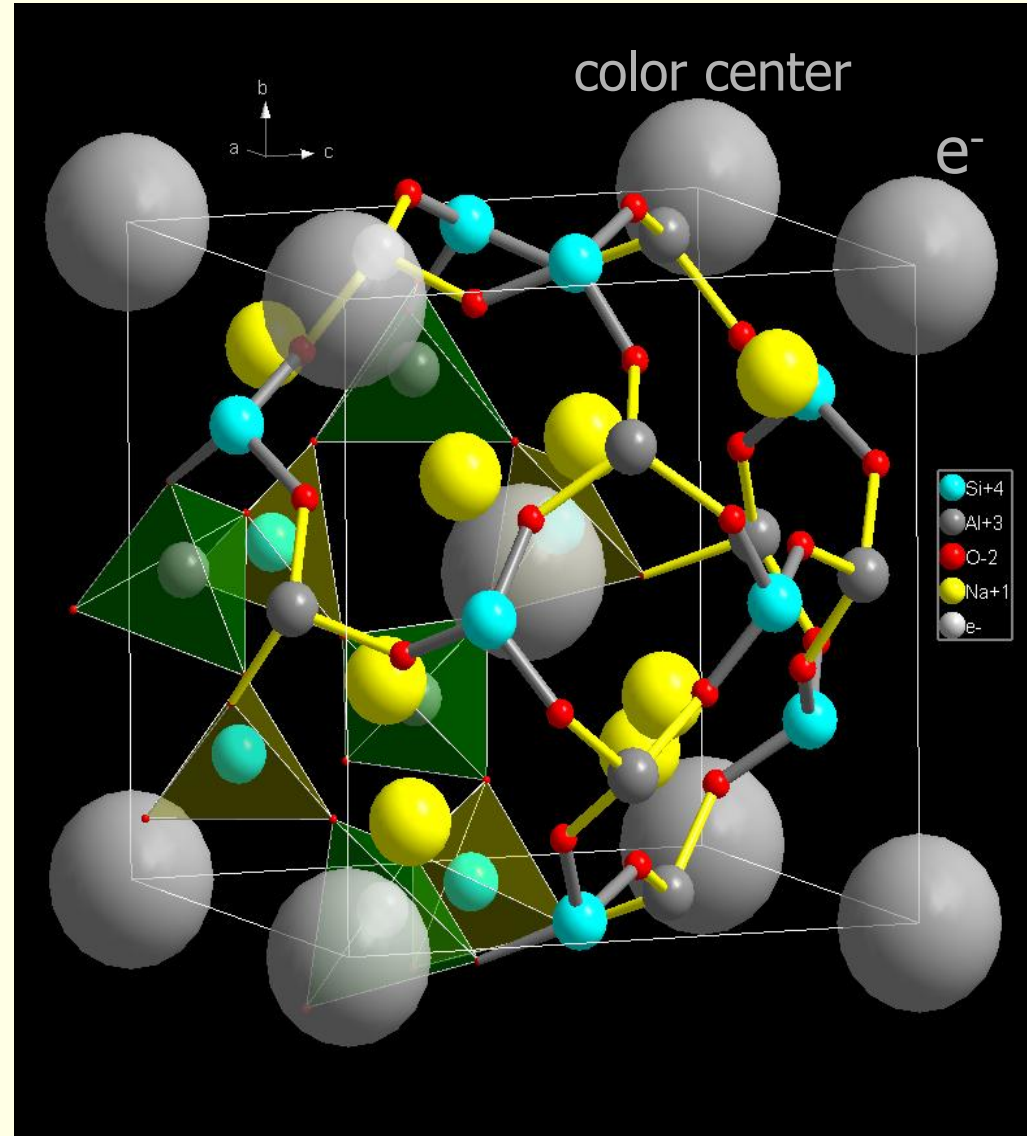
$$\text{Cr}_1 \downarrow = \text{Cr}_2 \uparrow$$

$$\text{Cr}_2 \downarrow = \text{Cr}_1 \uparrow$$

- Al-silicate
- corner shared
  - $SiO_4$  tetrahedra
  - $AlO_4$  tetrahedra
- $\beta$  cage
- Al / Si ratio 1
- alternating
- ordered (cubic)
- 3 e<sup>-</sup> per cage



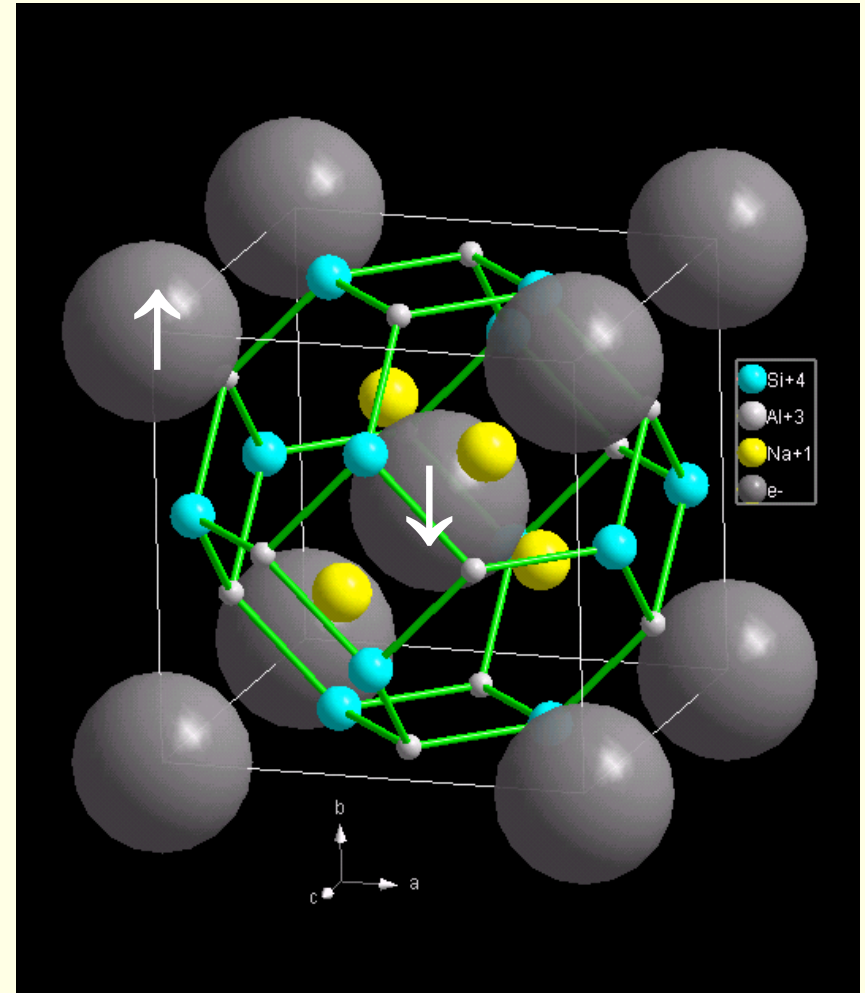
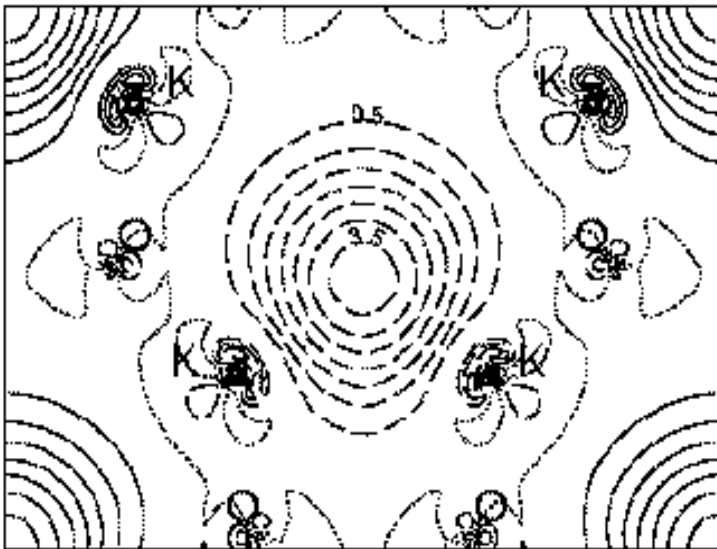
- **Si-Al zeolite (sodalite)**
  - Formed by corner-shared  $\text{SiO}_4$  and  $\text{AlO}_4$  tetrahedra
- **Charge compensated by doping with**
  - 4  $\text{Na}^+$
  - one  $e^-$  (color center)
- **antiferromagnetic (AFM) order of  $e^-$**



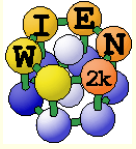
Energy (relative stability)

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



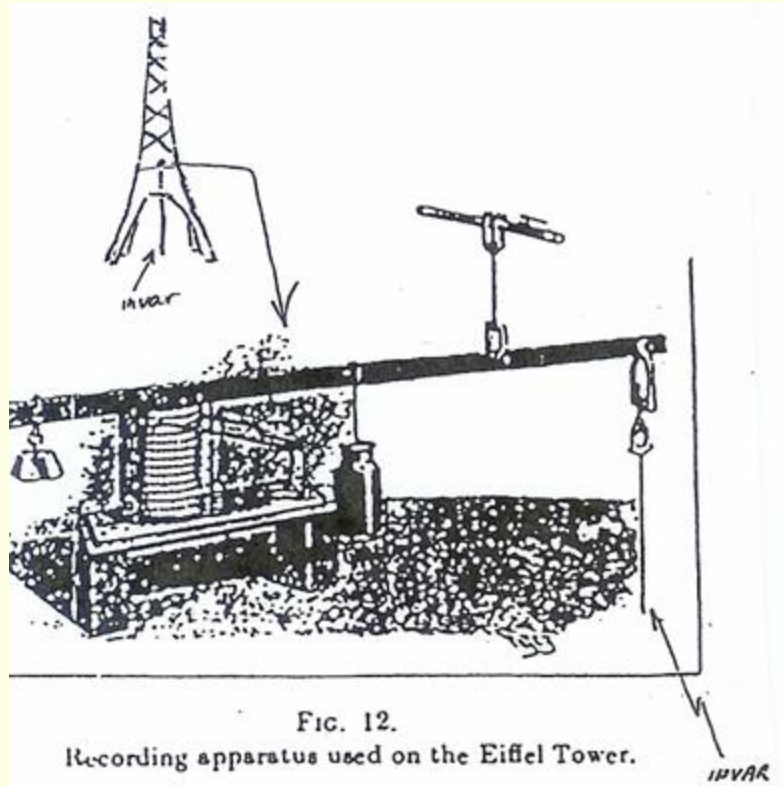
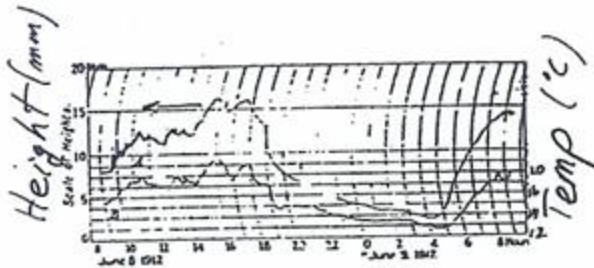


FIG. 12.

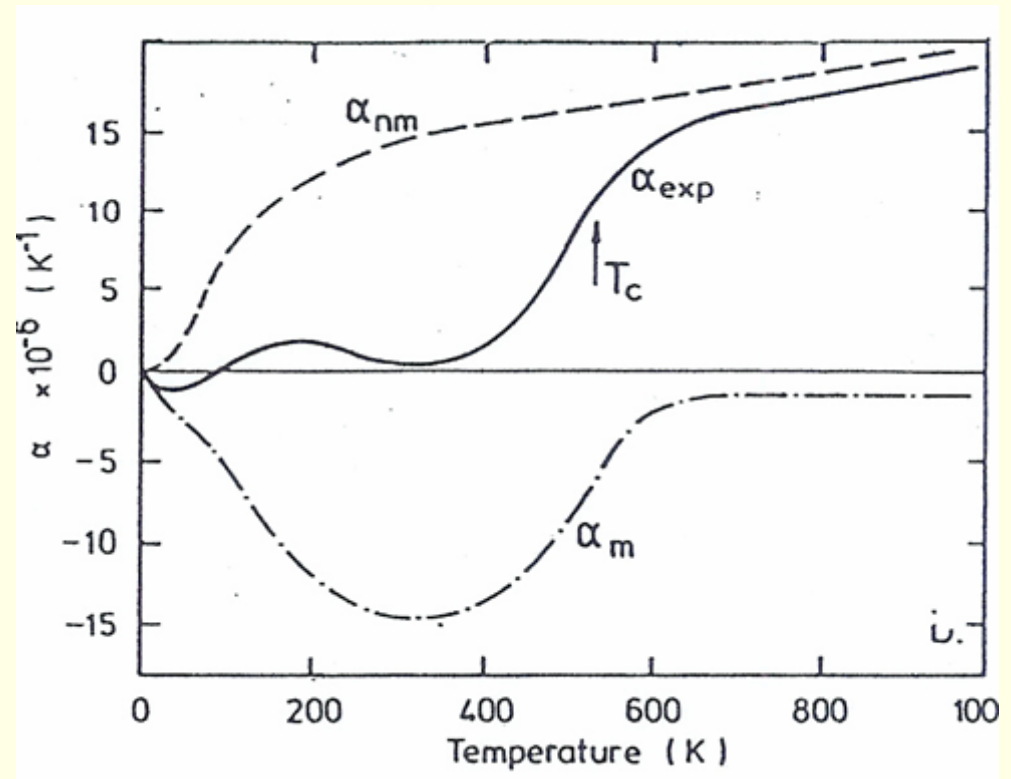
Recording apparatus used on the Eiffel Tower.

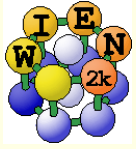
INVAR



Ch.E.Guillaume (1897)

- The thermal expansion of the Eiffel tower
- Measured with a rigid Fe-Ni INVAR wire
- The length of the tower correlates with the temperature
- **Fe<sub>65</sub>Ni<sub>35</sub>** alloy has vanishing thermal expansion around room temperature

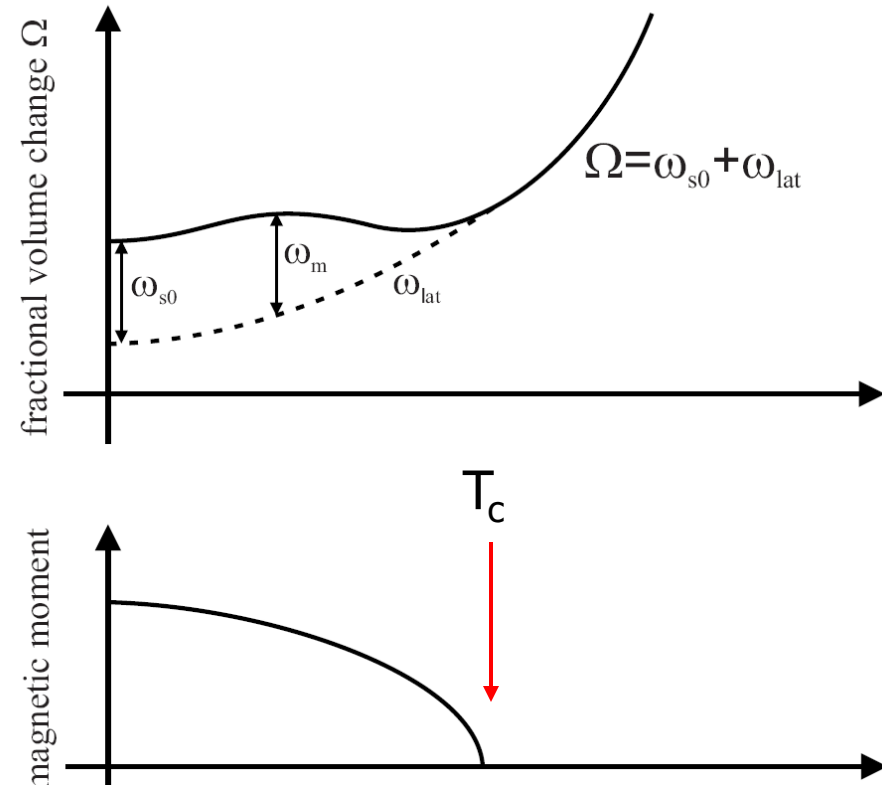


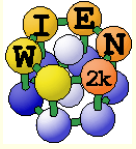


## What is magnetostriction?

Magnetostriction  $\omega_{s0}$  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  $\omega_m$  vanishes.

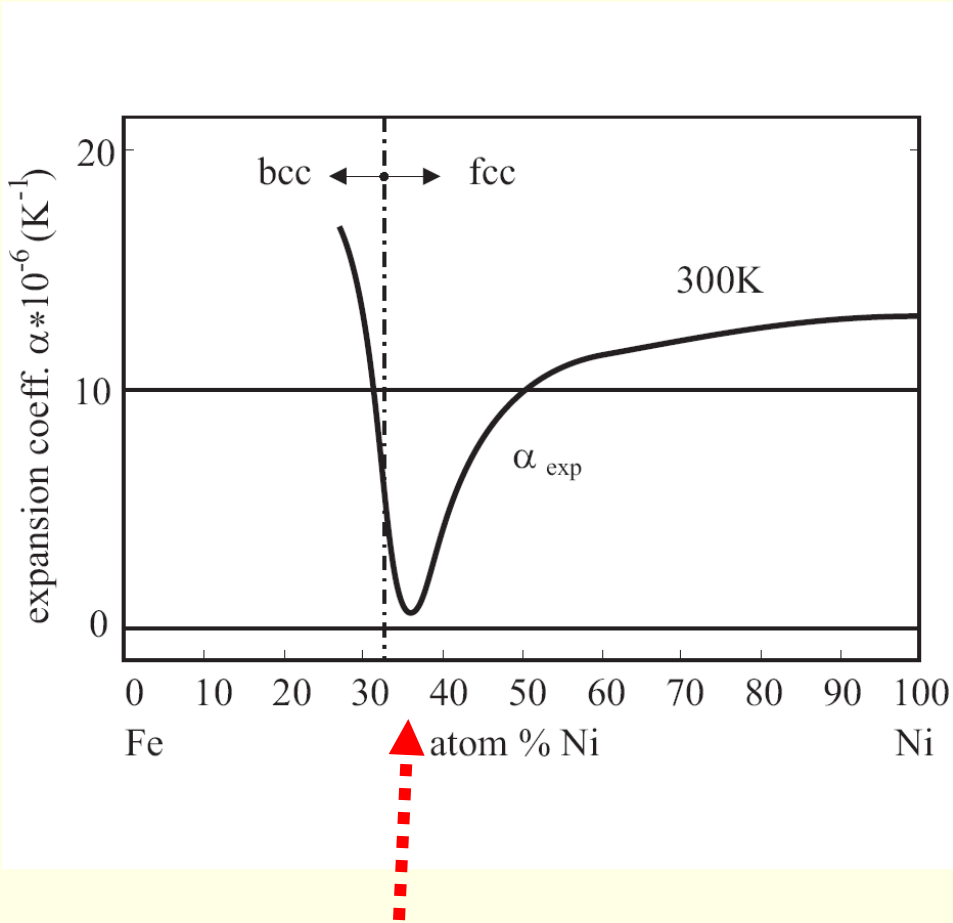




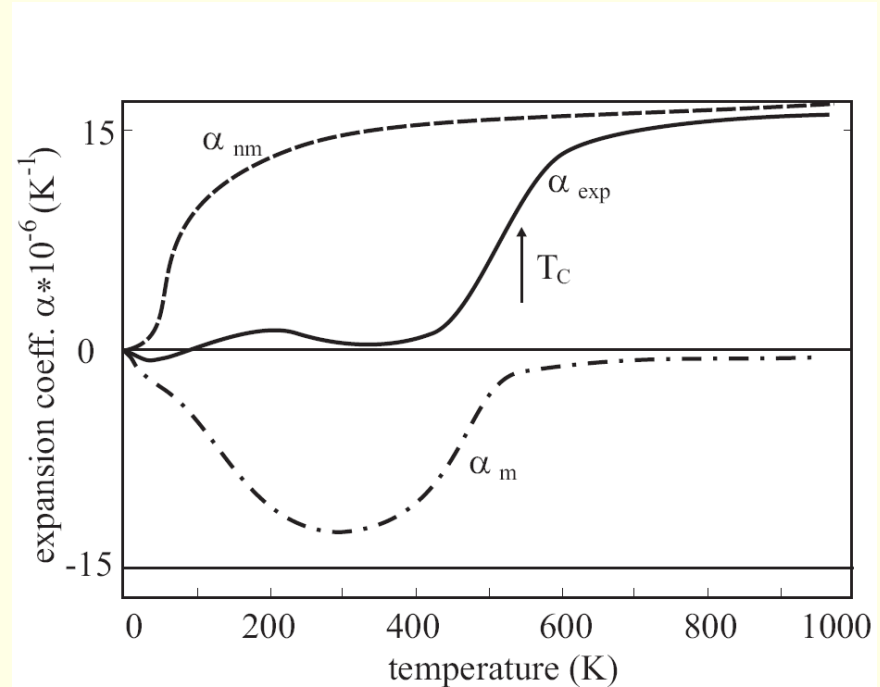
# Fe-Ni Invar alloys

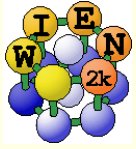


„classical“ Fe-Ni Invar



- **Fe<sub>65</sub>Ni<sub>35</sub>** 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**

$m=0.5 \mu_B$  AF

$a = 3.57 \text{ \AA}$

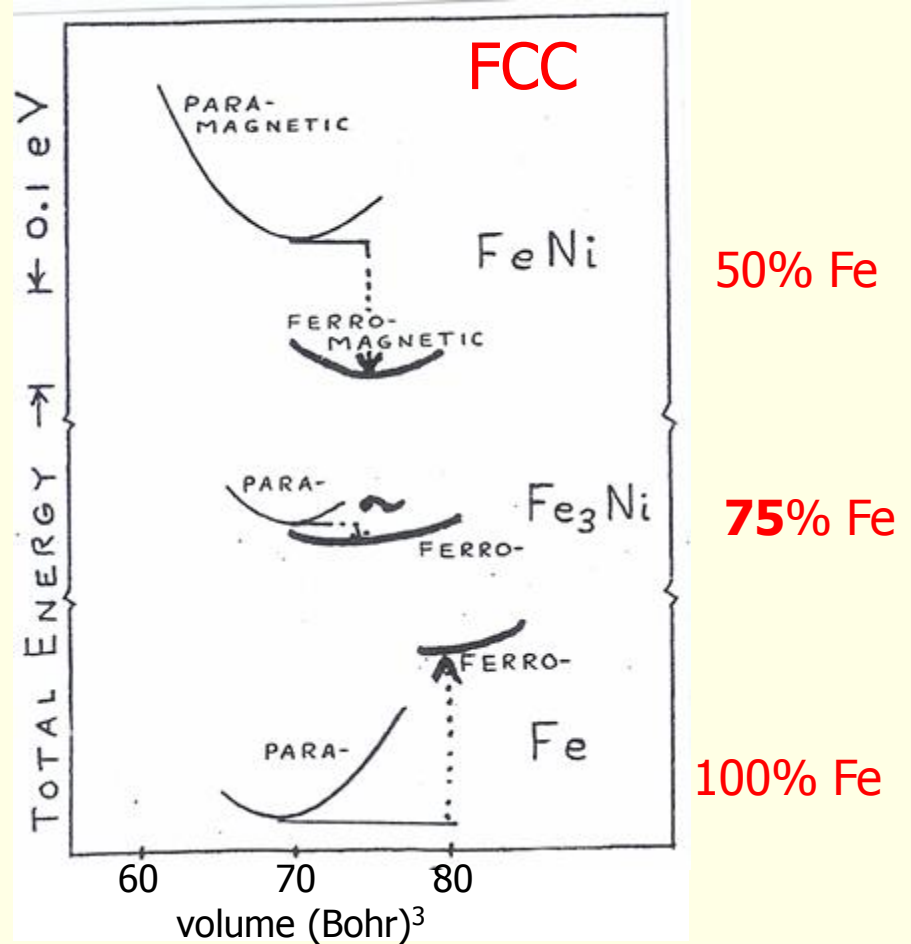
**high spin**

$m=2.8 \mu_B$  FM

$a = 3.64 \text{ \AA}$

small moment  
small volume  $\rightarrow Y_1$  AF

$kT$   
high moment  
large volume  $\rightarrow Y_2$  FM

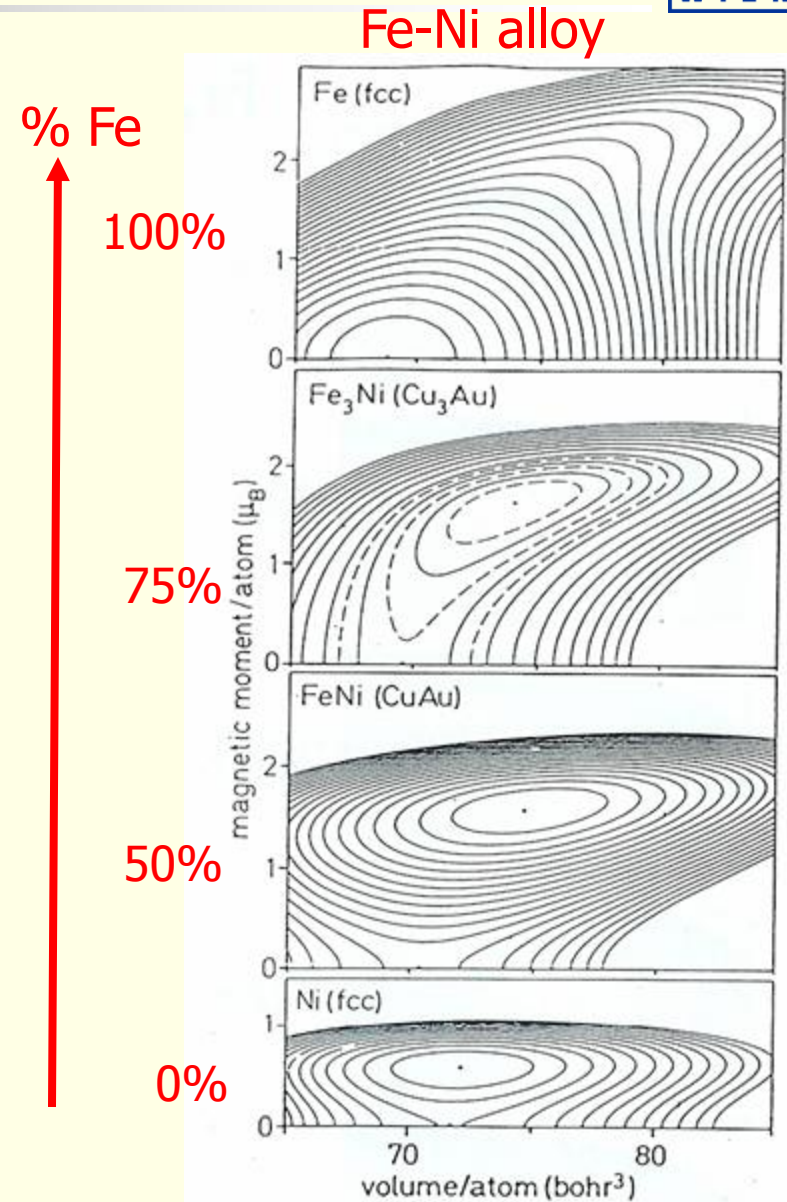


A.R.Williams, V.L.Moruzzi, G.D.Gelatt Jr., J.Kübler, K.Schwarz,  
*Aspects of transition metal magnetism*,  
J.Appl.Phys. **53**, 2019 (1982)



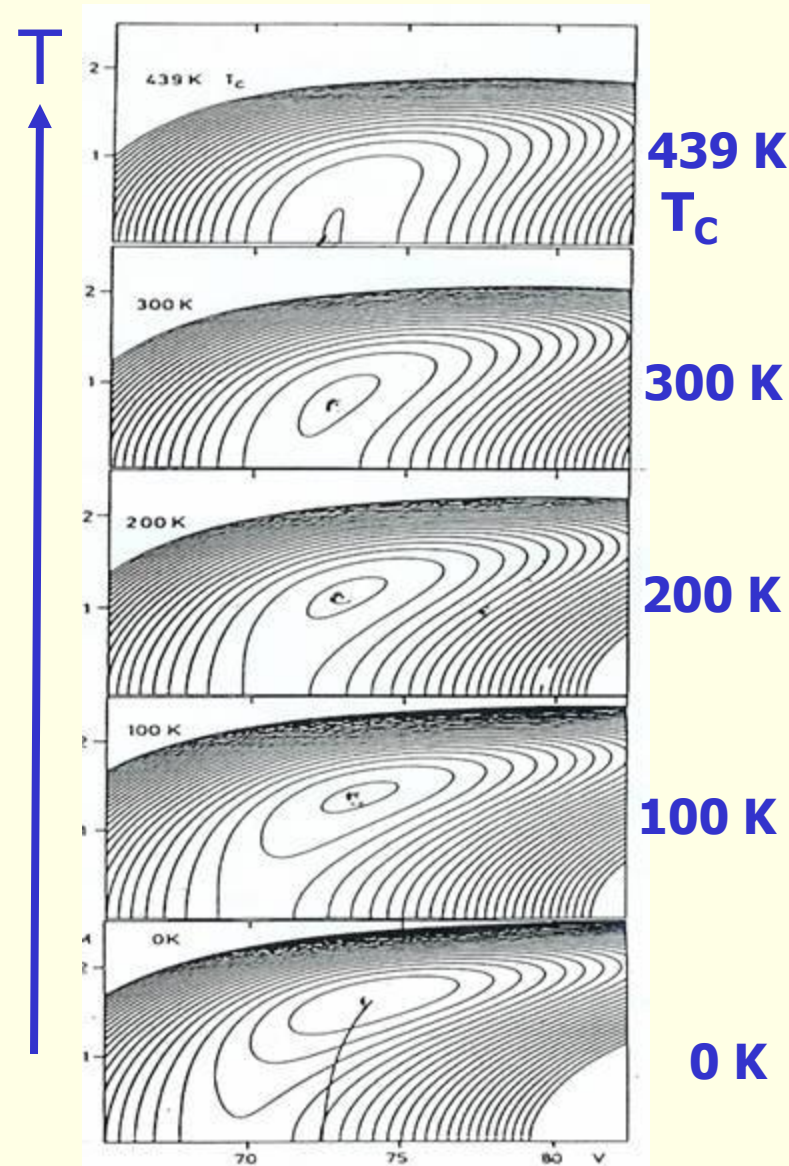
# Energy surfaces of Fe-Ni alloys

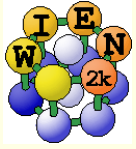
- This fcc structure
  - from *non magnetic Fe (fcc)*
  - to *ferromagnetic Ni*
  - as the composition changes
- At the INVAR composition
  - There is a flat energy surface
    - as function of volume and moment



- 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*

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





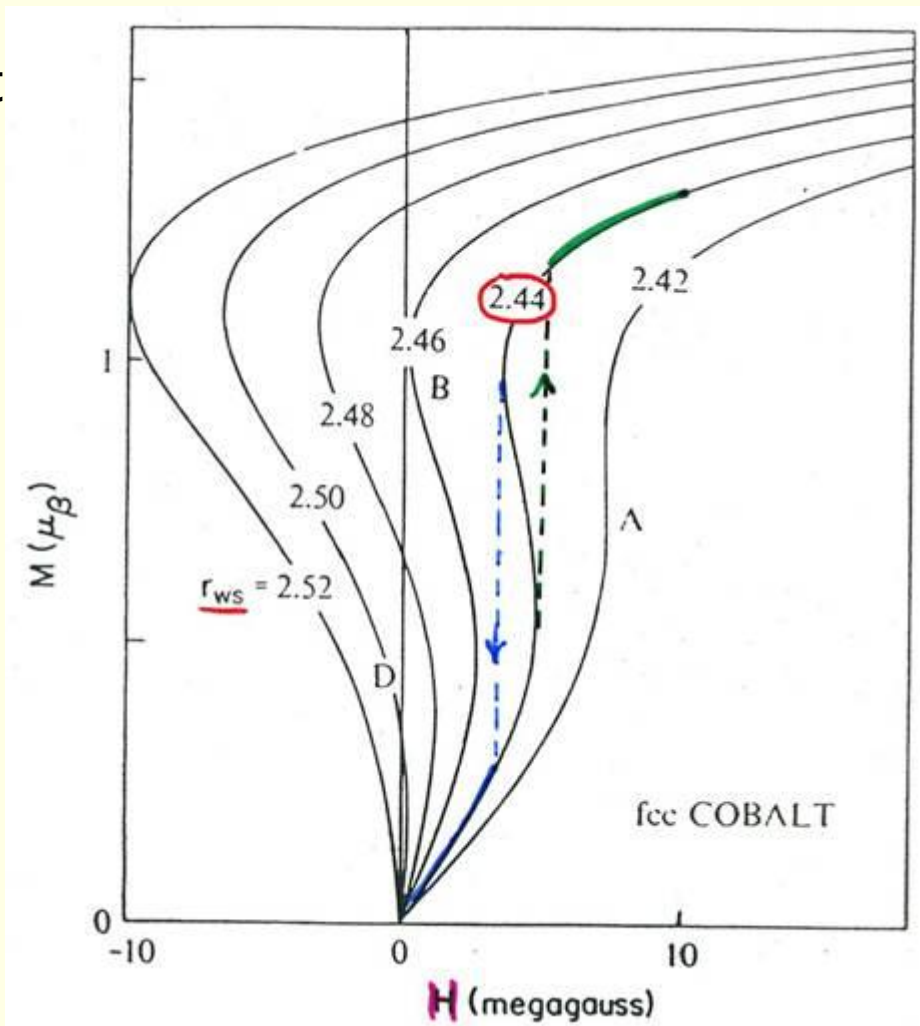
- fixed spin moment (FSM)  
e.g. **Fe-Ni alloy**
- allows to explore **energy surface**  $E(V, M)$   
as function of
  - *volume*  **$V$**
  - *magnetic moment*  **$M$**

- 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

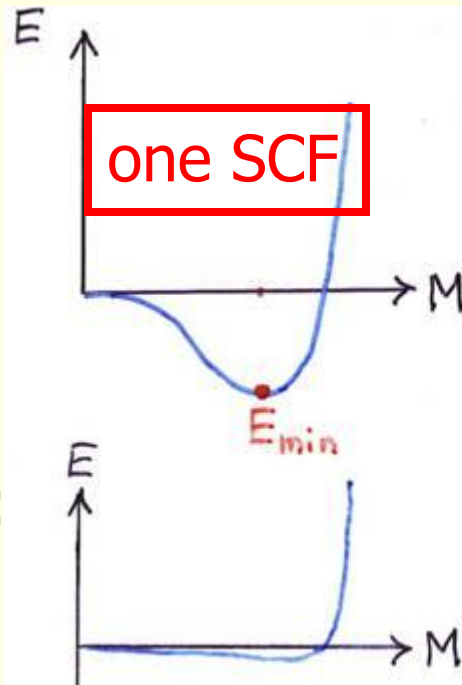
$$E_F^\uparrow = E_F^\downarrow$$

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

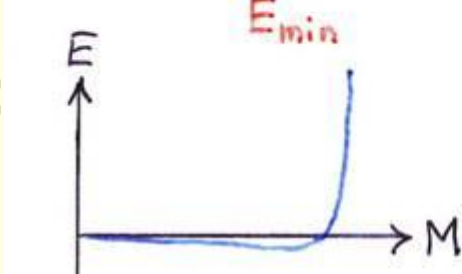
output

$$M = N^\uparrow - N^\downarrow$$

Simple case:  
bcc Fe



difficult case:  
 $Fe_3Ni$



poor convergence

## constrained (FSM) method

$$E_F^\uparrow \neq E_F^\downarrow$$

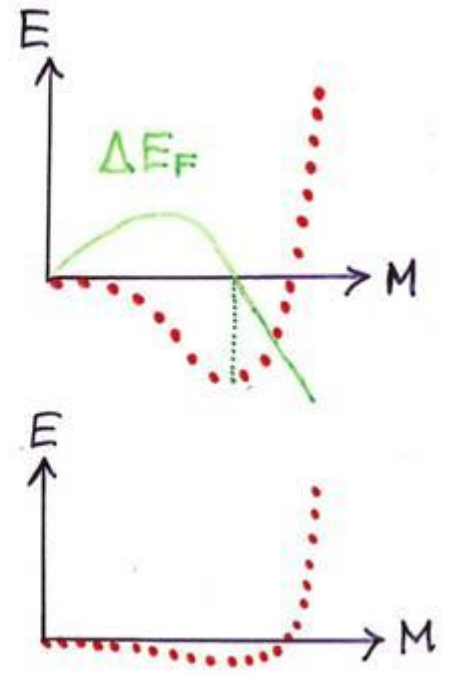
$$Z_v = N^\uparrow + N^\downarrow$$

output

$$M = N^\uparrow - N^\downarrow$$

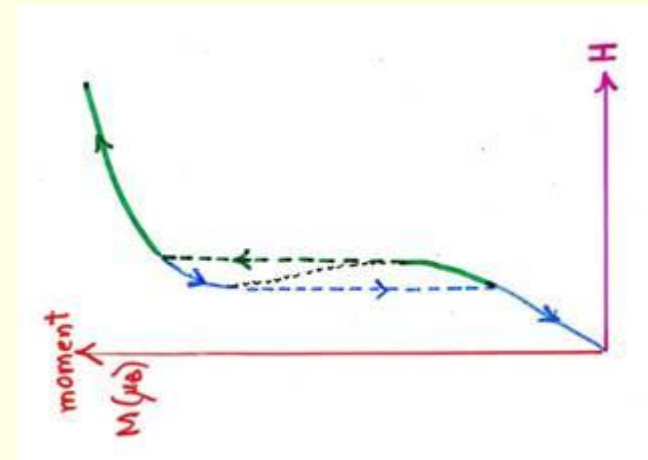
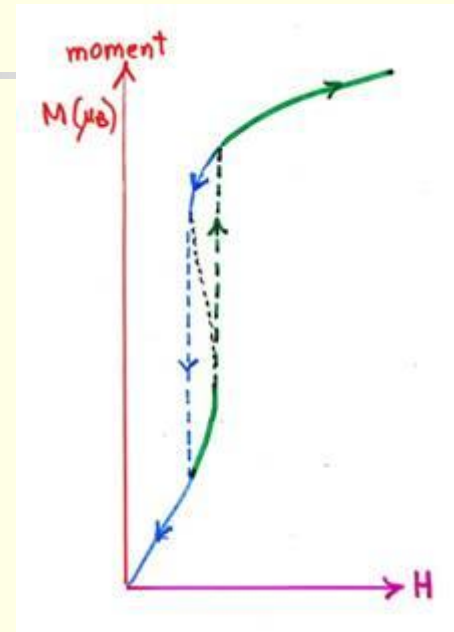
input

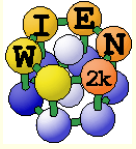
many  
calculations



good convergence

- **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*





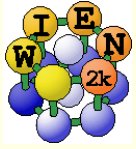
# FSM key references



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

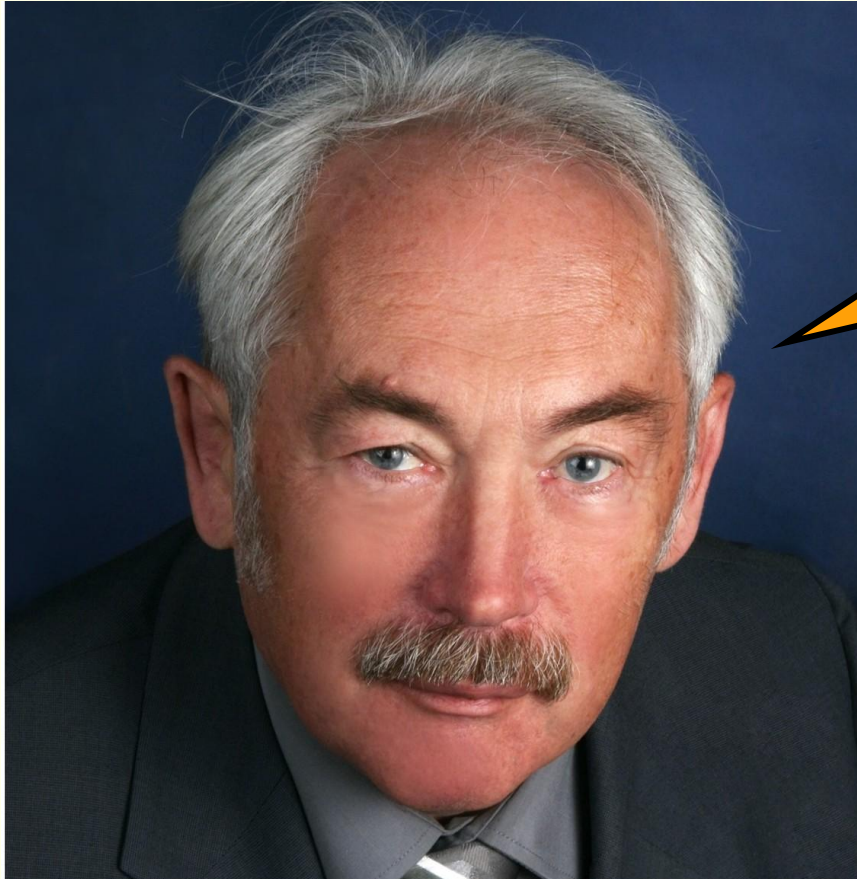
K.Schwarz, P.Mohn  
J.Phys.F **14**, L129 (1984)

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



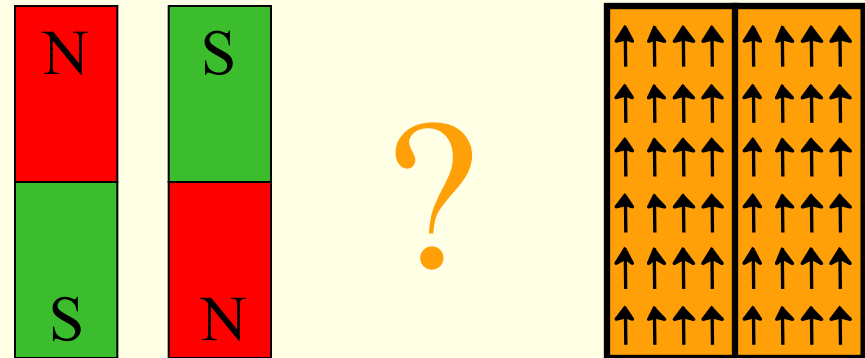
- GMR (Giant Magneto Resistance)
- half-metallic systems  
e.g.  $\text{CrO}_2$
- important for **spintronics**

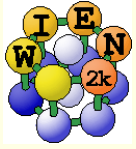
Once upon a time, in the early 1980's ...



Peter Grünberg

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





# Giant magnetoresistance (GMR)



Ferromagnet  
Metal  
Ferromagnet

Electrical  
resistance:

$$R_P$$

<( >)

$$R_{AP}$$

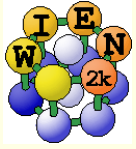
The electrical resistance depends on  
the **relative magnetic alignment** of the ferromagnetic layers

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

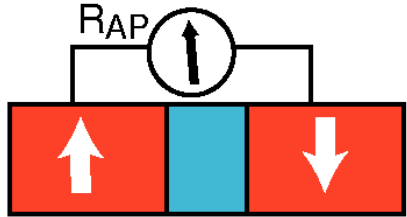
19% for trilayers @RT

80% for multilayers @ RT

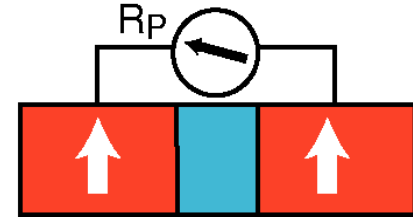
GMR is much **larger than the anisotropic magnetoresistance (AMR)**



1988: ... simultaneously, but independent ...



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



Albert Fert



Peter Grünberg



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

<http://www.kva.se/>

Scientific background

## The Discovery of Giant Magnetoresistance

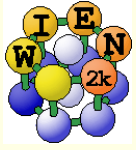
compiled by the Class for Physics of the Royal Swedish Academy of Sciences

### 4. Half-metals

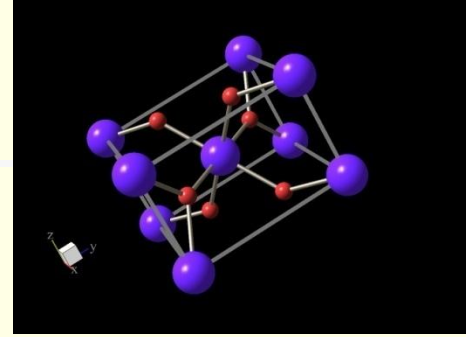
Since magnetoresistance deals with electrical conductivity it is obvious that it is the behaviour of the electrons at the Fermi surface (defined by the Fermi energy) which is of primary interest. The more spin-polarized the density of states (DOS) at the Fermi energy, i.e., the more  $N_{\uparrow}(E_F)$  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<sub>2</sub> 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<sub>2</sub> predicted as a half-metallic ferromagnet", J. Phys. F, **16**, L211 (1986).





# CrO<sub>2</sub> half-metallic ferromagnet

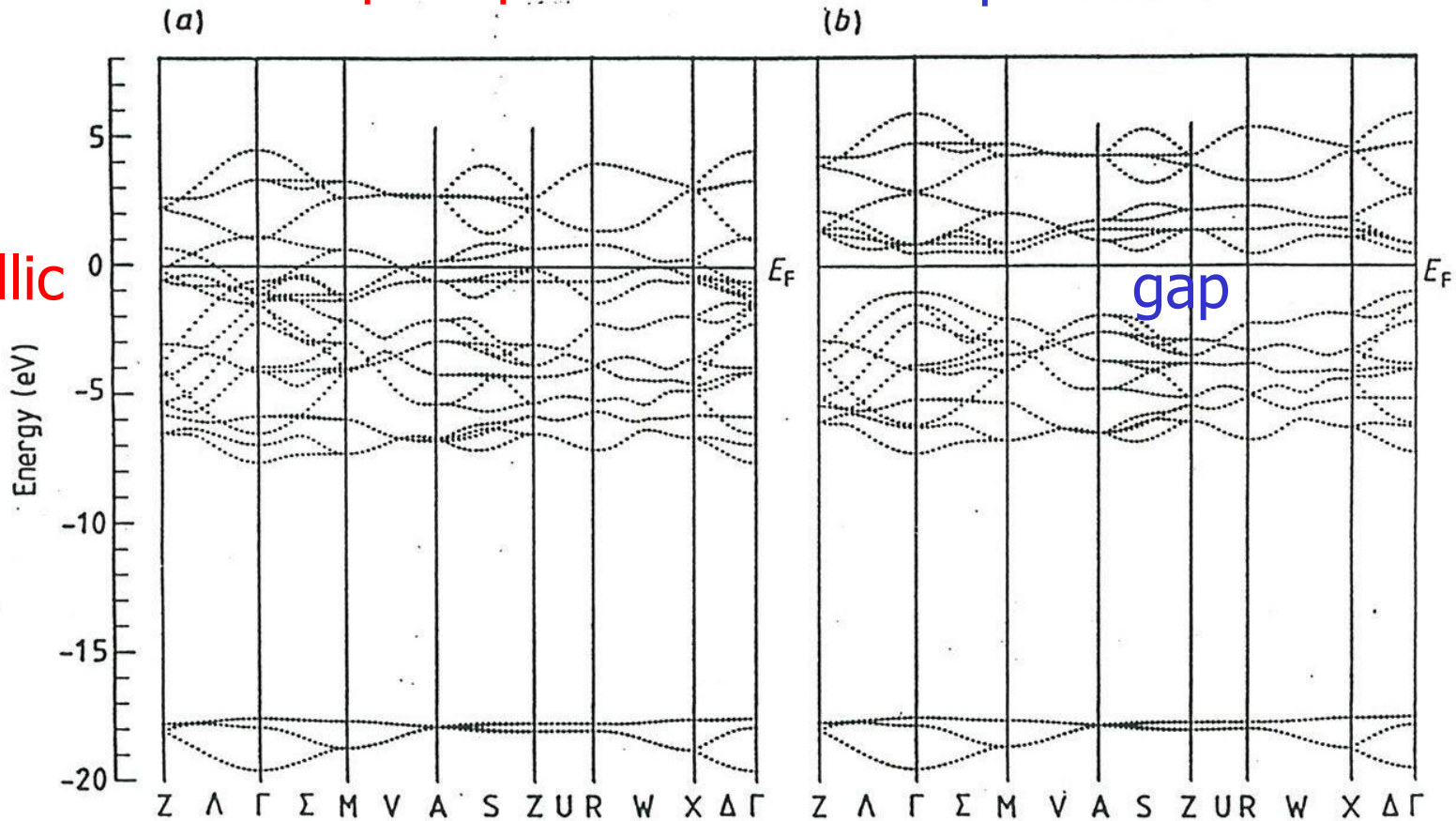


- CrO<sub>2</sub> (rutile structure)

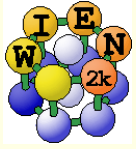
spin-up

spin-down

metallic



important for **spintronics**

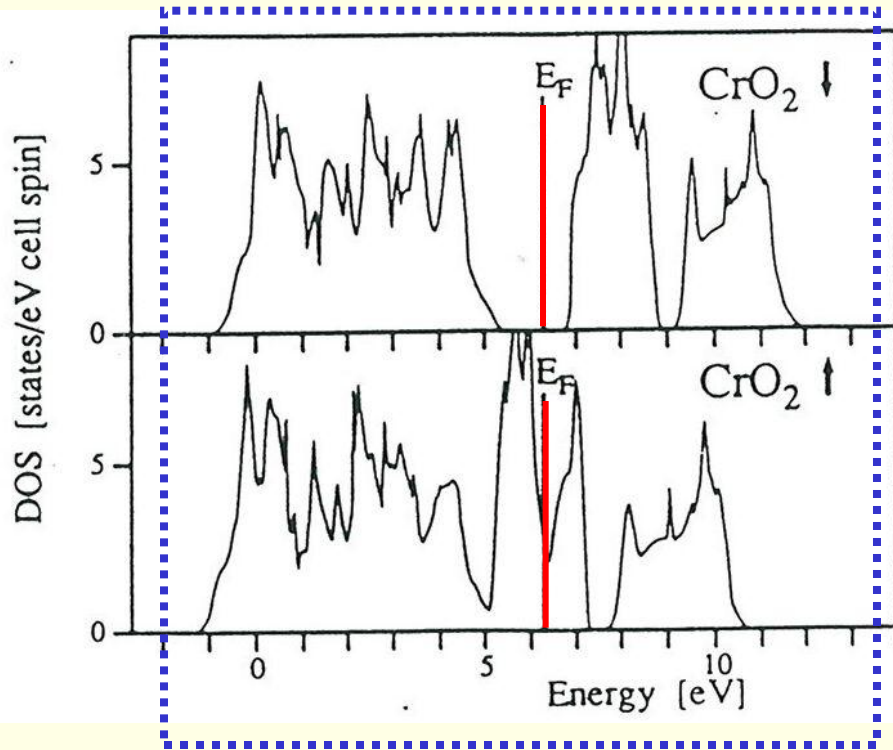


# CrO<sub>2</sub> DOS

K.Schwarz,  
*CrO<sub>2</sub> predicted as a  
half-metallic ferromagnet,*  
J.Phys.F:Met.Phys. **16**, L211 (1986)

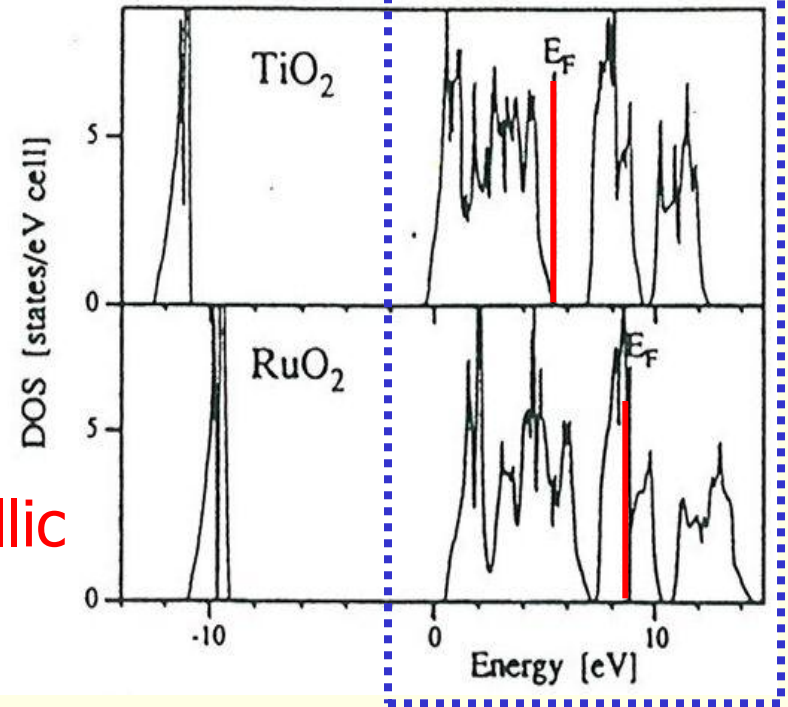
- The DOS features of CrO<sub>2</sub> are qualitatively like
  - TiO<sub>2</sub> (for spin-down)
  - RuO<sub>2</sub> (for spin-up)

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

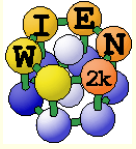


gap

metallic



all three compound crystallize in the rutile structure



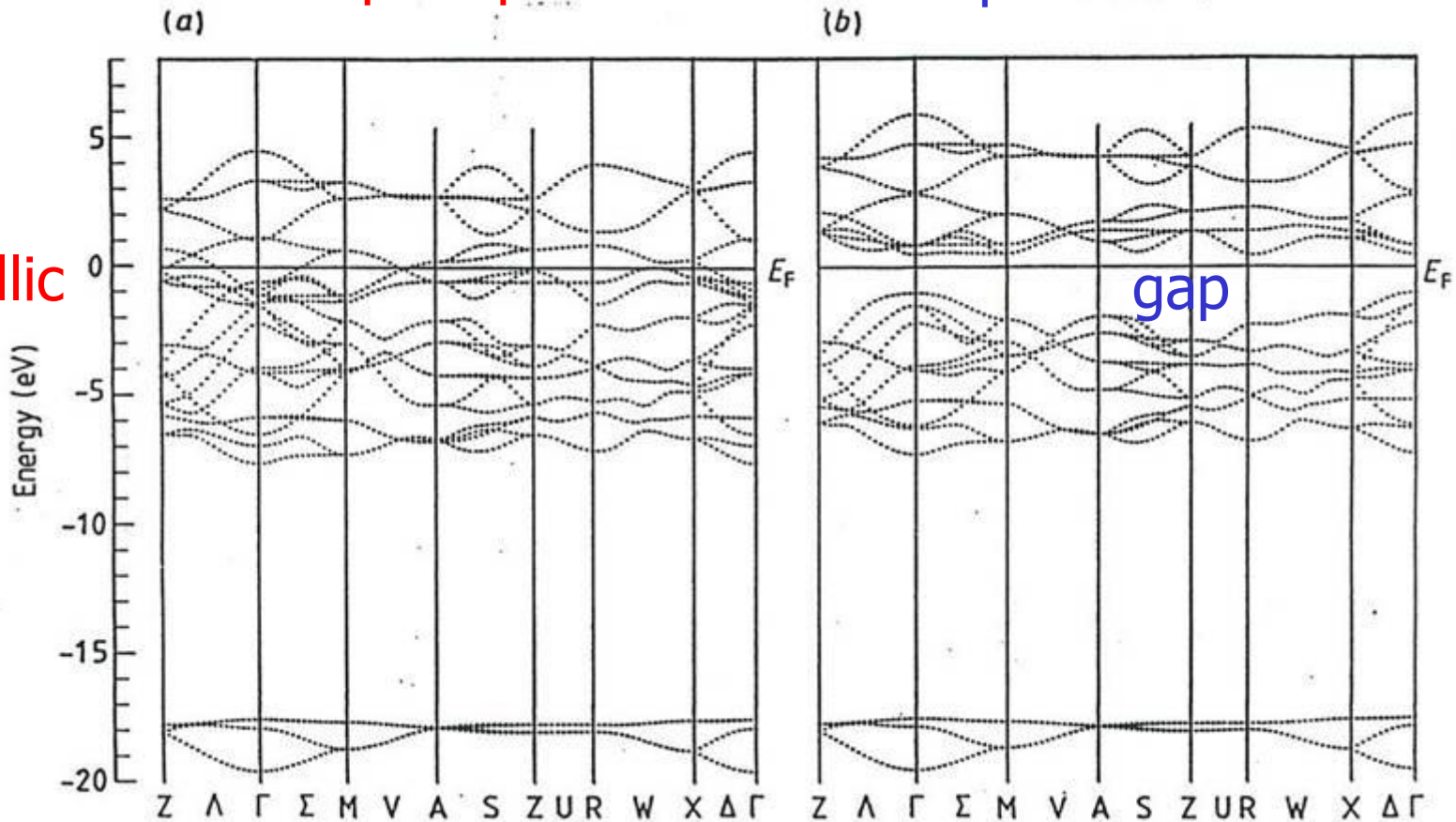
# Half-metallic ferromagnet

- CrO<sub>2</sub> (rutile structure)

spin-up

spin-down

metallic





# CrO<sub>2</sub> spin-down (TiO<sub>2</sub>) spin-up (RuO<sub>2</sub>)



Atomic number

Symbol

Atomic weight

Metal  
 Semimetal  
 Nonmetal

1 1 <b>H</b> 1.008	2 3 <b>Li</b> 6.941	4 4 <b>Be</b> 9.012											13 5 <b>B</b> 10.81	14 6 <b>C</b> 12.01	15 7 <b>N</b> 14.01	16 8 <b>O</b> 16.00	17 9 <b>F</b> 19.00	18 10 <b>Ne</b> 20.18
11 11 <b>Na</b> 22.99	12 12 <b>Mg</b> 24.31											13 13 <b>Al</b> 26.98	14 14 <b>Si</b> 28.09	15 15 <b>P</b> 30.97	16 16 <b>S</b> 32.07	17 17 <b>Cl</b> 35.45	18 18 <b>Ar</b> 39.95	
19 19 <b>K</b> 39.10	20 20 <b>Ca</b> 40.08	21 21 <b>Sc</b> 44.96	22 22 <b>Ti</b> 47.88	23 23 <b>V</b> 50.94	24 24 <b>Cr</b> 52.00	25 25 <b>Mn</b> 54.94	26 26 <b>Fe</b> 55.85	27 27 <b>Co</b> 58.93	28 28 <b>Ni</b> 58.69	29 29 <b>Cu</b> 63.55	30 30 <b>Zn</b> 65.39	31 31 <b>Ga</b> 69.72	32 32 <b>Ge</b> 72.61	33 33 <b>As</b> 74.92	34 34 <b>Se</b> 78.96	35 35 <b>Br</b> 79.90	36 36 <b>Kr</b> 83.80	
37 37 <b>Rb</b> 85.47	38 38 <b>Sr</b> 87.62	39 39 <b>Y</b> 88.91	40 40 <b>Zr</b> 91.22	41 41 <b>Nb</b> 92.91	42 42 <b>Mo</b> 95.94	43 43 <b>Tc</b> 98.91	44 44 <b>Ru</b> 101.1	45 45 <b>Rh</b> 102.9	46 46 <b>Pd</b> 106.4	47 47 <b>Ag</b> 107.9	48 48 <b>Cd</b> 112.4	49 49 <b>In</b> 114.8	50 50 <b>Sn</b> 118.7	51 51 <b>Sb</b> 121.8	52 52 <b>Te</b> 127.6	53 53 <b>I</b> 126.9	54 54 <b>Xe</b> 131.3	
55 55 <b>Cs</b> 132.9	56 56 <b>Ba</b> 137.3	71 71 <b>Lu</b> 175.0	72 72 <b>Hf</b> 178.5	73 73 <b>Ta</b> 180.9	74 74 <b>W</b> 183.8	75 75 <b>Re</b> 186.2	76 76 <b>Os</b> 190.2	77 77 <b>Ir</b> 192.2	78 78 <b>Pt</b> 195.1	79 79 <b>Au</b> 197.0	80 80 <b>Hg</b> 200.6	81 81 <b>Tl</b> 204.4	82 82 <b>Pb</b> 207.2	83 83 <b>Bi</b> 209.0	84 84 <b>Po</b> 209.0	85 85 <b>At</b> 210.0	86 86 <b>Rn</b> 222.0	
87 87 <b>Fr</b> 223.0	88 88 <b>Ra</b> 226.0	103 103 <b>Lr</b> 262.1	104 104 <b>Rf</b> 261.1	105 105 <b>Db</b> 262.1	106 106 <b>Sg</b> 263.1	107 107 <b>Bh</b> 264.1	108 108 <b>Hs</b> 265.1	109 109 <b>Mt</b> 268	110 110 <b>Uun</b> 269	111 111 <b>Uuu</b> 272	112 112 <b>Uub</b> 277	113 113 <b>Uut</b>	114 114 <b>Uuq</b> 289	115 115 <b>Uup</b>	116 116 <b>Uuh</b> 289	117 117 <b>Uus</b>	118 118 <b>Uuo</b> 293	
		57 57 <b>La</b> 138.9	58 58 <b>Ce</b> 140.1	59 59 <b>Pr</b> 140.9	60 60 <b>Nd</b> 144.2	61 61 <b>Pm</b> 146.9	62 62 <b>Sm</b> 150.4	63 63 <b>Eu</b> 152.0	64 64 <b>Gd</b> 157.3	65 65 <b>Tb</b> 158.9	66 66 <b>Dy</b> 162.5	67 67 <b>Ho</b> 164.9	68 68 <b>Er</b> 167.3	69 69 <b>Tm</b> 168.9	70 70 <b>Yb</b> 173.0			
		89 89 <b>Ac</b> 227.0	90 90 <b>Th</b> 232.0	91 91 <b>Pa</b> 231.0	92 92 <b>U</b> 238.0	93 93 <b>Np</b> 237.0	94 94 <b>Pu</b> 244.1	95 95 <b>Am</b> 243.1	96 96 <b>Cm</b> 247.1	97 97 <b>Bk</b> 247.1	98 98 <b>Cf</b> 251.1	99 99 <b>Es</b> 252.0	100 100 <b>Fm</b> 257.1	101 101 <b>Md</b> 258.1	102 102 <b>No</b> 259.1			



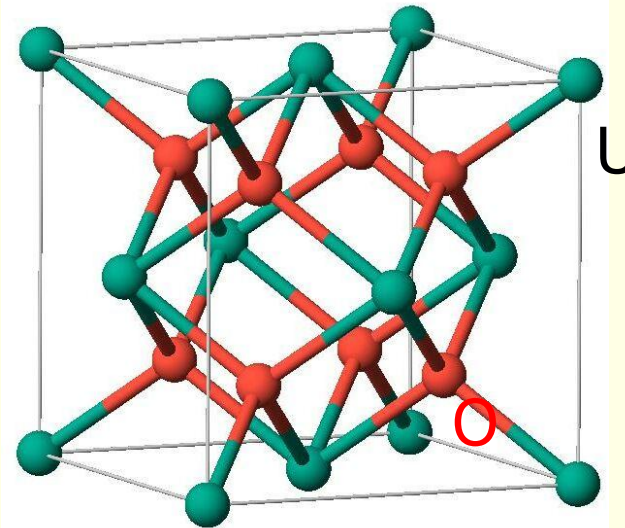
# Magnetic structure of uranium dioxide $\text{UO}_2$

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

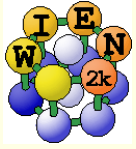


- topics

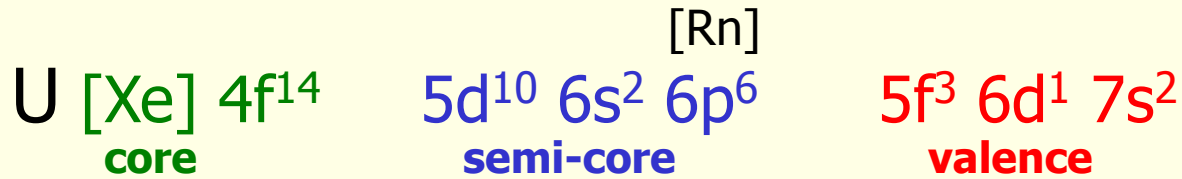
- *non-collinear magnetism*
- *spin-orbit coupling*
- *LDA+U (correlation of U-5f electrons)*
- *Structure relaxations*
- *electric field gradient (EFG)*



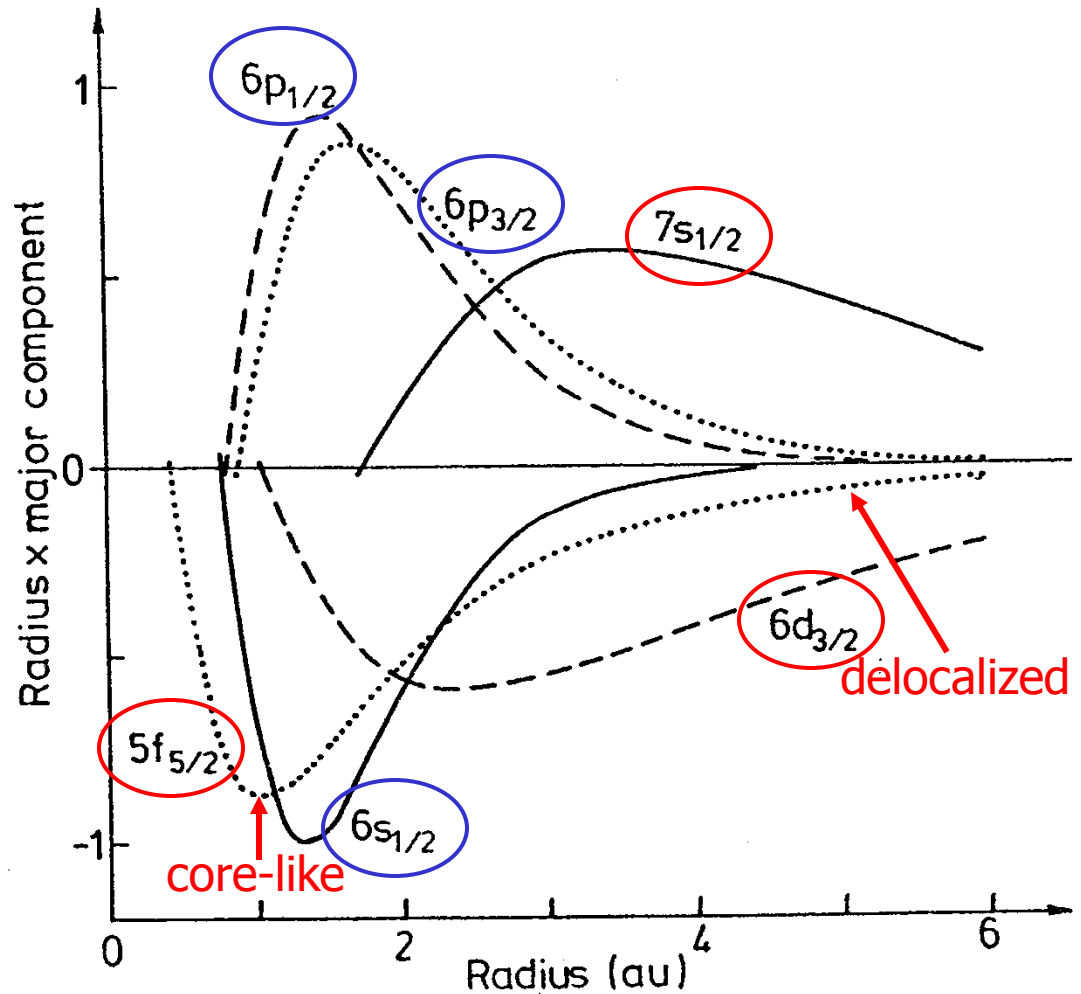
R.Laskowski, G.K.H.Madsen, P.Blaha, K.Schwarz:  
*Magnetic structure and electric-field gradients of uranium dioxide: An ab initio study*  
Phys.Rev.B **69**, 140408-1-4 (2004)



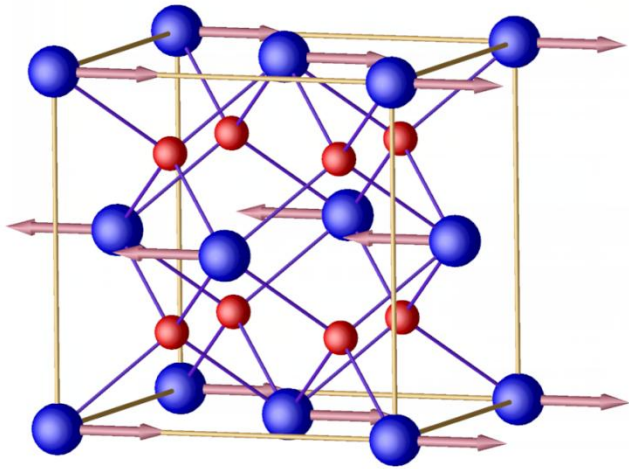
# Atomic configuration of uranium (Z=92)



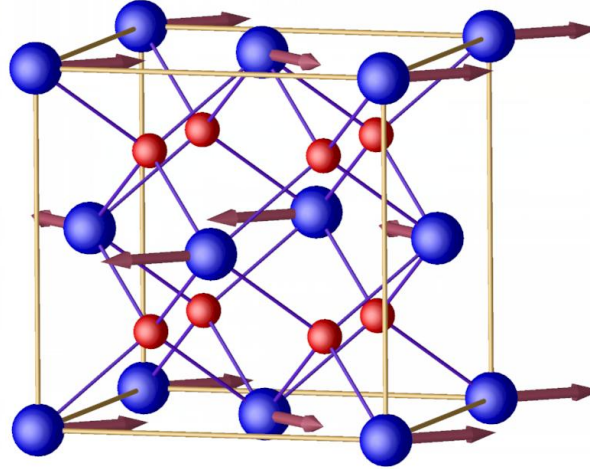
		E <sub>j</sub> (Ryd)	
		j (relativ.)	
n l		l-s	l+s
7s			-0.25
6d		-0.29	-0.25
5f		-0.17	-0.11
6p		-1.46	-2.10
6s			-3.40
5d		-7.48	-6.89
5p		-18.05	-14.06
5s			-22.57
4f		-27.58	-26.77
...			
1s			-8513.38



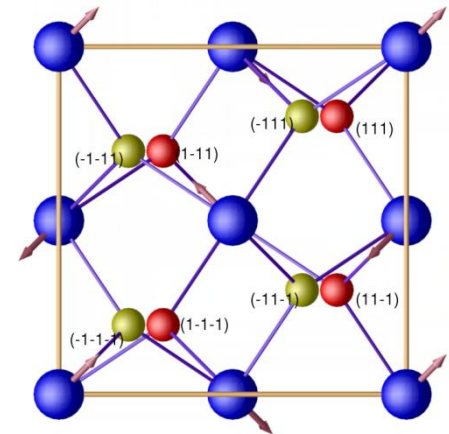
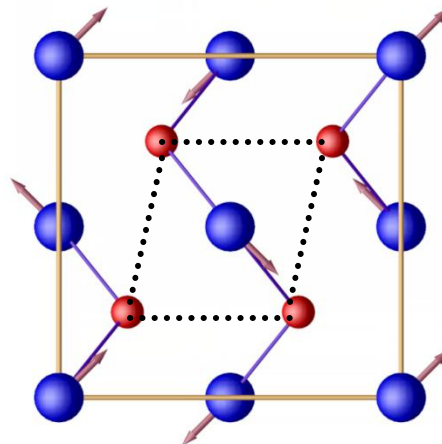
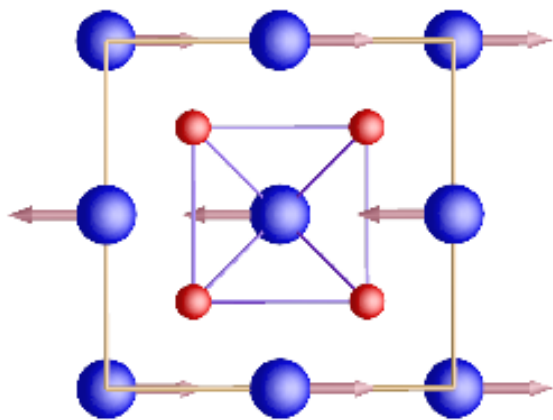
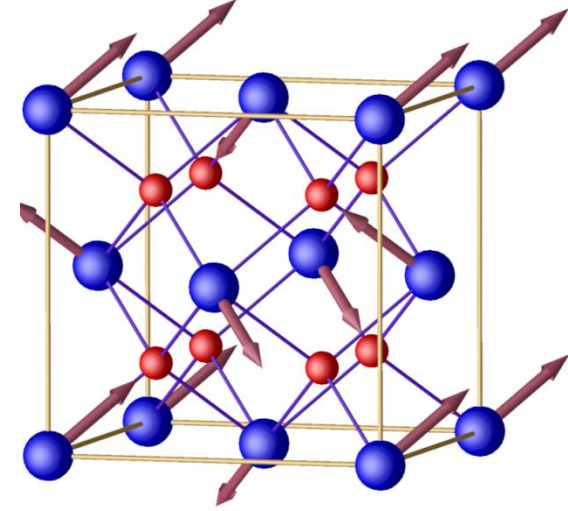
collinear 1k-

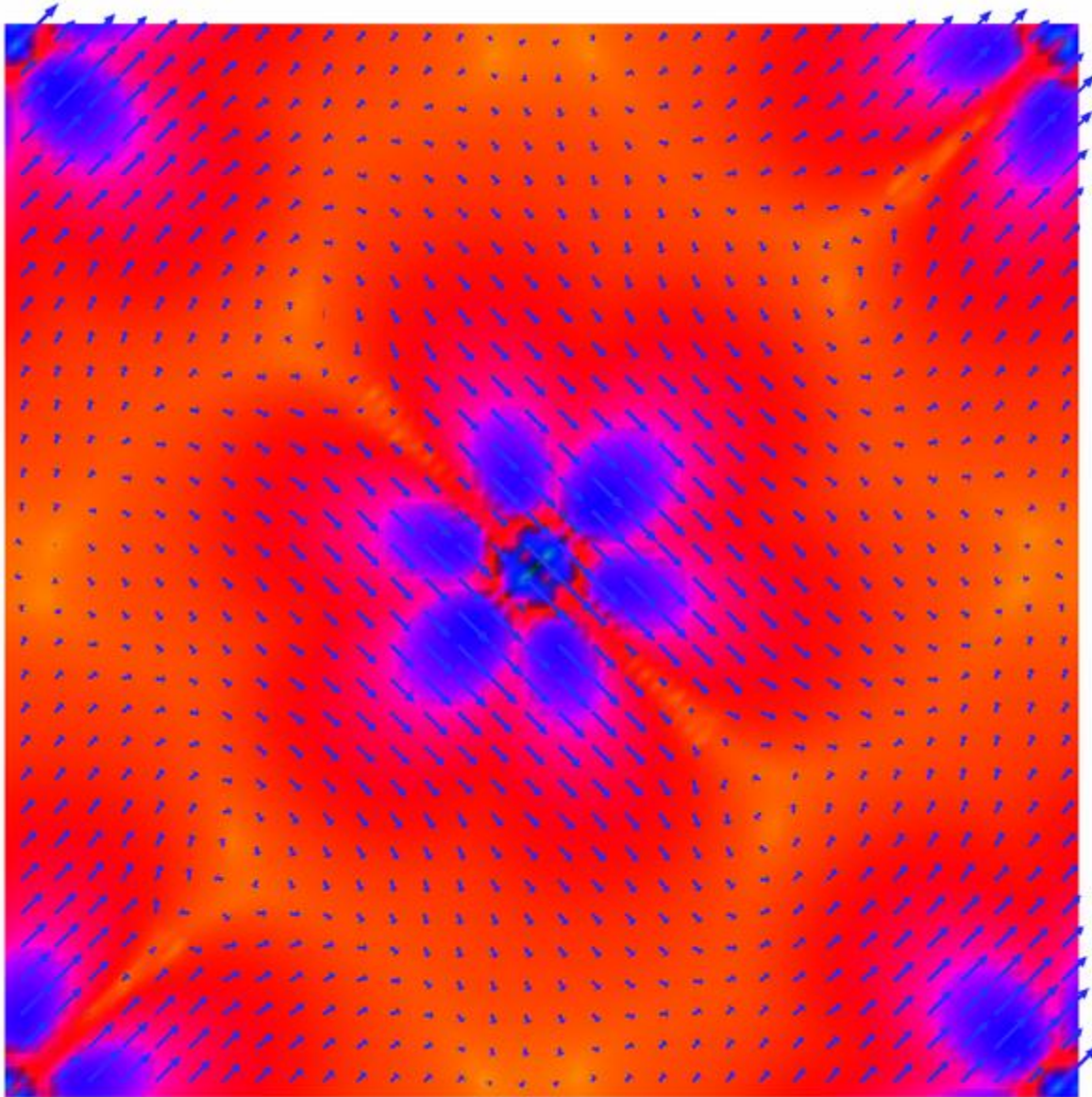


non-collinear 2k-

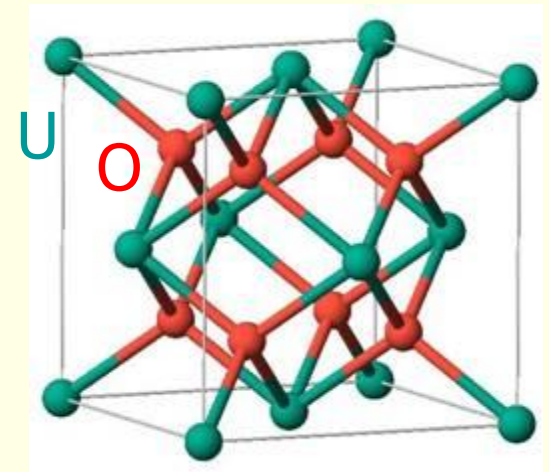


or 3k-structure



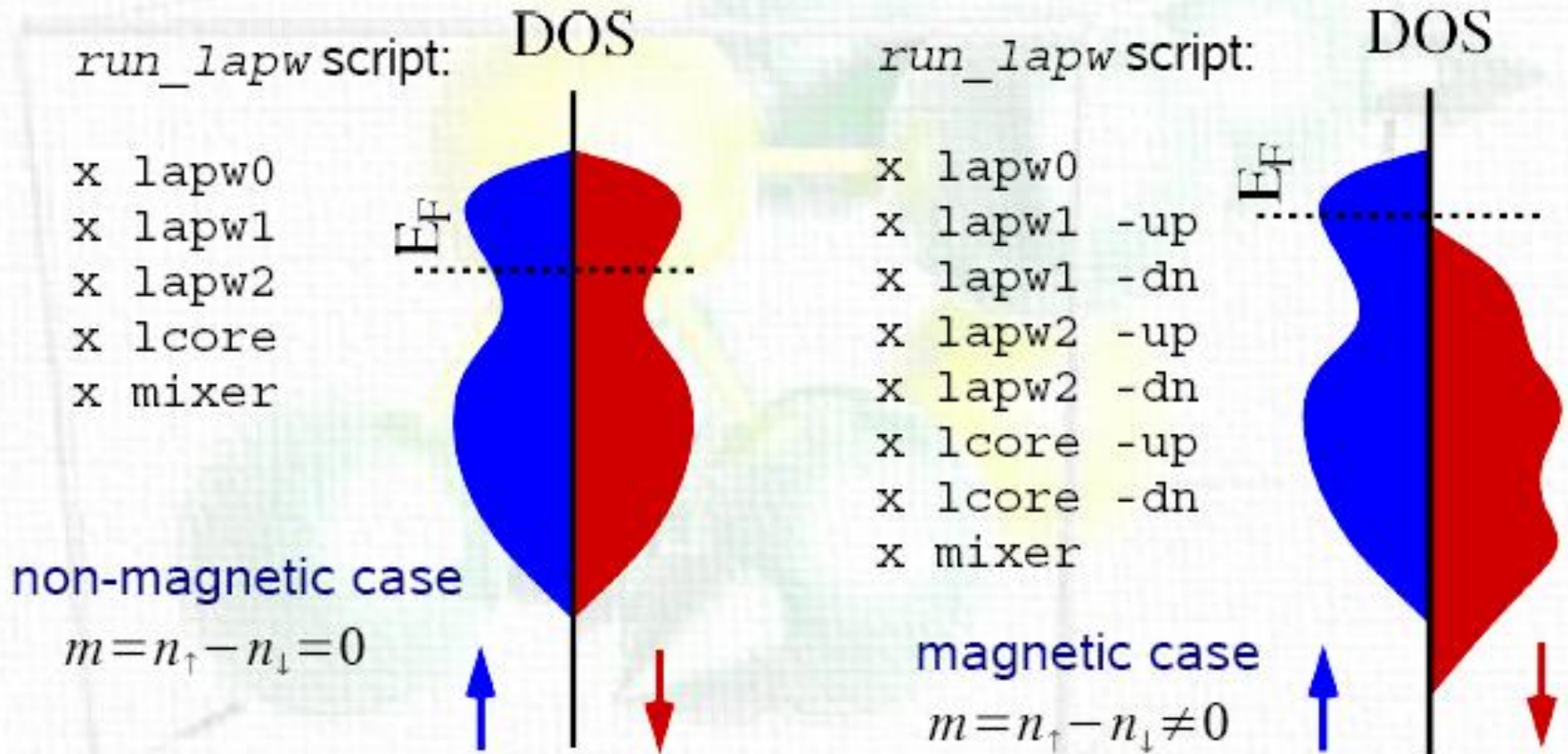


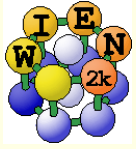
- Magnetisation direction perpendicular at the two U sites (arrows)
- Magnetisation density (color)





- Wien2k can only handle collinear or non-magnetic cases

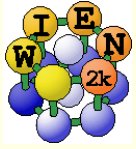




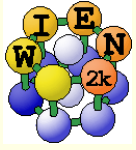
- *runsp\_lapw* script (unconstrained magnetic calc.)
  - runs lapw1/2 for both spins **independently**
  - case.scf contains extra information:
    - `grep :MMT case.scf` (for total moment)
    - `grep :MMI case.scf` (for atomic moments)
    - `grep :HFF case.scf` (for hyperfine fields)



- *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



- *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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