Radboud Universiteit

Theory of itinerant-electron magnetism

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Outline

1. Introduction
2. Exchange interactions in DFT
3. Localized vs itinerant behavior of d-electrons
4. DMFT theory for Fe, Co, and Ni
5. Correlations, magnetism and metallurgy
6. Half-metallic ferromagnets: many-body effects

Epigraphs

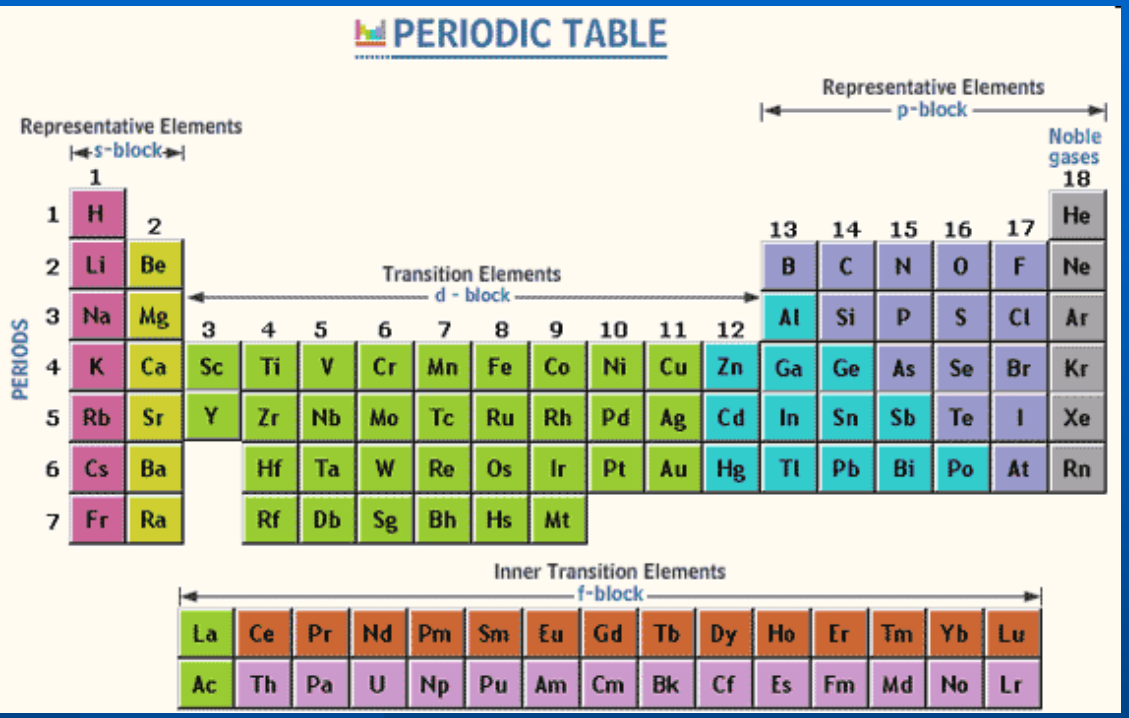
To the theoretical physicists, ferromagnetism presents a number of very interesting, unsolved and beautiful challenges. Our challenge is to understand why it exists at all.

(Feynman Lectures on Physics)

Make things as simple as possible but not simpler

(A. Einstein)

Long-standing problem



Ferromagnetism of iron is known from ancient times

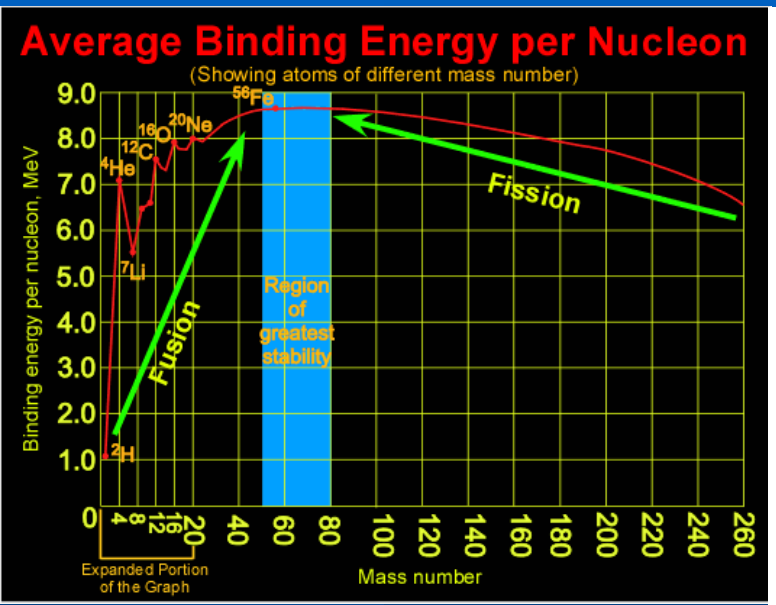
Iron

Cobalt

Nickel

Iron is special

^{56}Fe is the most stable nucleus, therefore there is a lot of iron (and nickel) in stars and planets



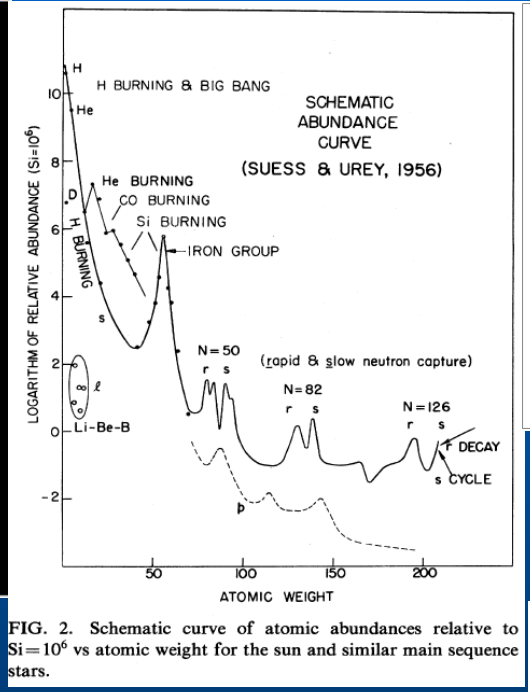
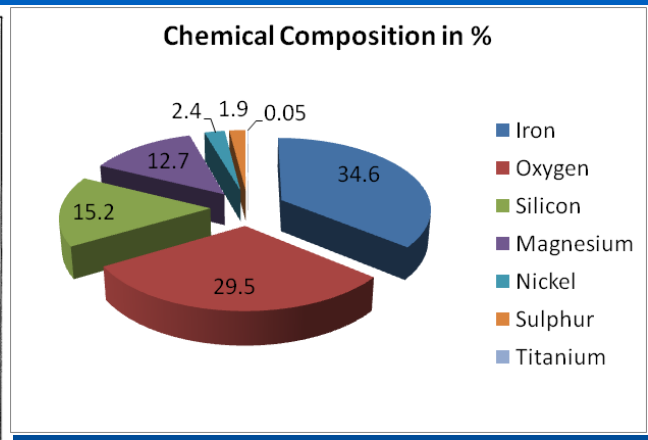
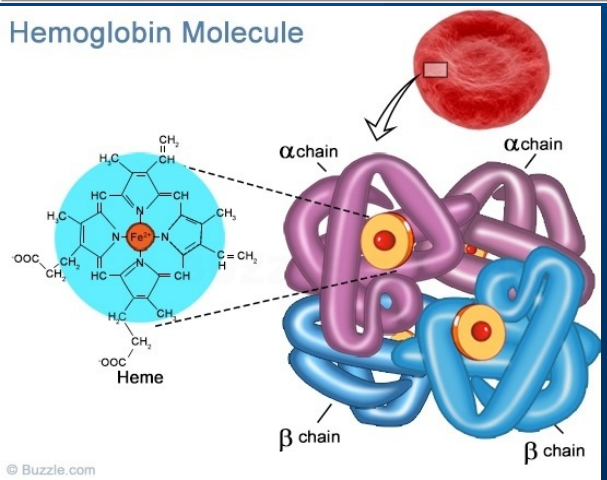


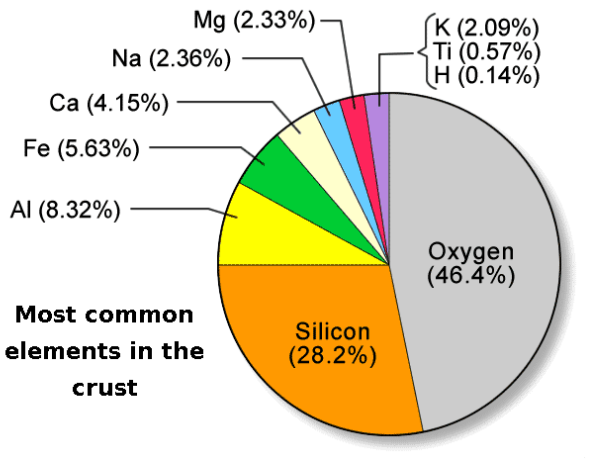
FIG. 2. Schematic curve of atomic abundances relative to Si=10^6 vs atomic weight for the sun and similar main sequence stars.



Chemical composition of Earth

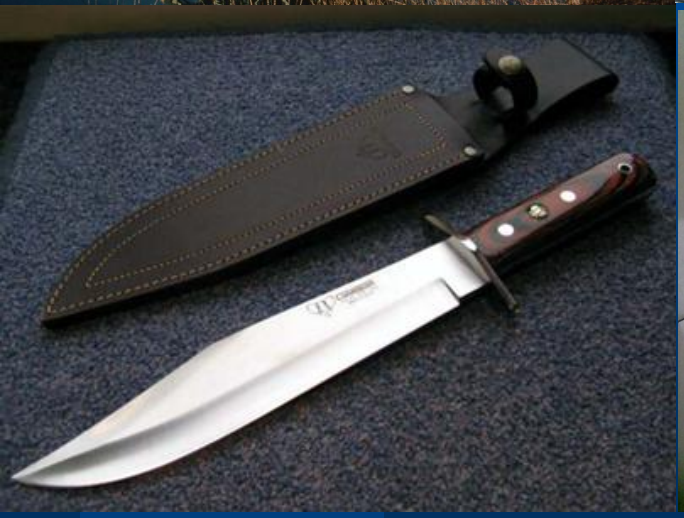


Crucially important for life (enzymes, oxygen trasfer, etc.)

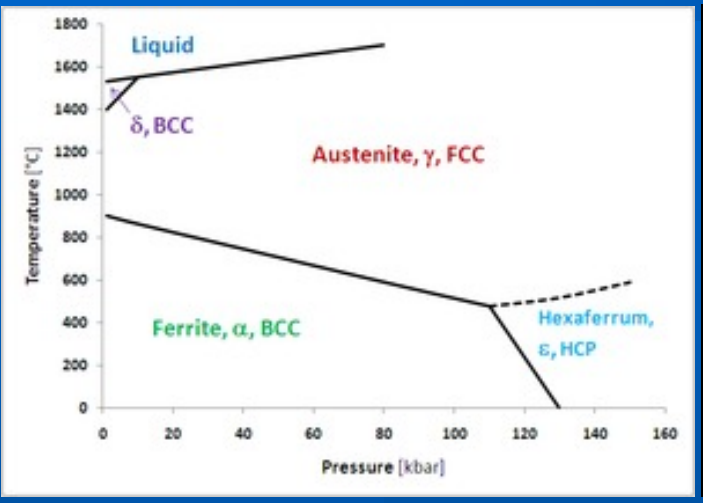


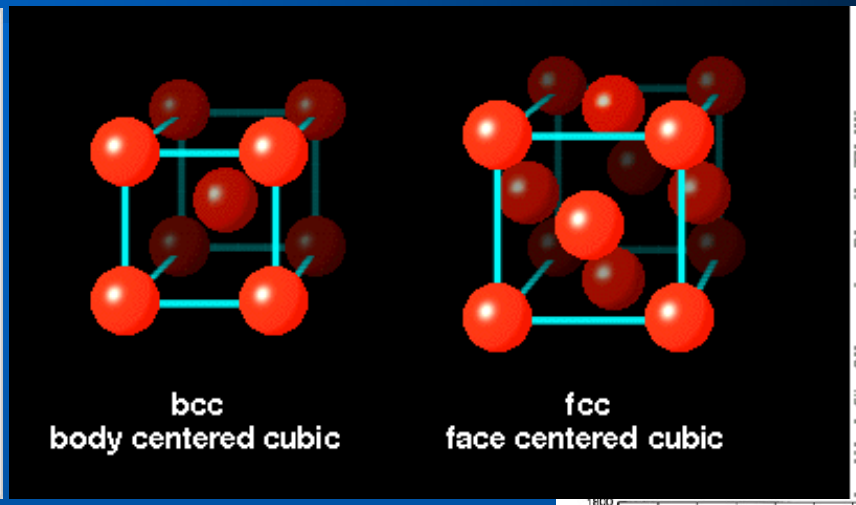
We are still in iron age

Steel (basically, Fe and a bit C) is one of the main materials of our civilization



Iron is polymorphous metal

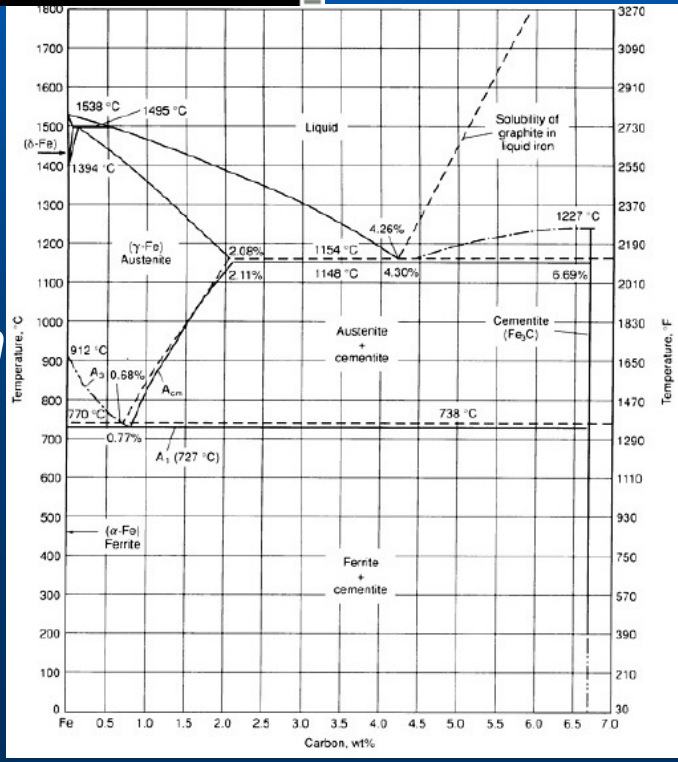




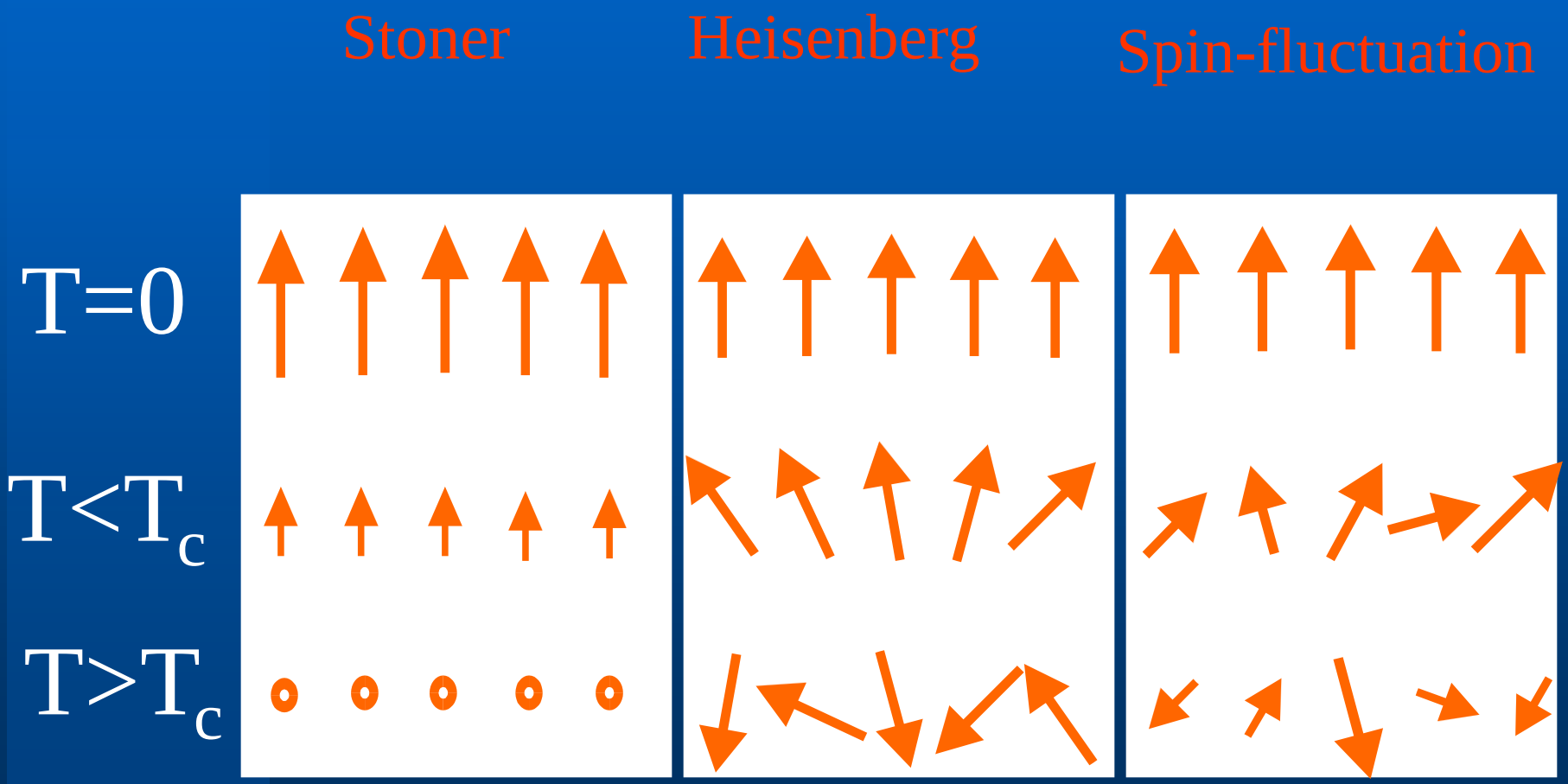
The only polymorphous metal where bcc phase is stable at lower temperatures than fcc or hcp: Role of magnetism (Zener)

Crucially important for Fe-C phase diagram and therefore for metallurgy

Should follow from electronic structure (quantum mechanical energy spectrum)



Itinerant-electron ferromagnetism



Stoner criterion

$$I_{\mathrm{eff}} N(E_{\mathrm{F}}) > 1$$

$N(E_{\mathrm{F}})$ is the density of one-electron states

I_{eff} is an on-site interaction parameter

Stoner parameter ≈ 0.9 eV for all 3d metals; DOS is crucially important

Equation for the Curie temperature:

f(E) Fermi function

$$I_{\mathrm{eff}} \int \mathrm{d}E \left(-\frac{\partial f}{\partial E} \right) N(E) = 1$$

If Fe would be Stoner magnet it would have T_C ≈ 4000 K (in reality 1043 K)

In reality, T_c is determined by spin fluctuations,
That is, exchange parameters

Density Functional Theory

SE for many-body wave function in configurational space is replaced by single-particle nonlinear self-consistent equation

Spinor $\Psi = \begin{pmatrix} \Psi_+ \\ \Psi_- \end{pmatrix}$

$$i\frac{\partial \Psi}{\partial t} = [H_L - \hat{\boldsymbol{\sigma}} \cdot \mathbf{B}(\mathbf{r},t)]\Psi$$

B is self-consistent magnetic field

$$H_L = -\nabla_{\mathbf{r}}^2 + \sum_{\mathbf{R}} V_{\mathbf{rR}} + 2\int d\mathbf{r}' \frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} + V_{\mathrm{xc}}$$

Simplifications

Adiabatic approx.: V_{xc} and B_{xc} are the same as in the equilibrium + local (spin) density approx.

$$\mathrm{i}\frac{\partial \psi}{\partial t} = H\psi$$

$$H = -\nabla^2 + V(\mathbf{r}) - \tfrac{1}{2}(\mathbf{B}_{\mathrm{xc}}(\mathbf{r}) + \mathbf{B}_{\mathrm{ext}}(\mathbf{r}))\sigma$$

$$V(\mathbf{r}) = V_{\mathrm{ext}}(\mathbf{r}) + \int \mathrm{d}\mathbf{r}' \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + \frac{\partial}{\partial n}[n\varepsilon_{\mathrm{xc}}]$$

$$\mathbf{B}_{\mathrm{xc}} = -2\frac{\mathbf{m}}{m}\frac{\partial}{\partial m}[n\varepsilon_{\mathrm{xc}}]$$

n,m are charge and spin densities

Magnetic force theorem

(Lichtenstein,MIK, Gubanov, J. Phys. F 1984; Sol. St. Comm. 1985)

Total energy in DFT

$$E = E_{sp} - E_{dc}$$

$$E_{sp} = \sum_{\nu}^{occ} \varepsilon_{\nu}$$

$$E_{dc} = E_{Hartree} + \int dr Tr\left[\rho \frac{\delta E_{xc}}{\delta \rho}\right] - E_{xc}$$

Variation

$$\delta E = \delta^* E_{sp} + \delta_1 E_{sp} - \delta E_{dc} = \delta^* E_{sp} = \delta^* \int_{-\infty}^{\varepsilon_F} d\varepsilon \left[\frac{1}{\pi} Tr\, \mathrm{Im}\, \hat{G}(\varepsilon)\right]$$

δ^* at fixed potential

δ_1 due to change of potential

Magnetic force theorem II

- Torque can be written in terms of variation of the density of states
- Decomposition of the torque in pair terms gives exchange integrals
- These exchange parameters are local (near given magnetic configuration)

Journal of Magnetism and Magnetic Materials 67 (1987) 65–74
North-Holland, Amsterdam

LOCAL SPIN DENSITY FUNCTIONAL APPROACH TO THE THEORY OF EXCHANGE INTERACTIONS IN FERROMAGNETIC METALS AND ALLOYS

A.I. LIECHTENSTEIN, M.I. KATSNELSON [+], V.P. ANTROPOV [+] and V.A. GUBANOV

Table 1
Values of exchange interaction parameters calculated by the cluster Green's function method

Metal	J_0 (meV)	T_c (K)	T_c^{expt} (K)	J_1 (meV)	J_2 (meV)	D (meV Å^2)	D^{expt} (meV Å^2)
Fe	155.7	1200	1040 [a]	20.5	−3.4	294	314 [b]
Ni	49.1	380	630 [a]	1.9	0.23	386	395 [c]

Non-Heisenberg character of exchange interactions in Fe and Ni

S.A. Turzhevskii, A.I. Lichtenstein, and M.I. Katsnelson, Fiz. Tverd. Tela **32**, 1952 (1990) [Sov. Phys. Solid State **32**, 1138 (1990)].

Rotation of a central spin: magnetic moment is not constant, energy change is not cosine

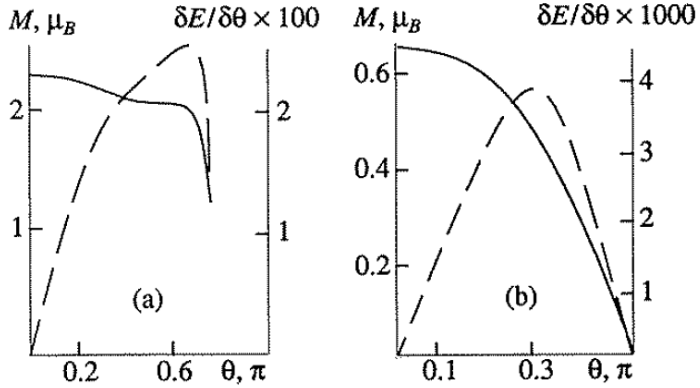


Fig. 4.4. *Magnetic moment in Bohr magnetons (the full curve) and the first derivative of energy with respect to angle of rotation in Ry (the dashed curve) according to calculations in [168]: (a) Fe, (b) Ni.*

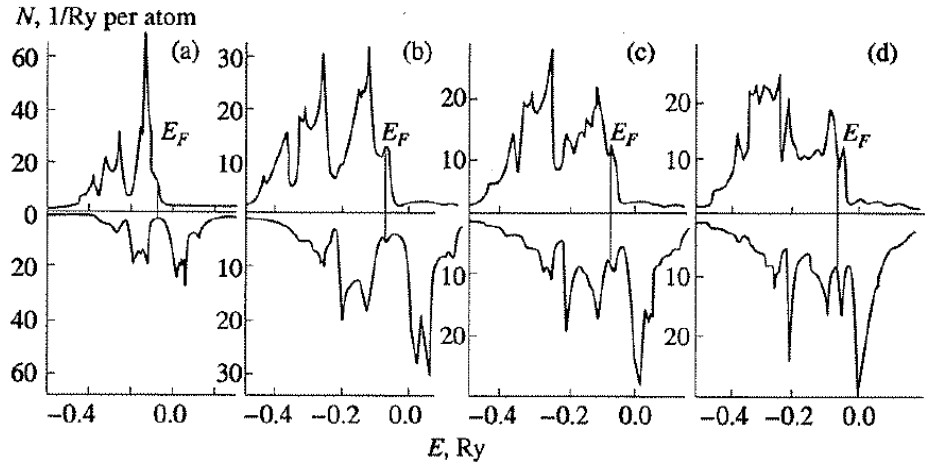
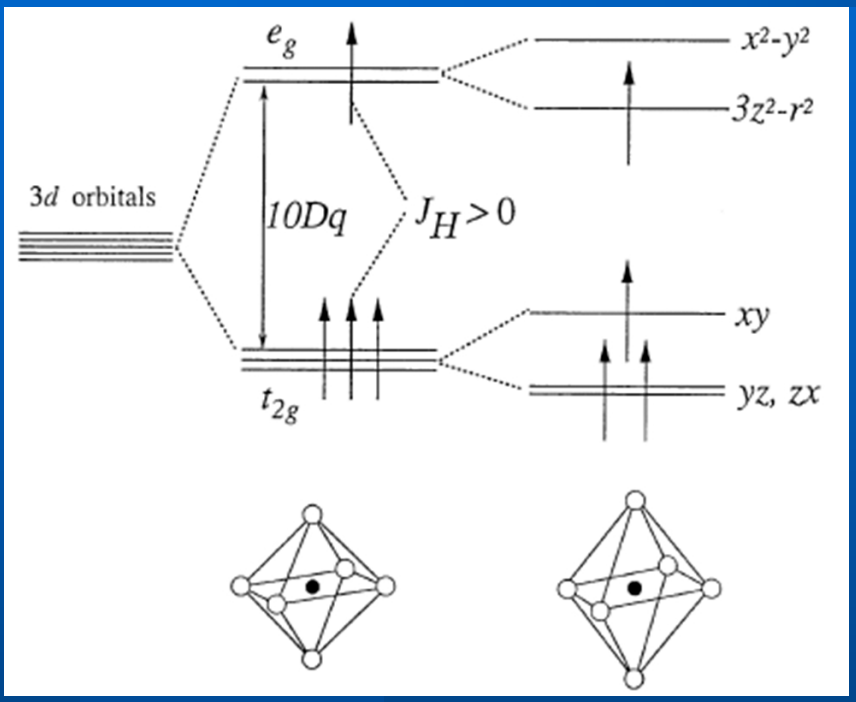


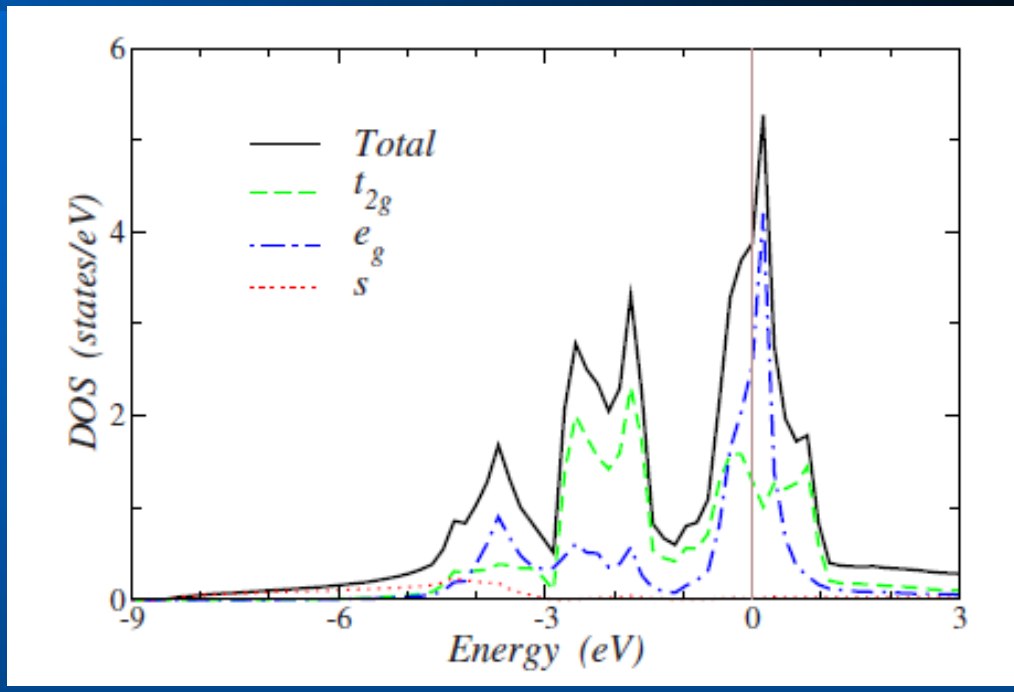
Fig. 4.5. *Electronic density of states for an Fe atom in a metal with the magnetic moment turned through θ = 0 (a), θ = 0.2π (b), θ = 0.35π (c), and θ = 0.5π (d).*

Electronic structure is angle-dependent

Iron: some details



Crystal field splitting



DOS for nonmagnetic bcc Fe

Stoner criterion is fulfilled due to e_g states only; they should play a special role in magnetism of Fe (Irkhin, Katsnelson, Trefilov, JPCM 5, 8763 (1993))

Iron: detailed analysis

PRL 116, 217202 (2016) PHYSICAL REVIEW LETTERS week ending 27 MAY 2016

Microscopic Origin of Heisenberg and Non-Heisenberg Exchange Interactions in Ferromagnetic bcc Fe

Y. O. Kvashnin,[1] R. Cardias,[2] A. Szilva,[1] I. Di Marco,[1] M. I. Katsnelson,[3,4] A. I. Lichtenstein,[4,5] L. Nordström,[1] A. B. Klautau,[2] and O. Eriksson[1]

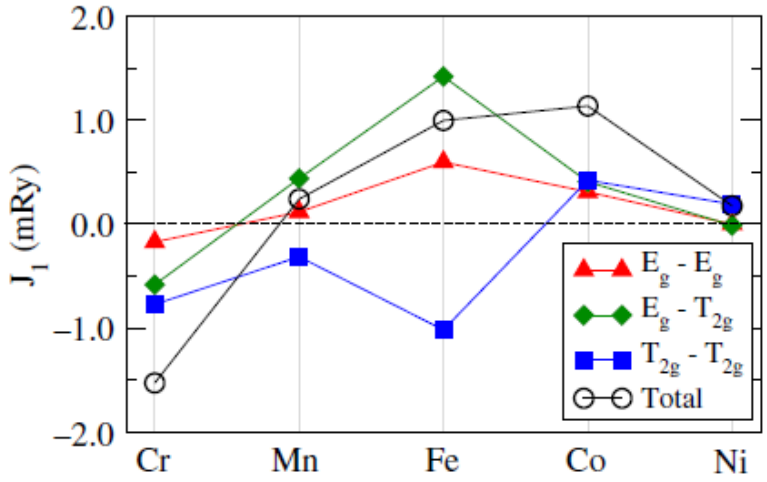
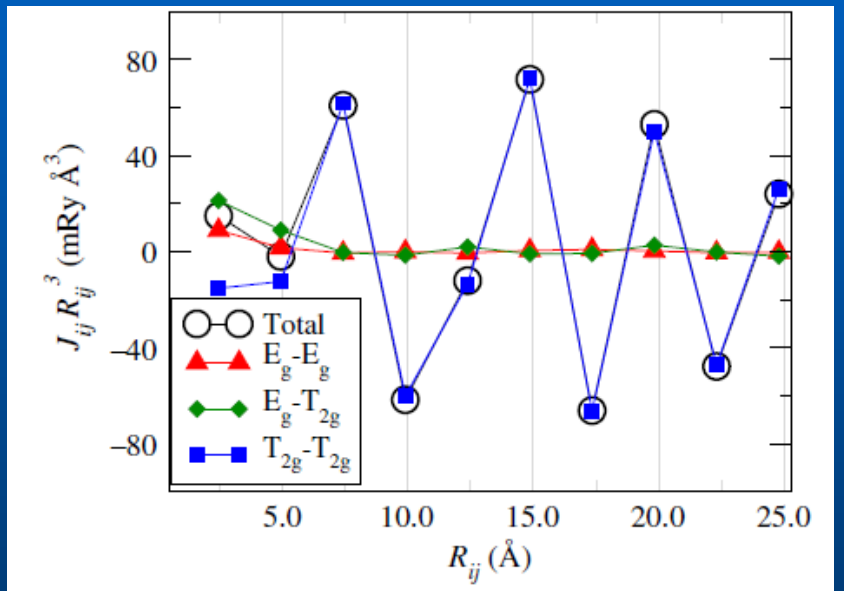
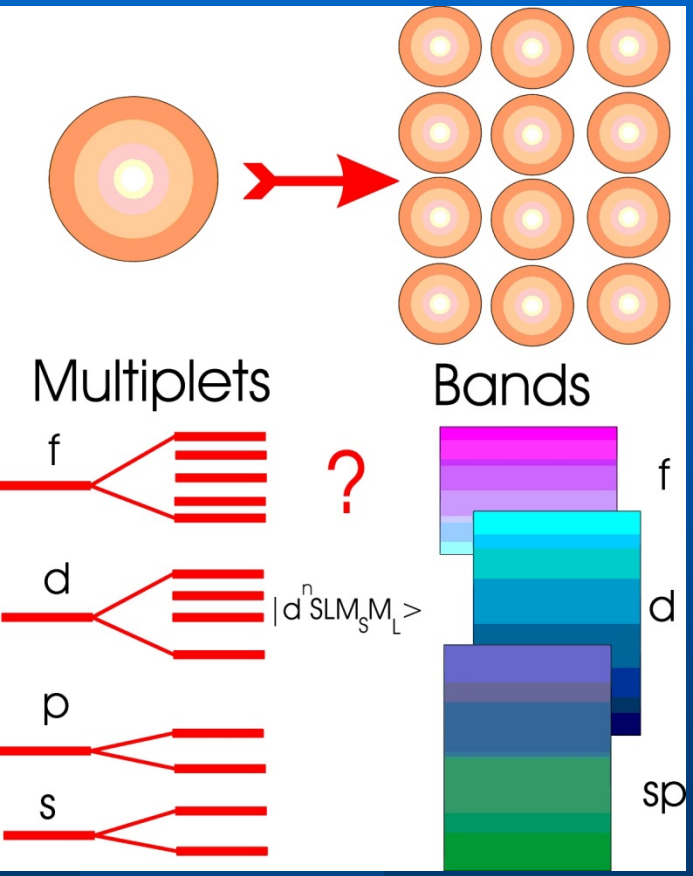


FIG. 1. Orbitally decomposed NN exchange interaction in elemental 3*d* metals in the bcc structure.



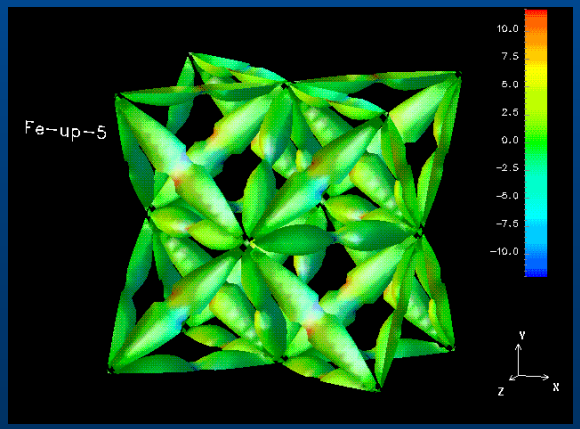
t_{2g} are itinerant electrons providing (Heisenberg-like) RKKY exchange with Friedel oscillations; e_g are more correlated providing (non-Heisenberg) "double exchange" typical for narrom-band systems

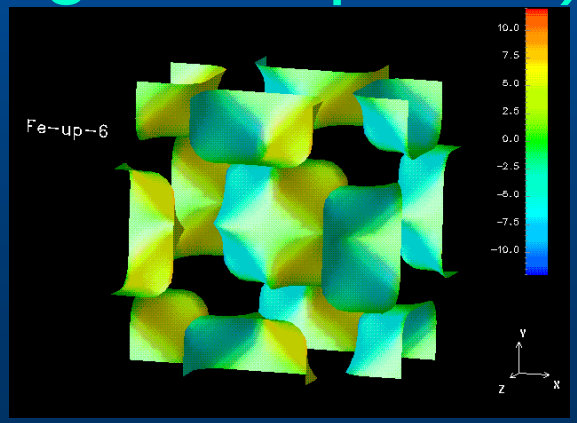
Problem: coexistence of localized and itinerant behavior



Local magnetic moments do exist above T_C (Curie-Weiss law, spectroscopy, neutrons…)

d electrons are itinerant (FS, chemical bonding, transport…)





Iron, majority spin FS

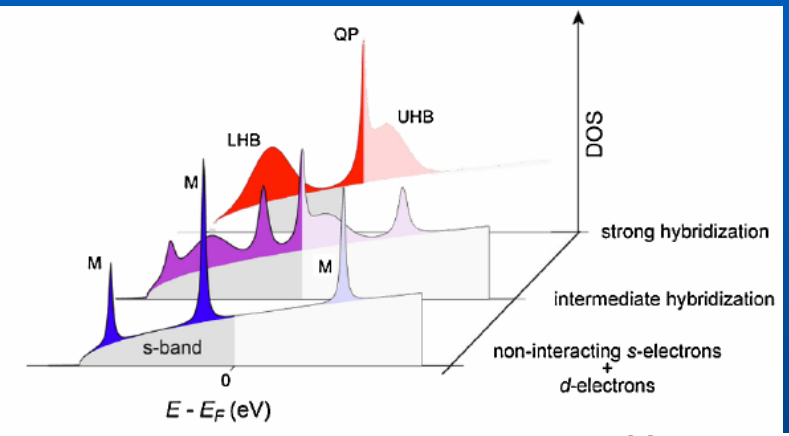
4f electrons are normally pure localized but not 3d

From atomic state to itinerant

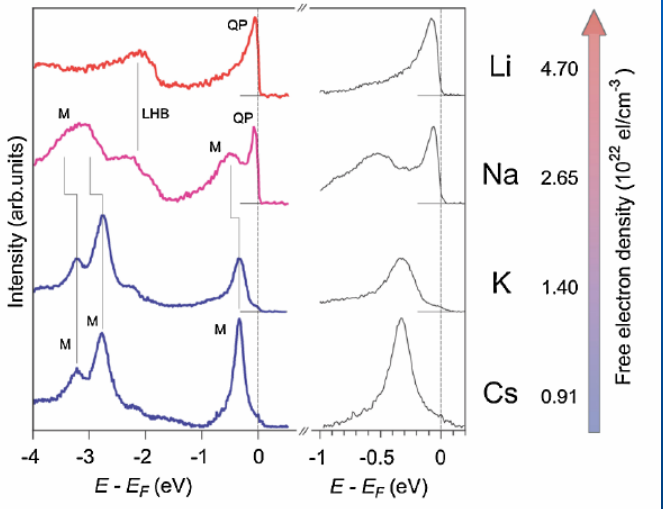
PRL **104,** 117601 (2010) PHYSICAL REVIEW LETTERS week ending 19 MARCH 2010

Correlated Electrons Step by Step: Itinerant-to-Localized Transition of Fe Impurities in Free-Electron Metal Hosts

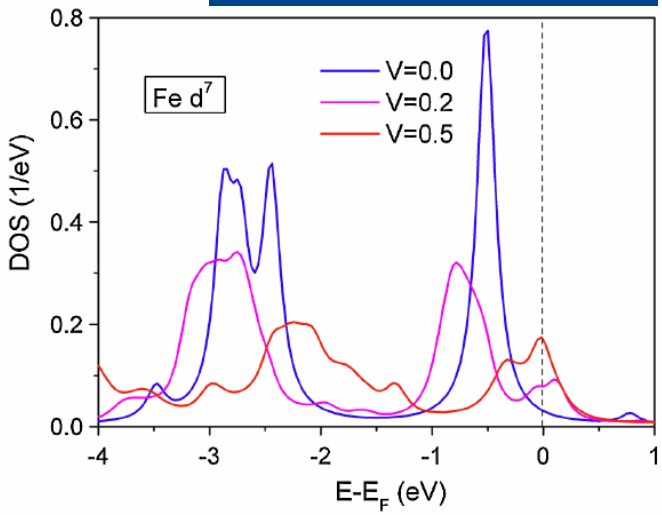
C. Carbone,[1] M. Veronese,[1] P. Moras,[1] S. Gardonio,[1] C. Grazioli,[1] P. H. Zhou,[2] O. Rader,[3] A. Varykhalov,[3] C. Krull,[4] T. Balashov,[4] A. Mugarza,[4] P. Gambardella,[4,5] S. Lebèque,[6] O. Eriksson,[7] M. I. Katsnelson,[8] and A. I. Lichtenstein[9]



Experiment: disappearance of multiplets



Calculations: increase of hybridization



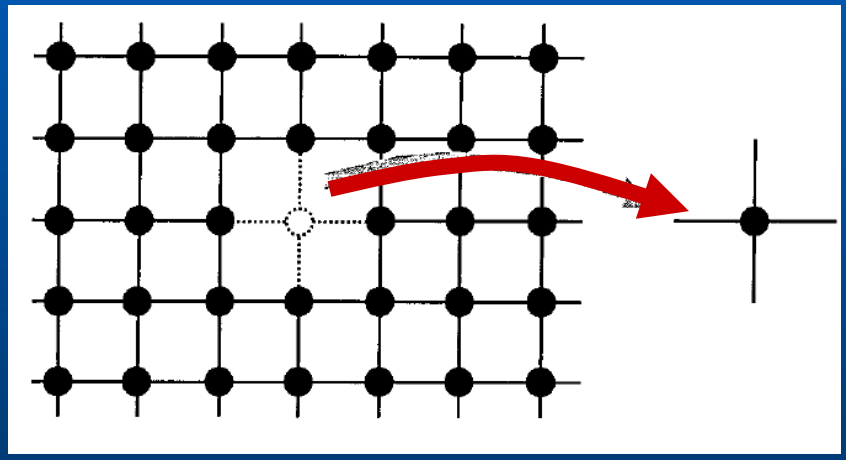
Blue line: exact diagonalization for free atom

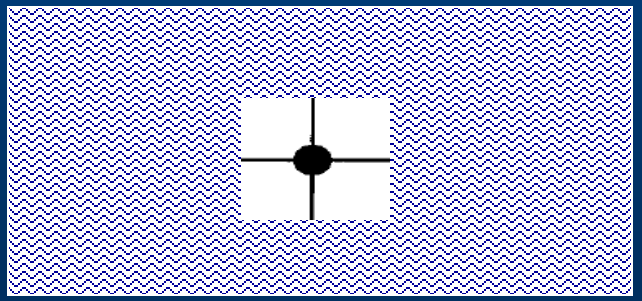
Dynamical Mean Field Theory I

A.Georges, G.Kotliar, W.Krauth and M.Rozenberg, Rev. Mod. Phys. ‘96

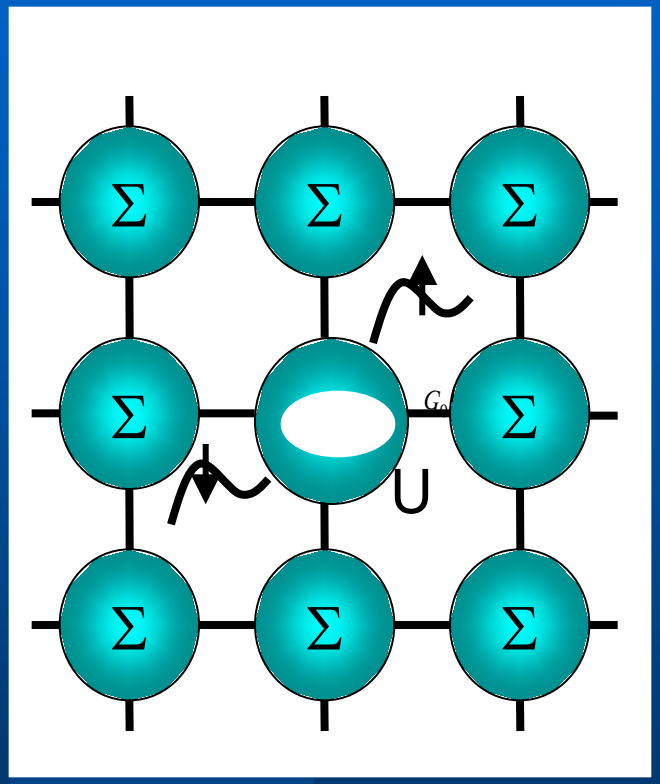
A natural generalization of the familiar MFT
to the problem of electrons in a lattice

Key idea: take one site out of a lattice and embed it in a self-consistent bath = mapping to an effective impurity problem



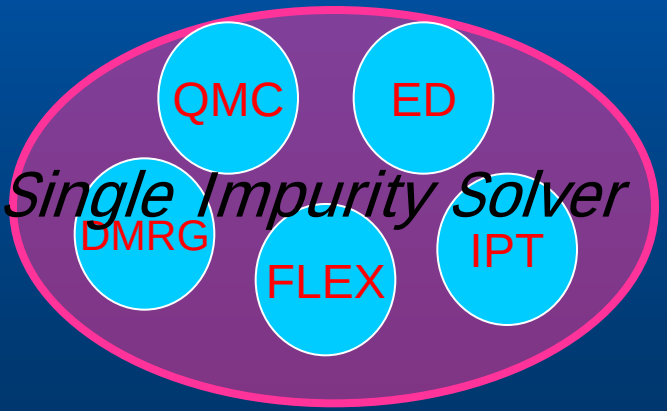


Dynamical Mean Field Theory II



$$\hat{G}(i\omega_n) = \frac{1}{\Omega}\sum_{\vec{k}}^{BZ} \hat{G}(\vec{k}, i\omega_n)$$

$$\hat{\mathcal{G}}_0^{-1}(i\omega_n) = \hat{G}^{-1}(i\omega_n) + \hat{\Sigma}(i\omega_n)$$



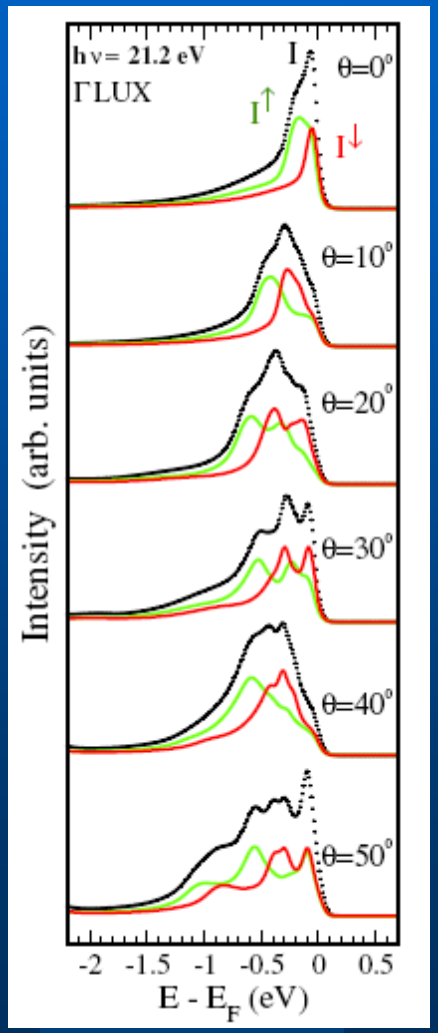
$$\hat{\Sigma}_{new}(i\omega_n) = \hat{\mathcal{G}}_0^{-1}(i\omega_n) - \hat{G}^{-1}(i\omega_n)$$

W. Metzner and D. Vollhardt (1987)
A. Georges and G. Kotliar (1992)

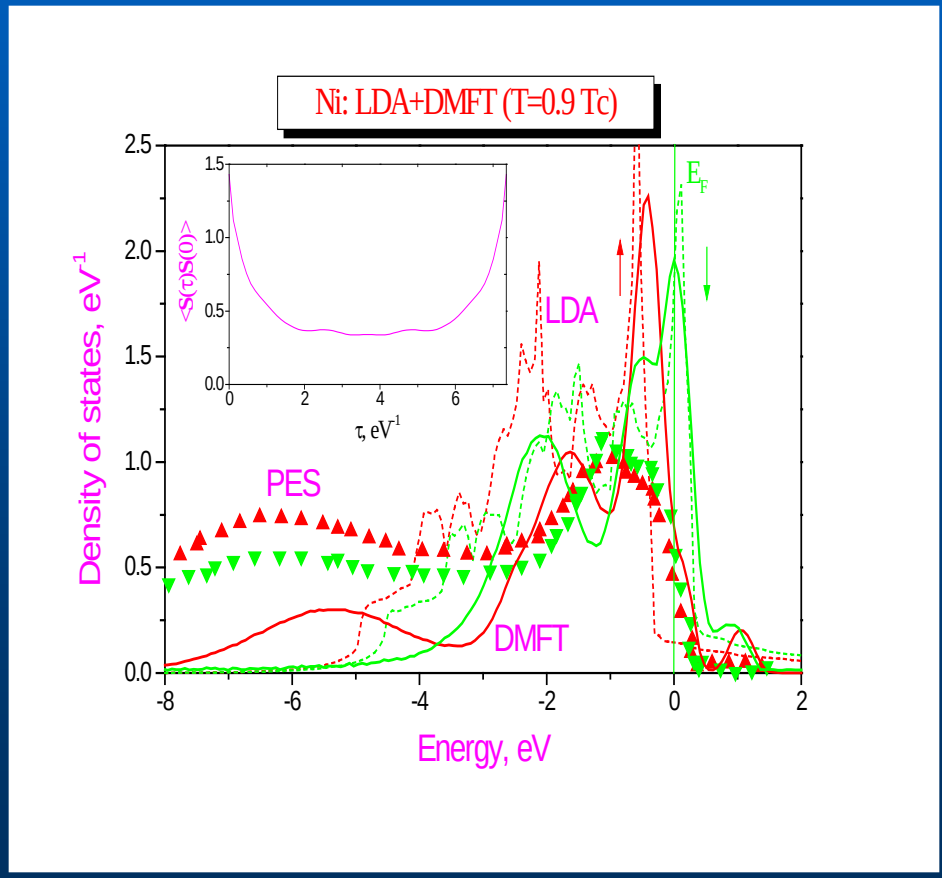
Ferromagnetism of transition metals: LDA+DMFT

Ferromagnetic Ni DMFT vs. LSDA:

- 30% band narrowing
- 50% spin-splitting reduction
- -6 eV sattellite



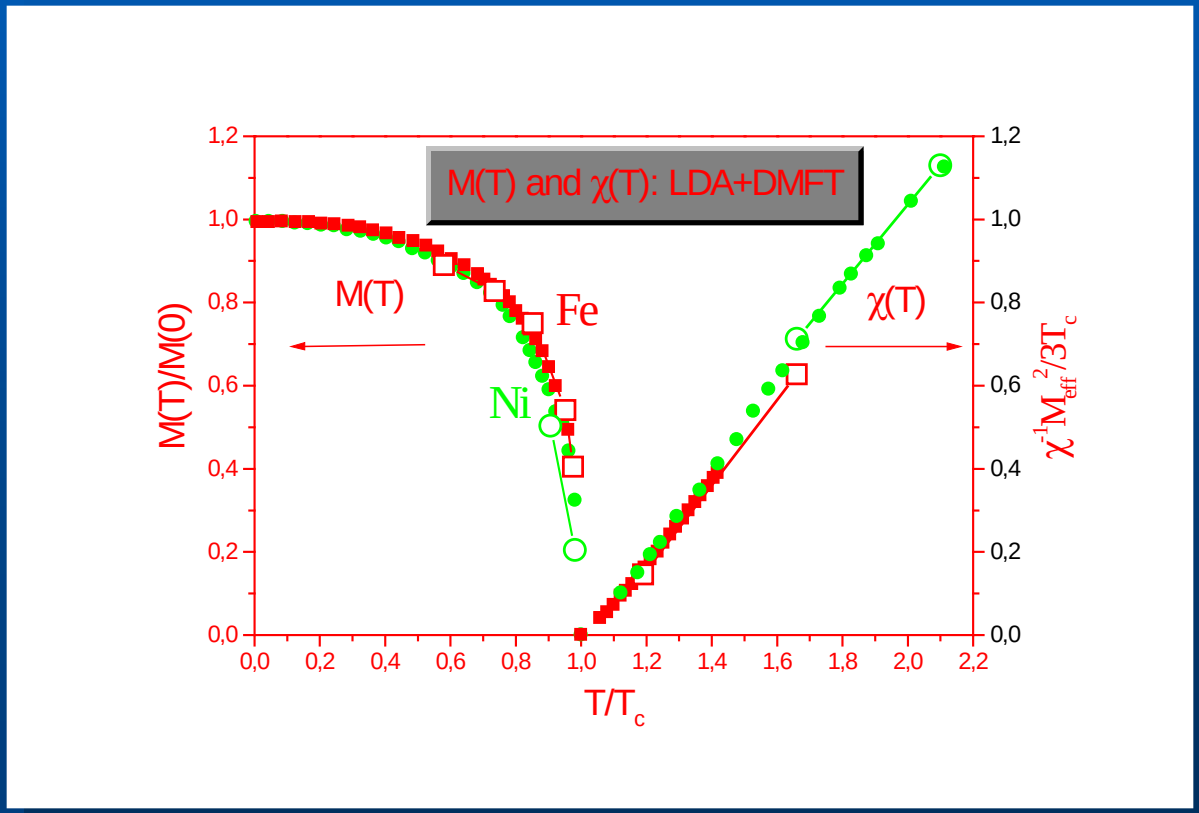
LDA+DMFT with ME
J. Braun *et al*
PRL (2006)



Lichtenstein, MIK, Kotliar, PRL (2001)

Effective Magnetic Moments: $T>T_c$

W	exp	eff	loc	DLM	Tc	exp
Fe	3.13	3.09	2.8	1.96	1900	1043
Ni	1.62	1.5	1.3	1.21	700	631



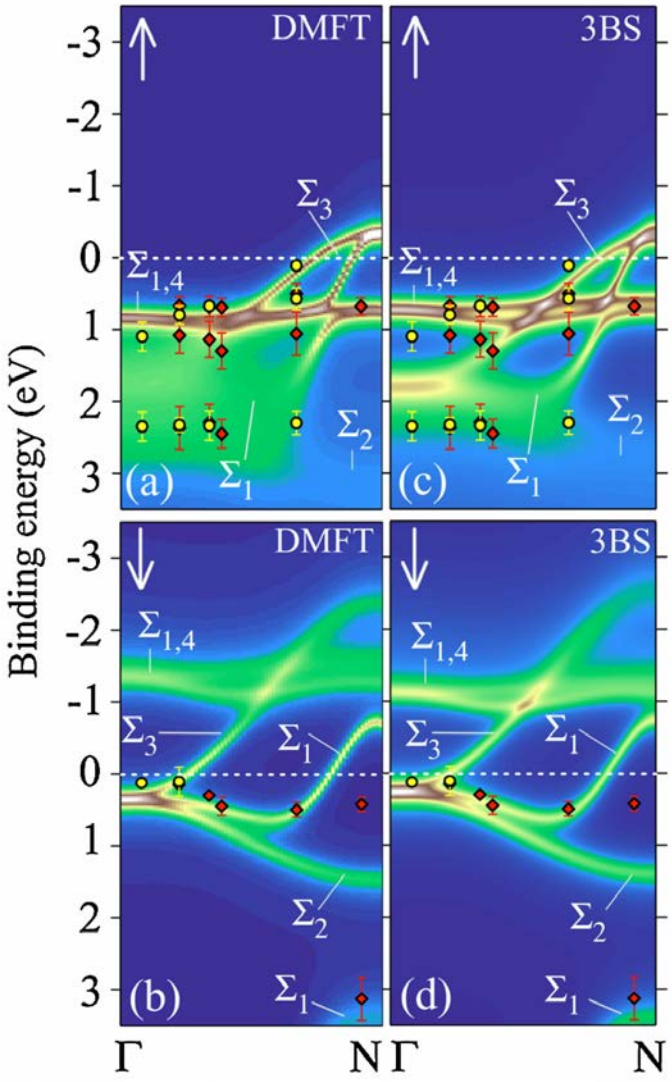
ARPES for iron

PRL 103, 267203 (2009) PHYSICAL REVIEW LETTERS week ending 31 DECEMBER 2009

Strength of Correlation Effects in the Electronic Structure of Iron

J. Sánchez-Barriga,[1] J. Fink,[1,2] V. Boni,[3] I. Di Marco,[4,5] J. Braun,[6] J. Minár,[6] A. Varykhalov,[1] O. Rader,[1] V. Bellini,[3] F. Manghi,[3] H. Ebert,[6] M. I. Katsnelson,[5] A. I. Lichtenstein,[7] O. Eriksson,[4] W. Eberhardt,[1] and H. A. Dürr[1]

Agreement is not bad (much better than LDA/GGA) but essentially worse than in nickel. Correlations in iron are not quite local

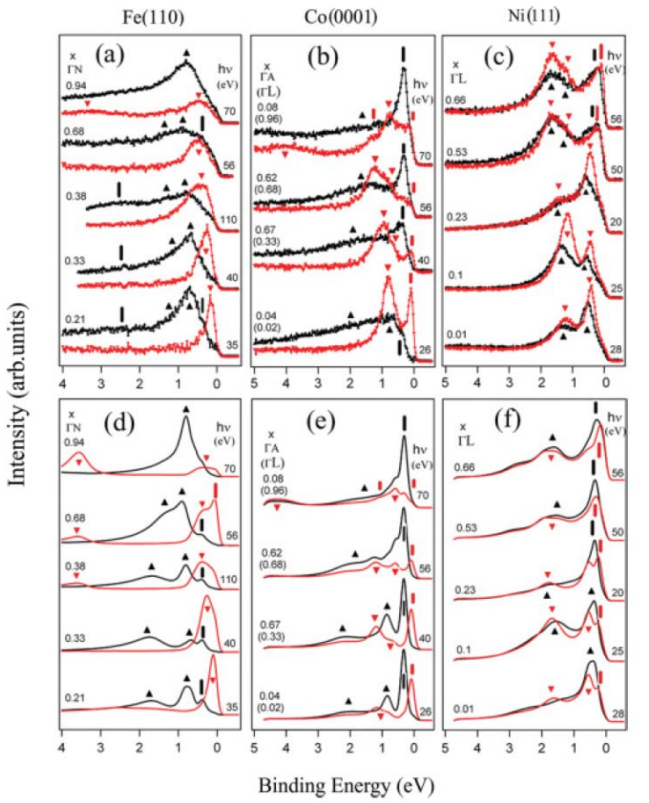


ARPES for 3d metals

PHYSICAL REVIEW B **85**, 205109 (2012)

Effects of spin-dependent quasiparticle renormalization in Fe, Co, and Ni photoemission spectra: An experimental and theoretical study

J. Sánchez-Barriga,[1] J. Braun,[2] J. Minár,[2] I. Di Marco,[3] A. Varykhalov,[1] O. Rader,[1] V. Boni,[4] V. Bellini,[5] F. Manghi,[4] H. Ebert,[2] M. I. Katsnelson,[6] A. I. Lichtenstein,[7] O. Eriksson,[3] W. Eberhardt,[1] H. A. Dürr,[1,8] and J. Fink[1,9]



Variation of U does not help too much for Fe

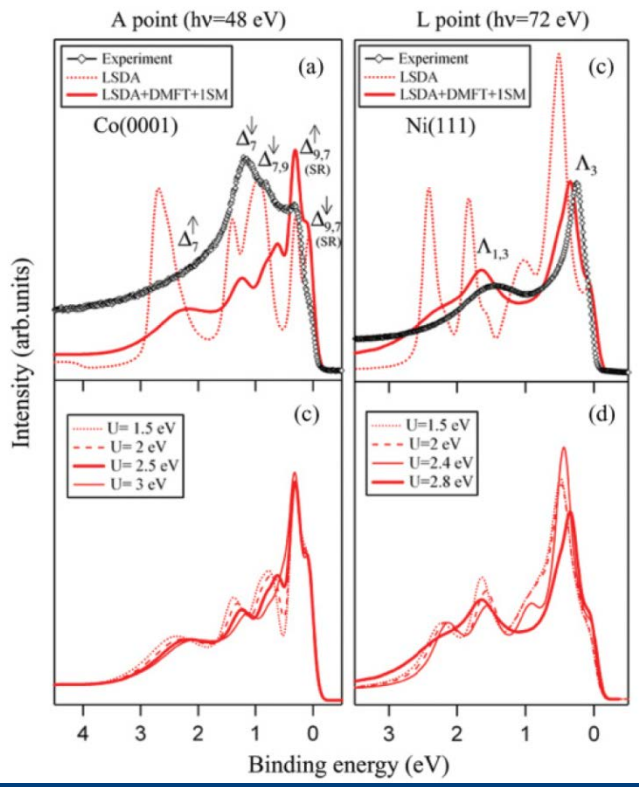
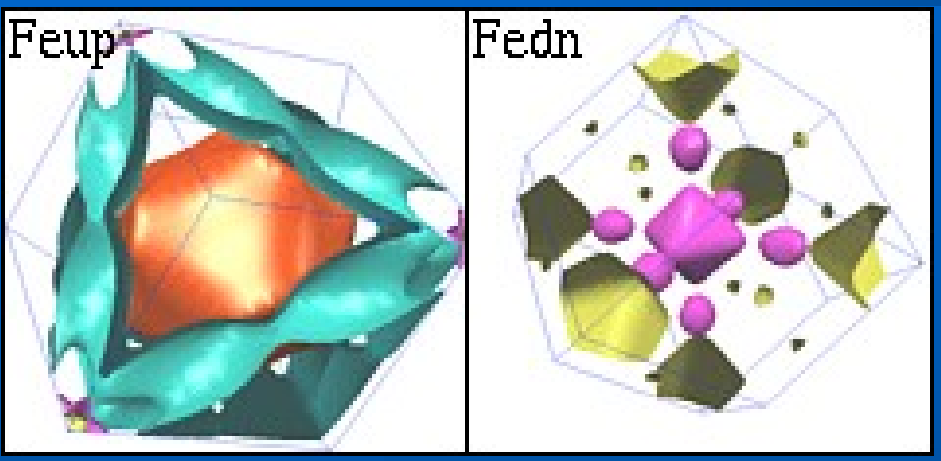


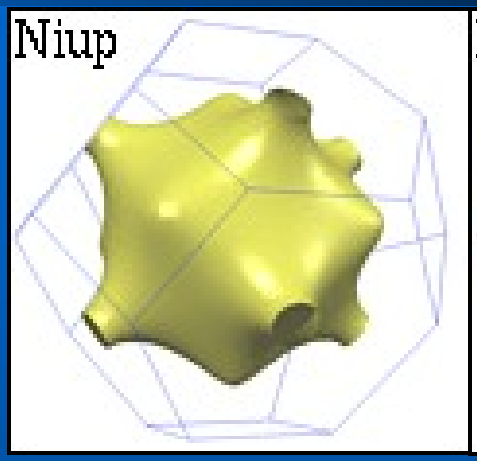
TABLE I. Values of the experimental and theoretical mass enhancement factors m^*/m_0 for majority spin states at high symmetry points of the BBZ of Fe, Co, and Ni, respectively. The theoretical values are derived for $U(\mathrm{Fe}) = 1.5$ eV, $U(\mathrm{Co}) = 2.5$ eV, $U(\mathrm{Ni}) = 2.8$ eV.

Fe			Co			Ni		
	Expt.	Theory		Expt.	Theory		Expt.	Theory
Γ	1.7	1.2	Γ	1.26	1.31	Γ	2.0	1.8
N	1.1	1.2	A	1.29	1.31	Λ	1.9	1.8

Black – spin up, red – spin down
Upper panel – exper,lower - DMFT

Why Ni is more local than Fe?





S. Hershfield ***http://www.phys.ufl.edu/fermisurface***

Nickel is almost half-metallic: majority-spin FS almost coincides with the boundaries of the Brillouin band

But the difference for minority spin is even more dramatic

Occupations for majority (minority) electrons

5 means full occupation

Fe: 4.6 (2.34) *Ni: 4.82 (4.15)*

Why Ni is more local than Fe II

Friedel oscillations originating from FS are much weaker in nickel

PHYSICAL REVIEW B, VOLUME 64, 174402

Ab initio calculations of exchange interactions, spin-wave stiffness constants, and Curie temperatures of Fe, Co, and Ni

M. Pajda,[1] J. Kudrnovský,[2,1] I. Turek,[3,4] V. Drchal,[2] and P. Bruno[1]

TABLE I. Effective Heisenberg exchange parameters J_{0j} for ferromagnetic Fe, Co, and Ni for the first 10 shells. Quantities $\mathbf{R}_{0j}$ and N_s denote, respectively, shell coordinates in units of corresponding lattice constants and the number of equivalent sites in the shell.

Fe (bcc)			Co (fcc)			Ni (fcc)		
$\mathbf{R}_{0j}$	N_s	J_{0j} (mRy)	$\mathbf{R}_{0j}$	N_s	J_{0j} (mRy)	$\mathbf{R}_{0j}$	N_s	J_{0j} (mRy)
$(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	8	1.432	$(\frac{1}{2}\frac{1}{2}0)$	12	1.085	$(\frac{1}{2}\frac{1}{2}0)$	12	0.206
(100)	6	0.815	(100)	6	0.110	(100)	6	0.006
(110)	12	−0.016	$(1\frac{1}{2}\frac{1}{2})$	24	0.116	$(1\frac{1}{2}\frac{1}{2})$	24	0.026
$(\frac{3}{2}\frac{1}{2}\frac{1}{2})$	24	−0.126	(110)	12	−0.090	(110)	12	0.012
(111)	8	−0.146	$(\frac{3}{2}\frac{1}{2}0)$	24	0.026	$(\frac{3}{2}\frac{1}{2}0)$	24	0.003
(200)	6	0.062	(111)	8	0.043	(111)	8	−0.003
$(\frac{3}{2}\frac{3}{2}\frac{1}{2})$	24	0.001	$(\frac{3}{2}1\frac{1}{2})$	48	−0.024	$(\frac{3}{2}1\frac{1}{2})$	48	0.007
(210)	24	0.015	(200)	6	0.012	(200)	6	−0.001
(211)	24	−0.032	$(\frac{3}{2}\frac{3}{2}0)$	12	0.026	$(\frac{3}{2}\frac{3}{2}0)$	12	−0.011
$(\frac{3}{2}\frac{3}{2}\frac{3}{2})$	8	0.187	$(2\frac{1}{2}\frac{1}{2})$	24	0.006	$(2\frac{1}{2}\frac{1}{2})$	24	0.001

As a result:

Magnons are much softer in Fe than in Ni (Curie temp. Higher but magnon frequencies lower)

	D_{ex} (meV Å^2)	T_C^{ex} (K)
Fe	280,[a] 330[b]	1044–1045
Co	580,[c, a] 510[b]	1388–1398[c]
Ni	555,[d] 422[a]	624–631

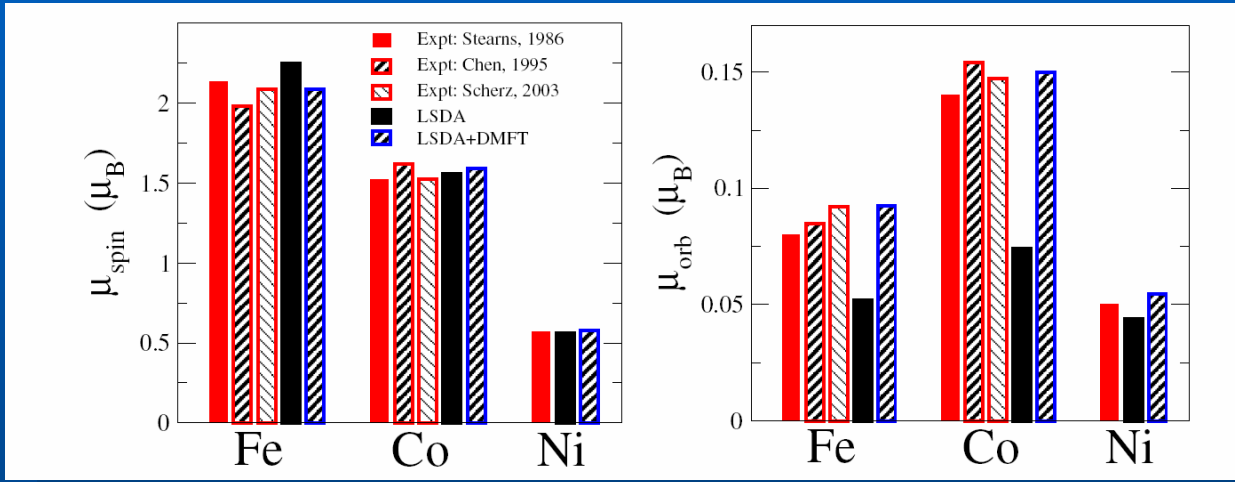
The softer magnons the stronger nonlocal e-m intercation

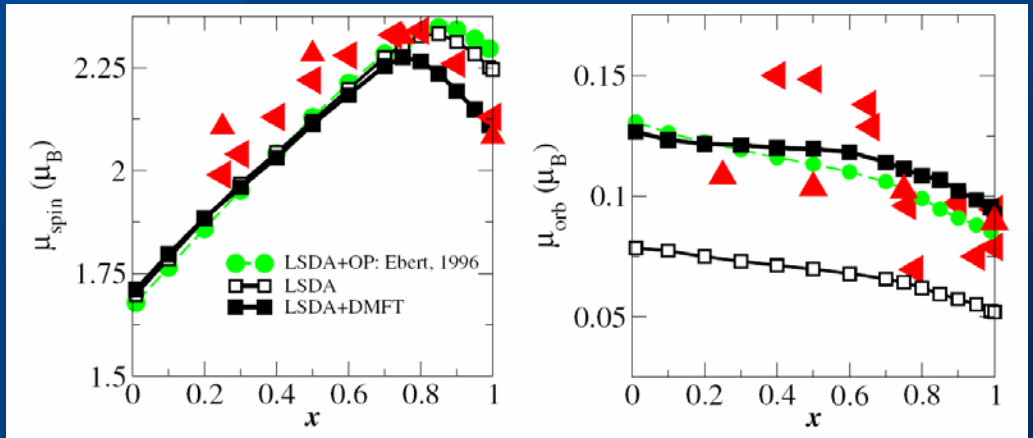
Orbital magnetic moments

Orbital magnetism in transition metal systems: The role of local correlation effects

S. Chadov, J. Minár, M. I. Katsnelson, H. Ebert, D. Ködderitzsch and A. I. Lichtenstein

EPL, **82** (2008) 37001





For Fe_xCo_{1-x} alloys

Exchange and Functionals

Magnetic force theorem

$$\begin{aligned} \Omega^d &= \Omega^d_{sp} - \Omega^d_{dc} \\ \Omega^d_{sp} &= -Tr\left\{\ln\left[\Sigma - G_0^{-1}\right]\right\} \\ \Omega^d_{dc} &= Tr\Sigma G - \Phi \end{aligned}$$

$$G^{-1} = G_0^{-1} - \Sigma$$

$$\Sigma = \frac{\delta\Phi}{\delta G}$$

$$\delta\Omega = \delta^*\Omega_{sp} + \delta_1\Omega_{sp} - \delta\Omega_{dc}$$

$$\delta_1\Omega_{sp} = \delta\Omega_{dc} = TrG\delta\Sigma$$

$$\delta\Omega = \delta^*\Omega_{sp} = -\delta^* Tr\ln\left[\Sigma - G_0^{-1}\right]$$

LDA+DMFT

(Lichtenstein & MIK 1997, 1998,1999; Anisimov et al 1997)

LSDA	LDA++
Density functional	Baym-Kadanoff functional
Density $\rho(\mathbf{r})$	Green-Function $G(\mathbf{r},\mathbf{r}',E)$
Potential $V_{xc}(\mathbf{r})$	Self-energy $\Sigma_i(E)$
$E_{tot} = E_{sp} - E_{dc}$	$\Omega = \Omega_{sp} - \Omega_{dc}$
$E_{sp} = \sum_{\lambda<\lambda_F} \varepsilon_\lambda$	$\Omega_{sp} = -Tr\ln[-G^{-1}]$
$E_{dc} = E_H + \int \rho V_{xc} d\mathbf{r} - E_{xc}$	$\Omega_{dc} = Tr\Sigma G - \Phi_{LW}$
Temperature:	Matsubara frequencies: real-T
in the Fermi function	for collective excitations

Exchange interactions from DMFT

Heisenberg exchange:

$$H = -\sum_{ij} J_{ij} S_i S_j$$

$$\delta\Omega = \delta^* \Omega_{sp} = \mathbf{V}_i \delta\varphi_i$$

Magnetic torque:

$$\delta \mathbf{e}_i = \delta\varphi_i \times \mathbf{e}_i$$

$$\mathbf{V}_i = 2Tr_{\omega L}\left[\Sigma_i^s \times \mathbf{G}_{ii}^s\right]$$

Exchange interactions:

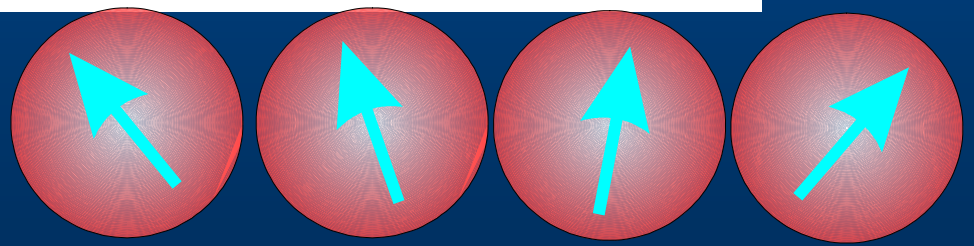
$$J_{ij} = -Tr_{\omega L}\left(\Sigma_i^s G_{ij}^{\uparrow} \Sigma_j^s G_{ji}^{\downarrow}\right)$$

$$\Sigma_i^s = \frac{1}{2}\left(\Sigma_i^{\uparrow} - \Sigma_i^{\downarrow}\right)$$

Spin wave spectrum:

$$\omega_{\mathbf{q}} = \frac{4}{M}\sum_j J_{0j}\left(1 - \cos \mathbf{q}\mathbf{R}_j\right) \equiv \frac{4}{M}[J(0) - J(\mathbf{q})]$$

Non-collinear magnetism :



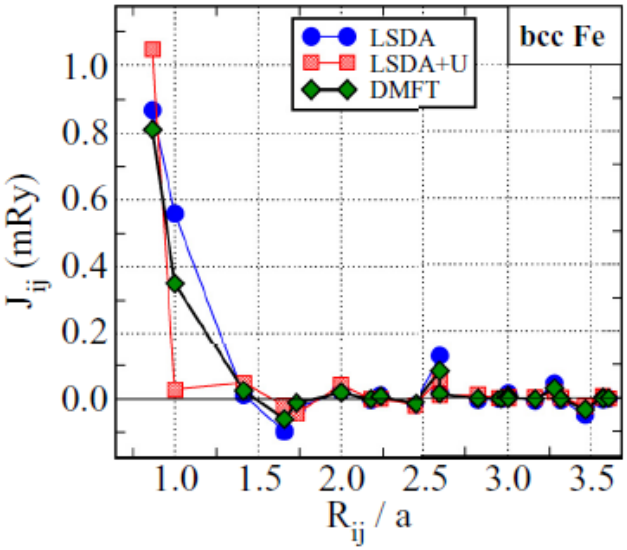
MIK & Lichtenstein Phys. Rev. B 61, 8906 (2000)

Applications

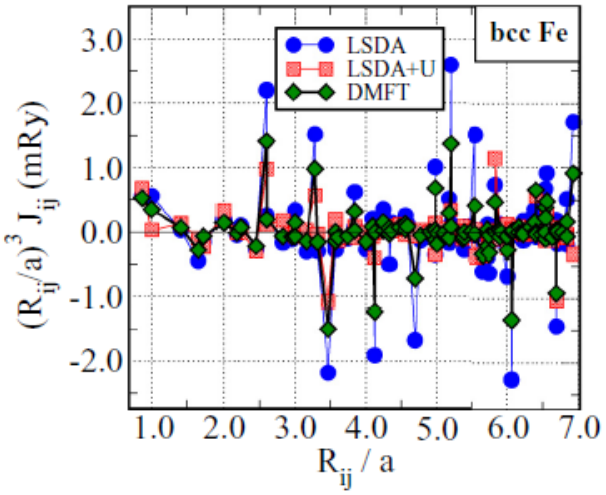
PHYSICAL REVIEW B **91**, 125133 (2015)

Exchange parameters of strongly correlated materials: Extraction from spin-polarized density functional theory plus dynamical mean-field theory

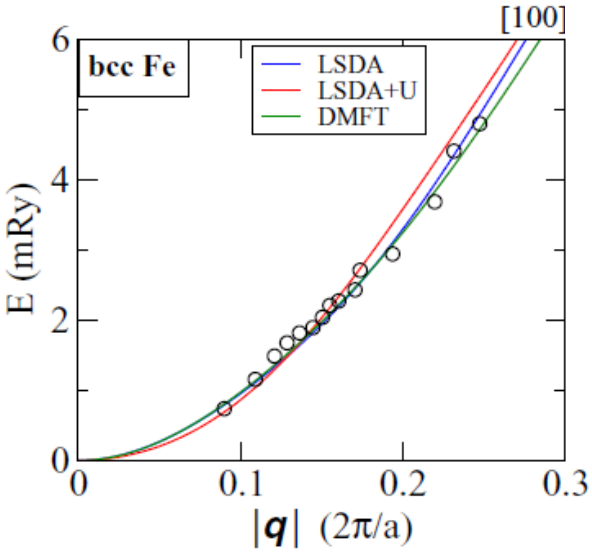
Y. O. Kvashnin,[1] O. Grånäs,[1,2] I. Di Marco,[1] M. I. Katsnelson,[3,4] A. I. Lichtenstein,[4,5] and O. Eriksson[1]



For Fe (and Ni) quite small difference between DFT and DMFT



Nontrivial: electronic structure is very different!



←Spin-wave spectrum

Error cancellation?!

α-γ transformation in Fe: role of magnetism

Zener: bcc phase of Fe is stabilized by magnetism (DOS peaks destabilizing crystal lattice are moved from the Fermi energy)

SCIENTIFIC REPORTS

OPEN

SUBJECT AREAS:
MAGNETIC PROPERTIES AND MATERIALS
ELECTRONIC PROPERTIES AND MATERIALS

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Electronic correlations determine the phase stability of iron up to the melting temperature

I. Leonov[1], A. I. Poteryaev[2,3], Yu. N. Gornostyrev[2,3], A. I. Lichtenstein[4], M. I. Katsnelson[5,6], V. I. Anisimov[2,6] & D. Vollhardt[1]

[1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135

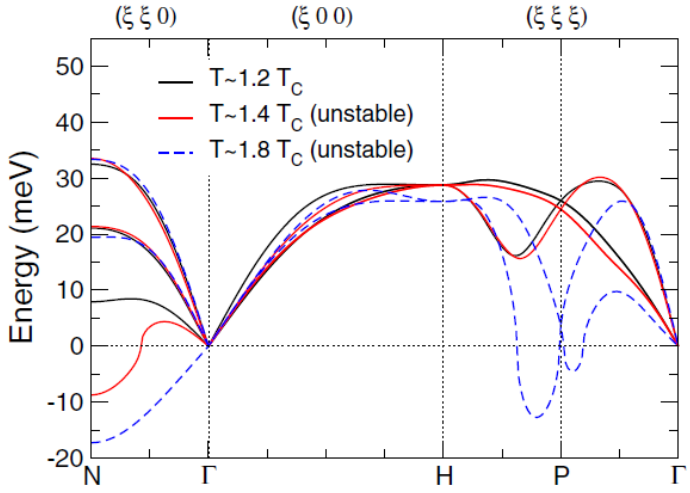


Figure 2 | Calculated phonon dispersions of paramagnetic bcc iron near the α-to-γ and γ-to-δ phase transitions for different temperatures.

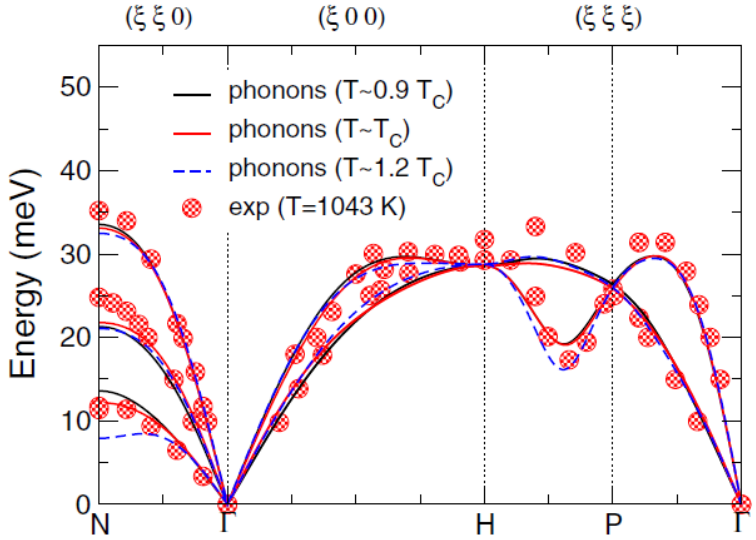


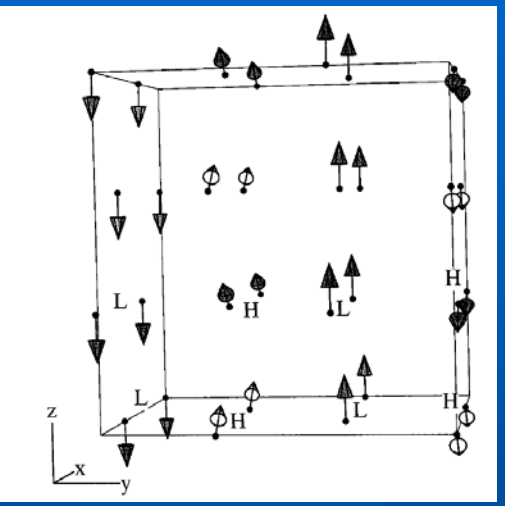
Figure 1 | Calculated phonon dispersion curves for bcc iron near the Curie temperature T_C. The results are compared with neutron inelastic scattering measurements at 1043 K.

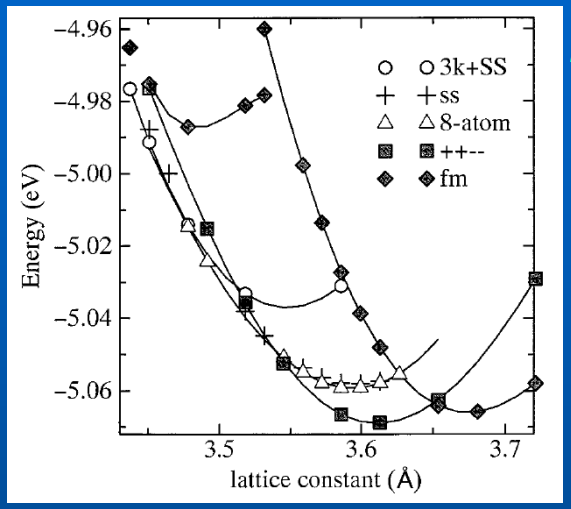
Dynamical instability as a result of disappearance of magnetic moments

DMFT is essential!!!

Frustrated magnetism in γ-Fe

Antropov et al, PRL 1995 - first practical application of ab initio SD





Many magnetic structures with very close energies (frustration); strong dependence on lattice constants

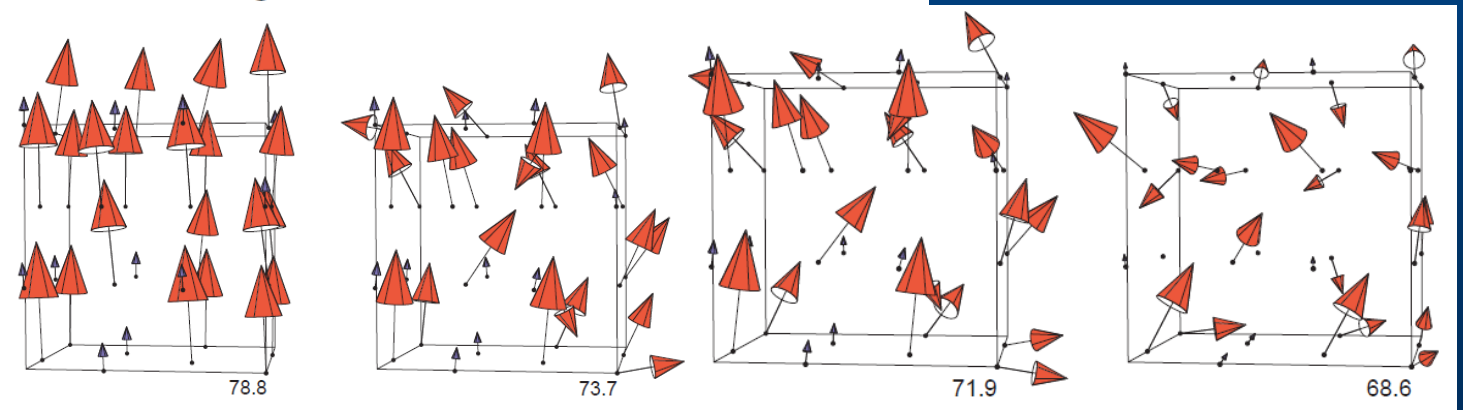
Also in Fe-Ni alloys

Origin of the Invar effect in iron–nickel alloys

NATURE | VOL 400 | 1 JULY 1999

Mark van Schilfgaarde*, I. A. Abrikosov† & B. Johansson†

Application to Invar problem



Fe-Ni

Atomic volumes in a.u.

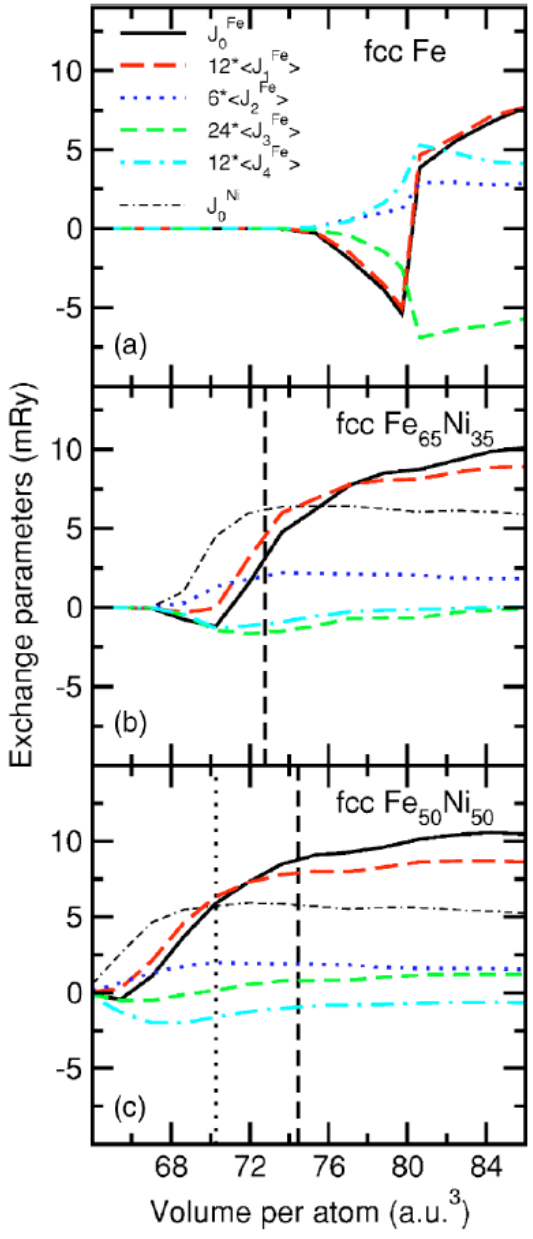
Frustrated magnetism in γ-Fe II

PHYSICAL REVIEW B **71**, 054402 (2005)

Origin of magnetic frustrations in Fe-Ni Invar alloys

A. V. Ruban,[1] M. I. Katsnelson,[2,3] W. Olovsson,[3] S. I. Simak,[3,4] and I. A. Abrikosov[4]

FIG. 1. (Color online) Effective exchange parameters for Fe J_0^{Fe} (thick black solid line) and Ni J_0^{Ni} (thin black dot-double dashed line), as well as average pair exchange parameters $\langle J_p^{\mathrm{Fe}} \rangle = (1/z_p)\Sigma_{j\in p}[cJ_{0j}^{\mathrm{Fe\text{-}Fe}} + (1-c)J_{0j}^{\mathrm{Fe\text{-}Ni}}]$ for the first (red long-dashed line), second (dark blue dotted line), third (green short-dashed line), and fourth (light blue dot-dashed line) shells in (a) fcc Fe, (b) $Fe_{65}Ni_{35}$ alloy, and (c) $Fe_{50}Ni_{50}$ alloy as a function of the volume per atom. z_p is the coordination number of the pth coordination shell, and c is the Fe concentration. In the figure $\langle J_p^{\mathrm{Fe}} \rangle$ are multiplied with z_p in order to show their actual contribution to J_0^{Fe}. Vertical dashed lines in (b) and (c) show calculated equilibrium volume at corresponding concentrations. The vertical dotted line in (c) indicates estimated volume where fcc $Fe_{50}Ni_{50}$ alloy shows Invar behavior under pressure, Ref. 5. Calculations are done within the coherent potential approximation (see text for the discussion).



Total exchange is determined by J_1; long-range oscillating tail favors frustrations. J_1 strongly depend on volume

Frustrated magnetism in γ-Fe III

Okatov, Gornostyrev, Lichtenstein & MIK, PR B 84, 214422 (2011)

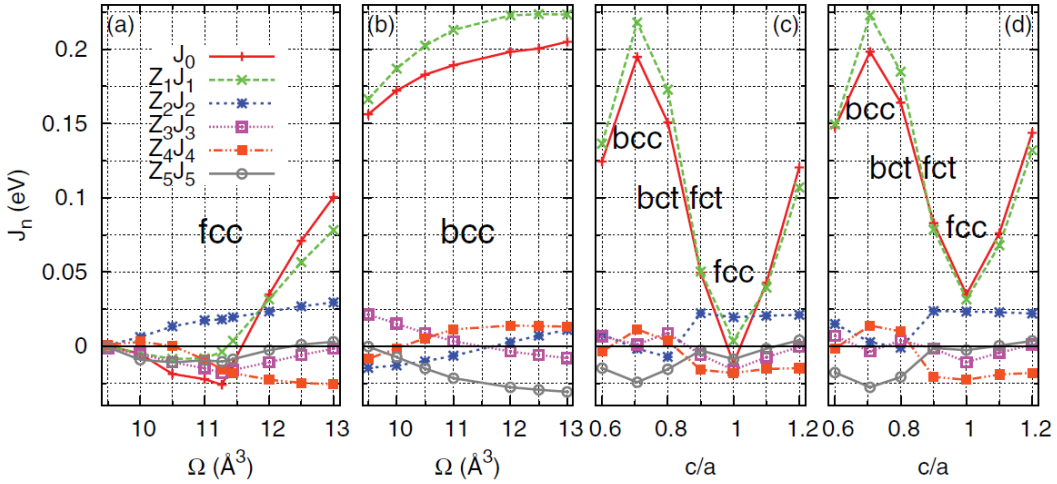


FIG. 3. (Color online) Exchange parameters J_n for $n = 1,2,3,4,5$ for different lattice parameters: dependence J_n on a volume of fcc (a) and bcc (b) Fe; dependence J_n on (c/a) at fixed volumes $\Omega = 11.44$ Å^3 (c) and $\Omega = 12.0$Å^3 (d), respectively.

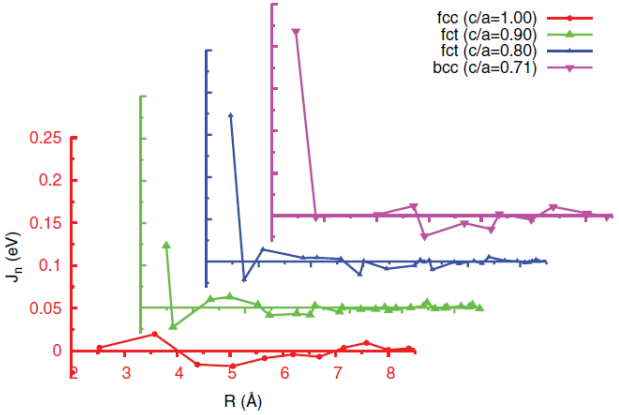


FIG. 5. (Color online) The exchange parameter as a function of interatomic distance to the nth neighbor $J_n(R_n)$ for different c/a ratios.

Exchange parameters are very sensitive not only to volume but also to tetragonal deformations – stabilization of fct phase

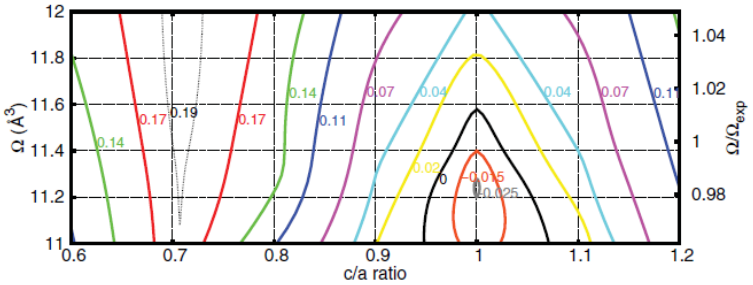
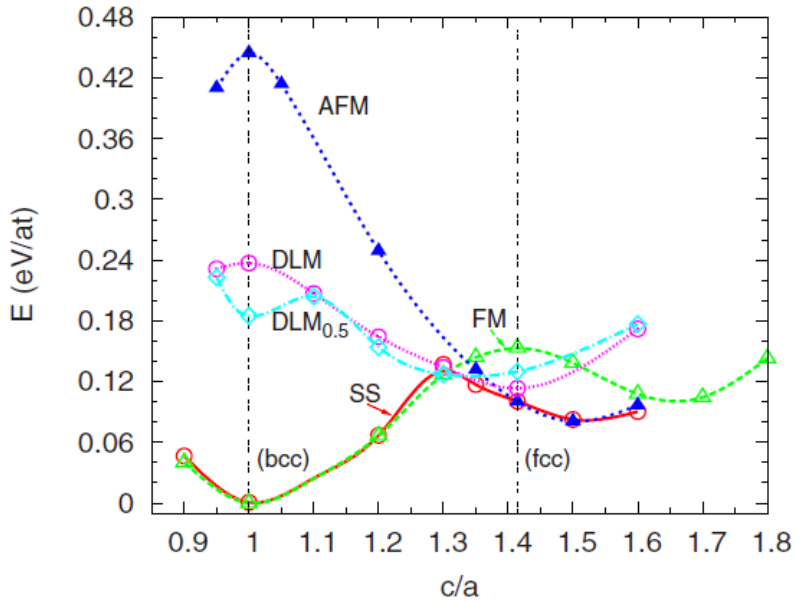


FIG. 4. (Color online) Dependence of the total exchange parameter J_0 on volume Ω and c/a ratio as a contour plot $J_0(\Omega, c/a)$.

Magnetism along the Bain path in Fe

Okatov, Kuznetsov, Gornostyrev, Urtsev & MIK, PR B 79, 094011 (2011)



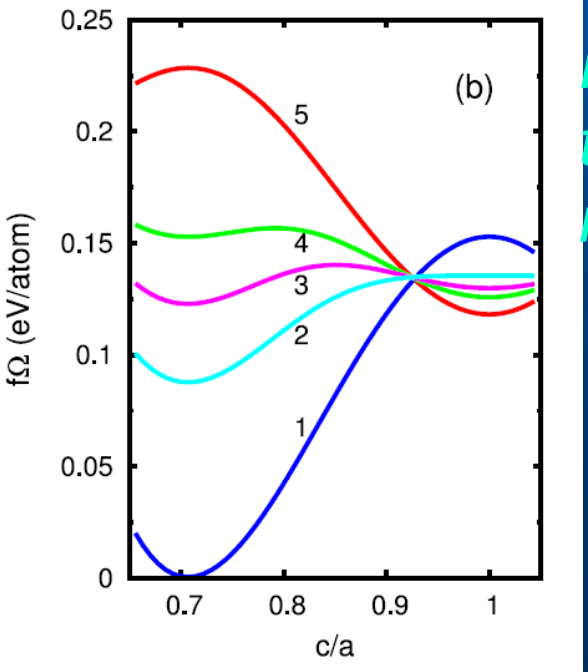
Transition without barrier starting from FM state

A very important consequences for morphology of the transformation

J. Phys.: Condens. Matter 25 (2013) 135401 (9pp) doi:10.1088/0953-8984/25/13/135401

Effect of magnetism on kinetics of γ–α transformation and pattern formation in iron

I K Razumov[1,2], Yu N Gornostyrev[1,2] and M I Katsnelson[3]

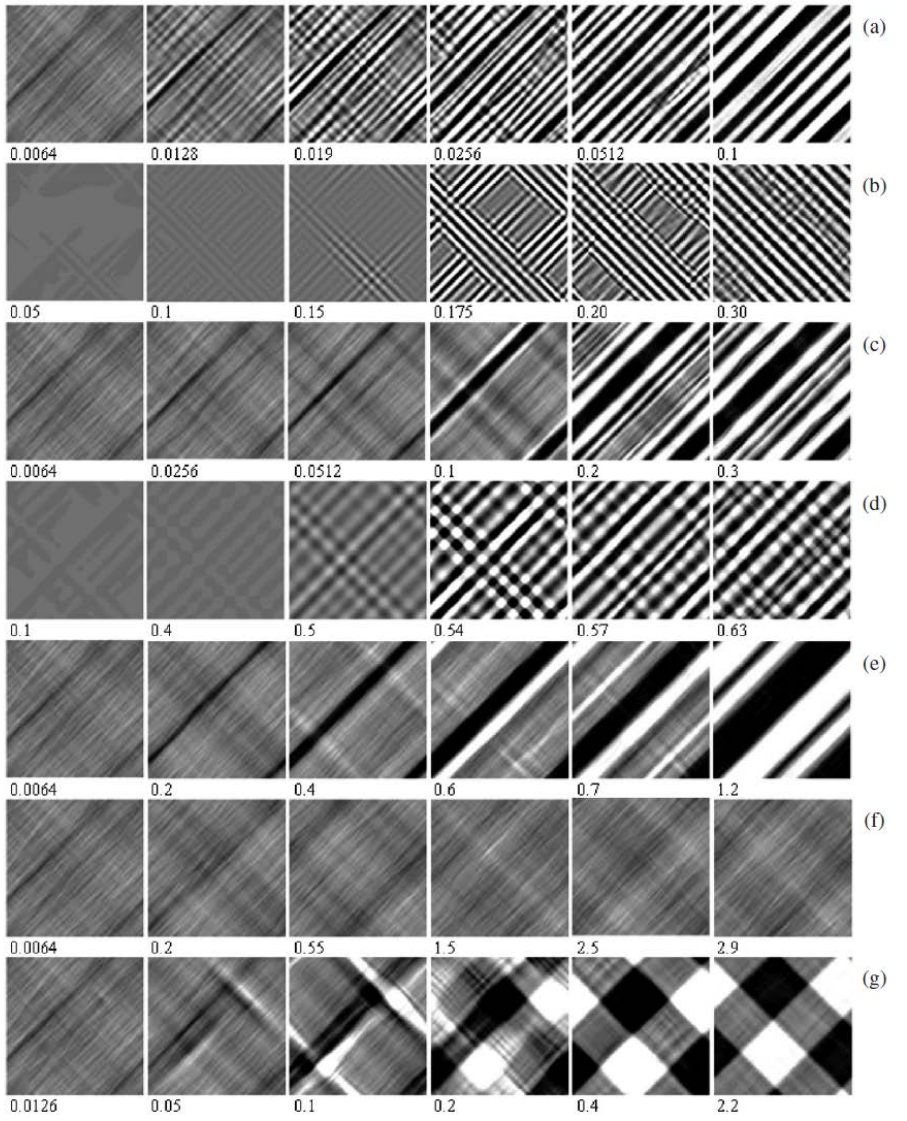


Free energy to be used in phase field

1-5: T=0K; 700; 1000; 1300; ∞

Magnetic temperature

Phase field simulations



Magnetic free energy plays crucial role in kinetics of transformation and morphology of the final structure in pure iron

J. Phys.: Condens. Matter **25** (2013) 135401 (9pp) doi:10.1088/0953-8984/25/13/135401

Effect of magnetism on kinetics of γ–α transformation and pattern formation in iron

I K Razumov[1,2], Yu N Gornostyrev[1,2] and M I Katsnelson[3]

Figure 2. Time evolution of the structure at exposure at $T = 400$ K ((a), (b)), 700 K ((c), (d)), 950 K (e), 1000 K ((f), (g)) after quenching of the high-temperature state ((a), (c), (e), (f)) or development of instability of the uniform fcc state ((b), (d)), under homogeneous ((a)–(f)) and heterogeneous nucleation (g). Gradations of gray color correspond to the values for the order parameter ϕ; black and white colors show the regions for the α-phase with two possible orientations ($\phi = \pm 1$).

Carbon impurity in γ-Fe: Role of exchange interactions

PRL 99, 247205 (2007) PHYSICAL REVIEW LETTERS week ending 14 DECEMBER 2007

Magnetism and Local Distortions near Carbon Impurity in γ-Iron

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Institut für Theoretische Physik, Universität Hamburg, 20355 Hamburg, Germany
(Received 25 June 2007; published 13 December 2007)

Long-standing problem: solution enthalpy of C in γ-Fe

Solution: local tetragonal distortions and local FM ordering

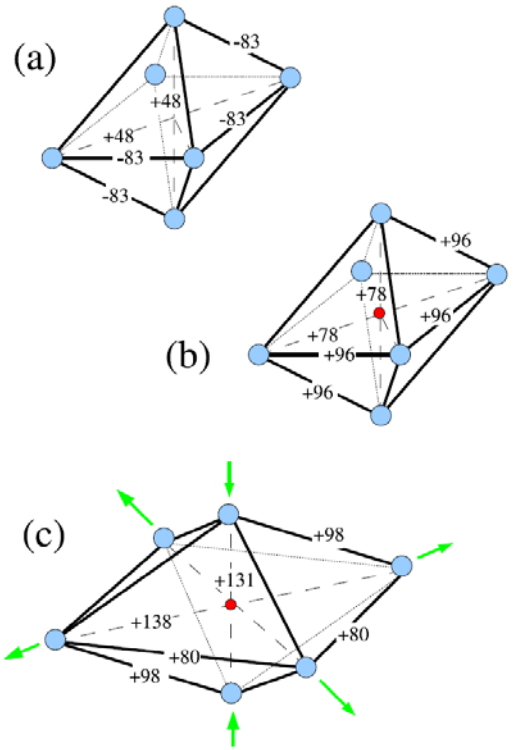


FIG. 2 (color online). Exchange parameters (in K) for different Fe-Fe pairs in original fcc lattice (a); in fcc lattice with carbon interstitial impurity without (b) and with (c) relaxation taken into account. Arrows indicate direction of atomic displacements during the relaxation.

Solution enthalpy 0.55 eV (exp. 0.4 eV)

Deformations make C-C interaction much stronger (not pure dilatation centers)

Model and phase field simulations for steel

PHYSICAL REVIEW B **90**, 094101 (2014)

Role of magnetic degrees of freedom in a scenario of phase transformations in steel

I. K. Razumov,[1,2,*] D. V. Boukhvalov,[3] M. V. Petrik,[2] V. N. Urtsev,[4] A. V. Shmakov,[4]
M. I. Katsnelson,[5,6] and Yu. N. Gornostyrev[1,2]

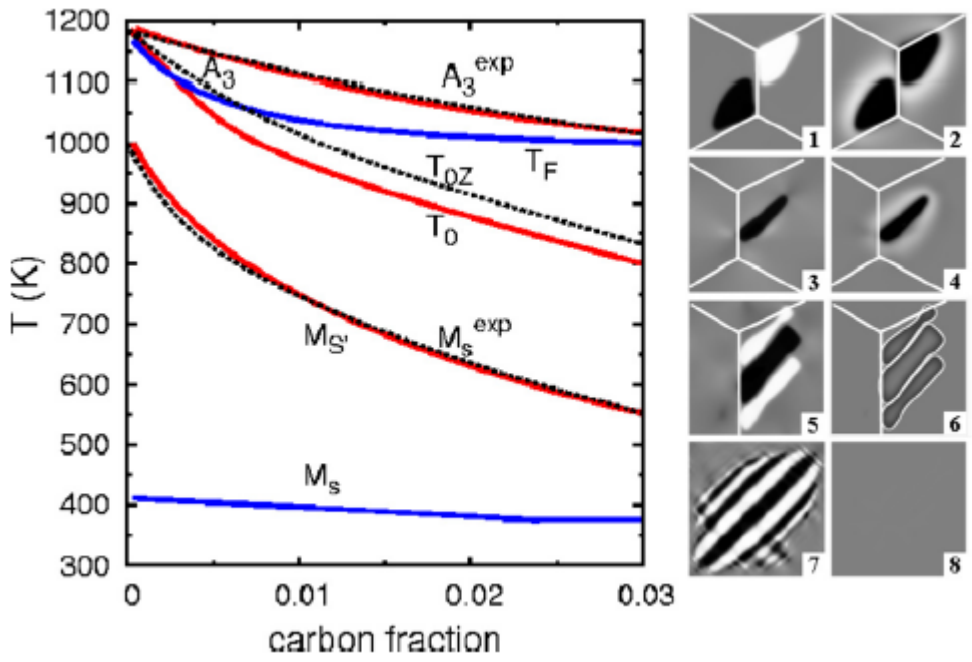


FIG. 4. (Color online) The left panel shows calculated lines (solid) corresponding to the start of ferrite transformation, paraequilibrium, and the start of martensitic transformation. M_s and $M_{s'}$ are the temperatures at the start of lattice instability and martensitic-like transformation. Dashed lines show the experimental boundary of the two-phase region (A_3) [36], the experimental paraequilibrium temperature (T_{0Z}) [37], and the experimental temperature of the start of martensitic transformation ($M_s^{\text{expt.}}$) [35]. The right panel shows microstructures forming as a result of transformation at various temperatures: $T_0 < T < A_3$ (1,2), $M_{s'} < T < T_0$ (3,4; 5,6), and $T < M_{s'}$ (7,8). The left and right columns in this panel correspond to tetragonal strain (black and white are two orthogonal directions of tetragonal deformation in bcc phase; gray shows fcc regions) and carbon distribution (the darker the smaller), respectively.

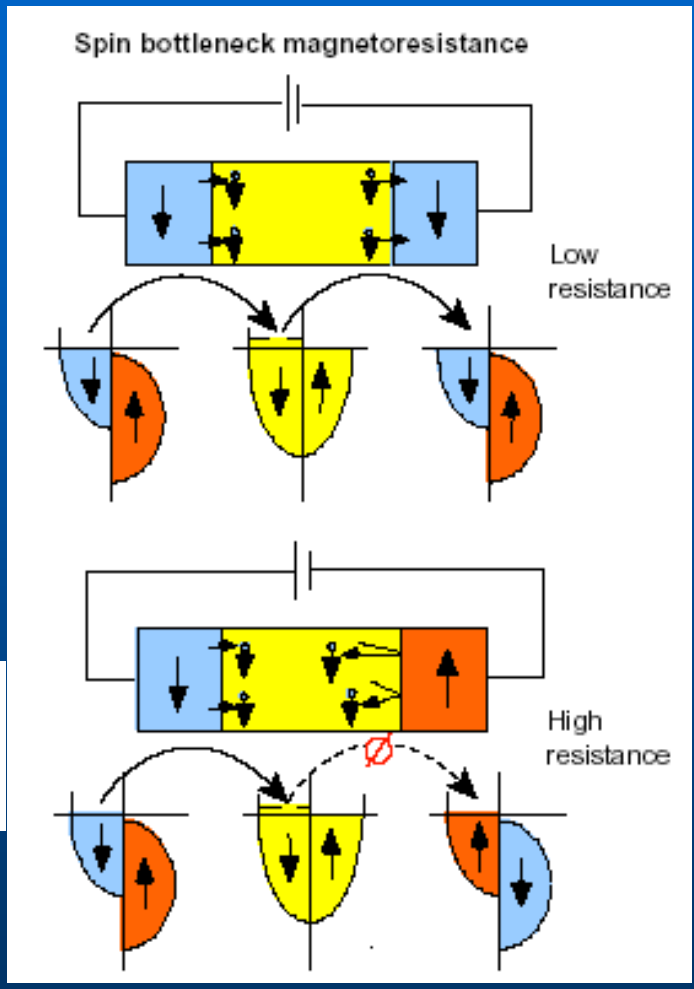
Quantitative description of boundaries of martensitic, baynite and ferrite transformations – crucial for metallurgy

Half-metallic ferromagnets

Metal for one spin projection and semiconductor for other spin projection

R. de Groot et al, PRL 50, 2024 (1983)

Heussler alloys (NiMnSb, PtMnSb…); CrO_2, CoS_2, Fe_3O_4, $(La,Ca)MnO_3$....



REVIEWS OF MODERN PHYSICS, VOLUME 80, APRIL–JUNE 2008

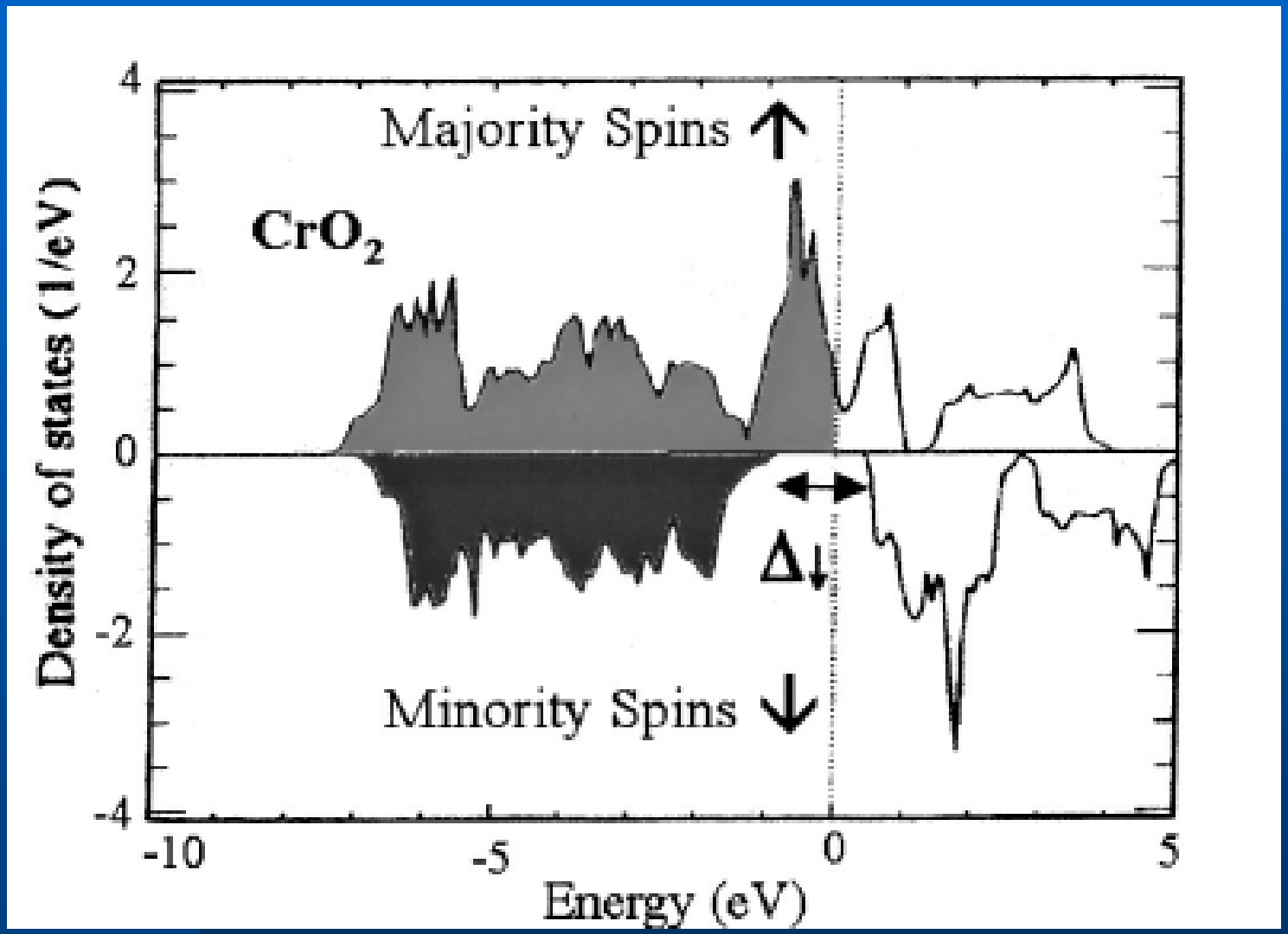
Half-metallic ferromagnets: From band structure to many-body effects

MIK, Irkhin, Chioncel, Lichtenstein, de Groot

Prinz, Science (1998)

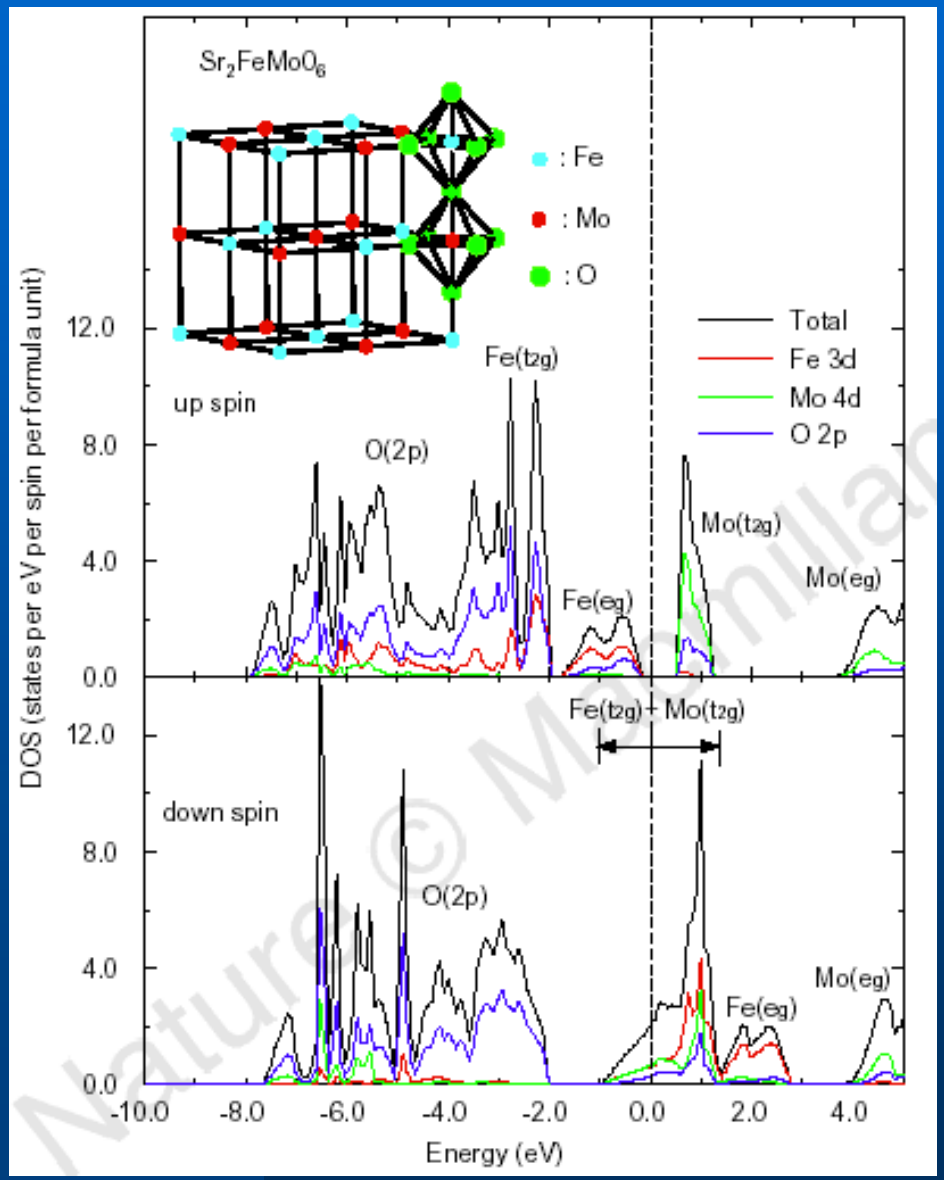
CrO_2

Lewis et al, PRB (1997)



Majority spin gap (typical case; also Heussler alloys etc.)

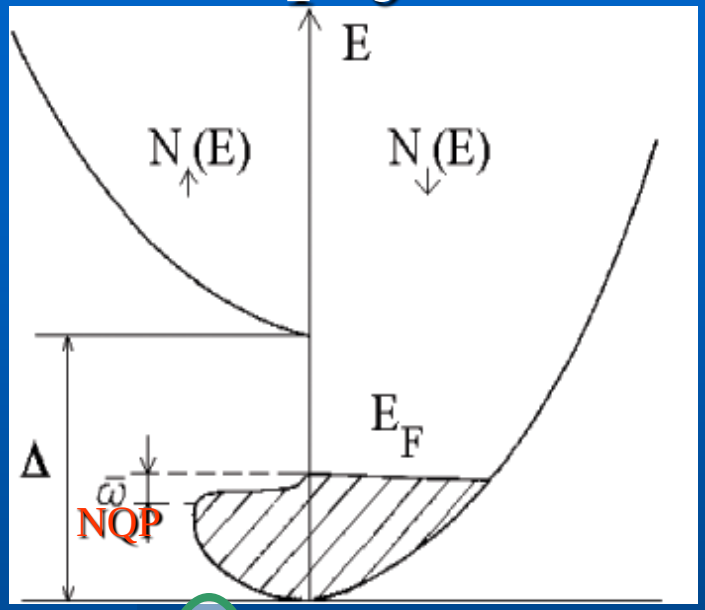
Sr_2FeMoO_6 Kobayashi et al, Nature (1988)



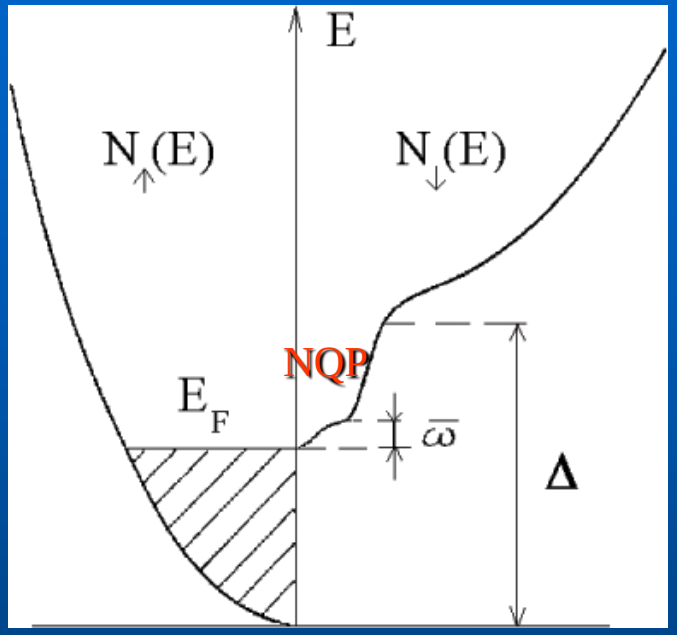
Minority spin gap

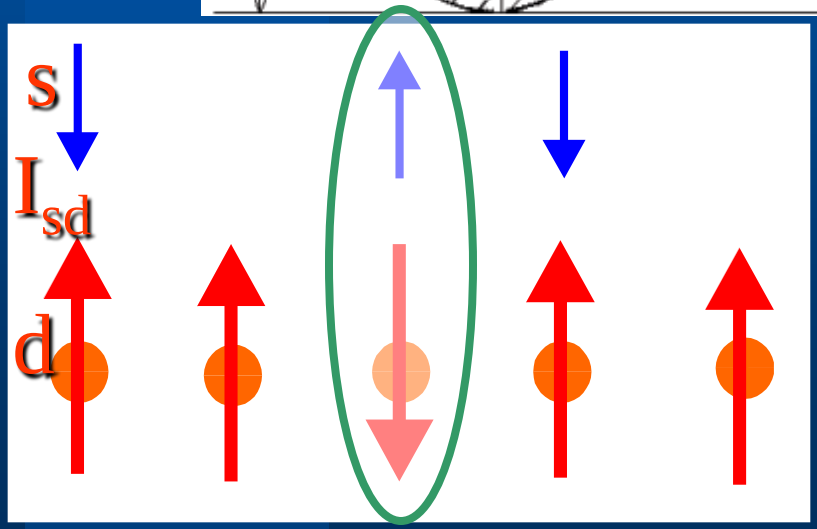
The *s-d* exchange model and NQP

I<0



I>0



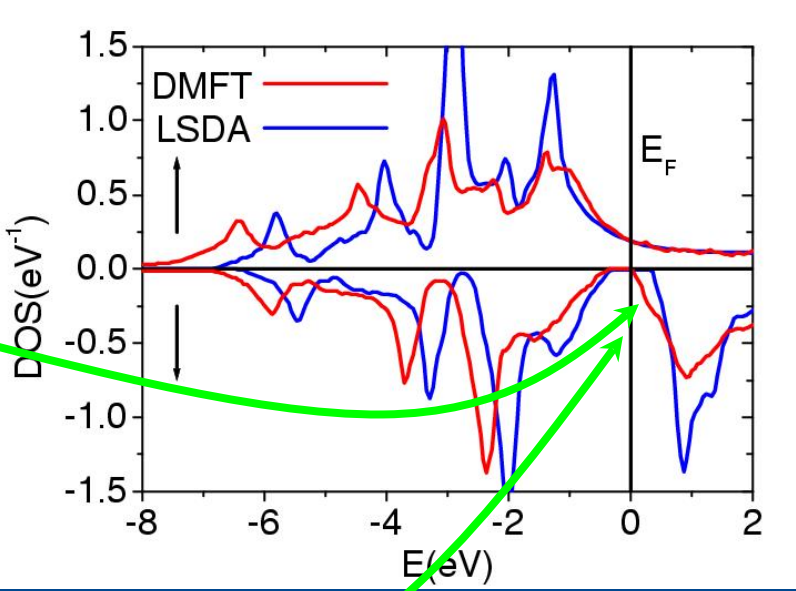


Nonquasiparticle states.
Quantum effects !

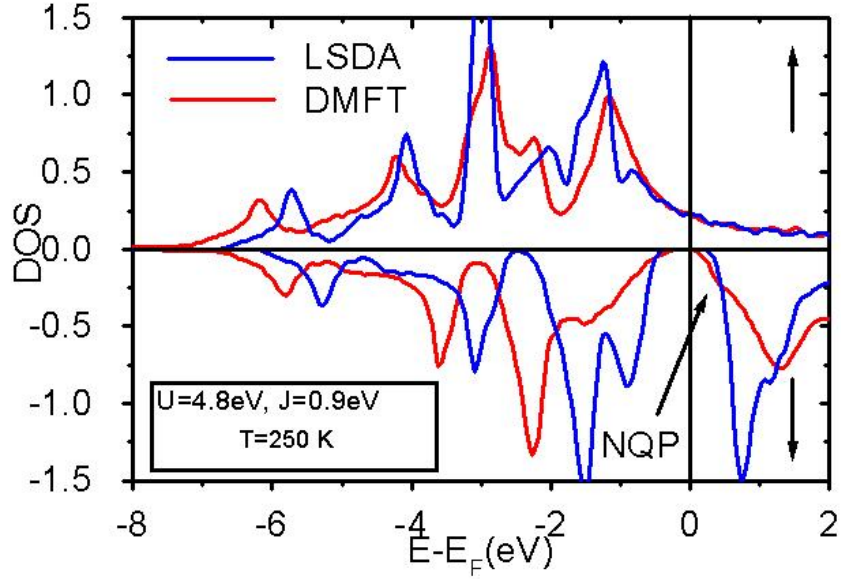
LDA+DMFT for NiMnSb

$$\Sigma_{12}^{\sigma}(\tau) = \sum_{34} W_{13,42}^{\sigma\sigma'}(\tau) G_{34}^{\sigma'}(\tau)$$

$$W^{\sigma\sigma'}(i\omega_n) = \begin{bmatrix} W^{++} & W^{+-} \\ W^{-+} & W^{--} \end{bmatrix}$$



U=2 eV, J=0.9 eV, T=300 K

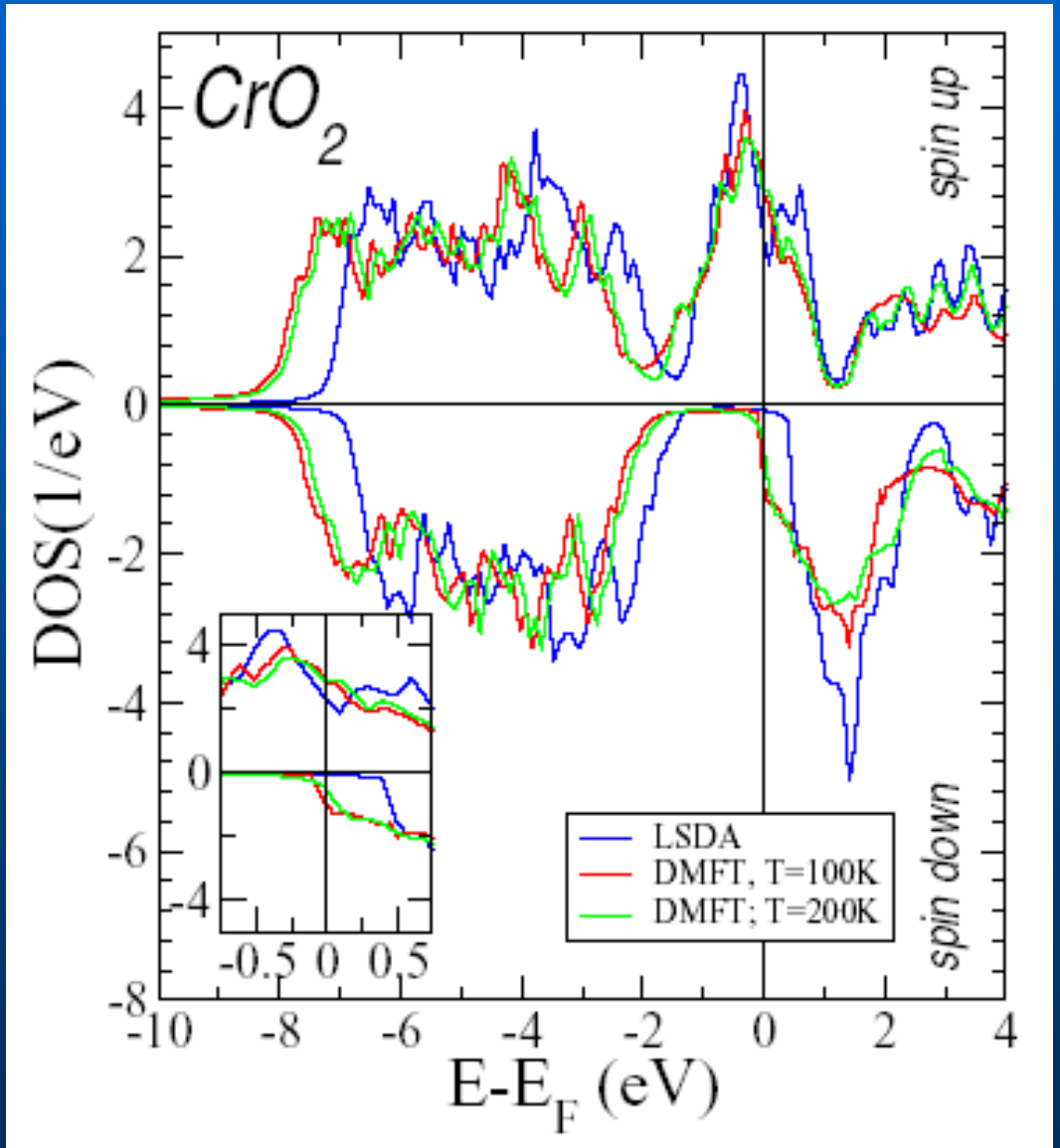


NQP states created in the minority channel just above the Fermi level

U=4.8 eV, J=0.9 eV, T=250 K

CrO_2

L. Chioncel et al, PRB 2006



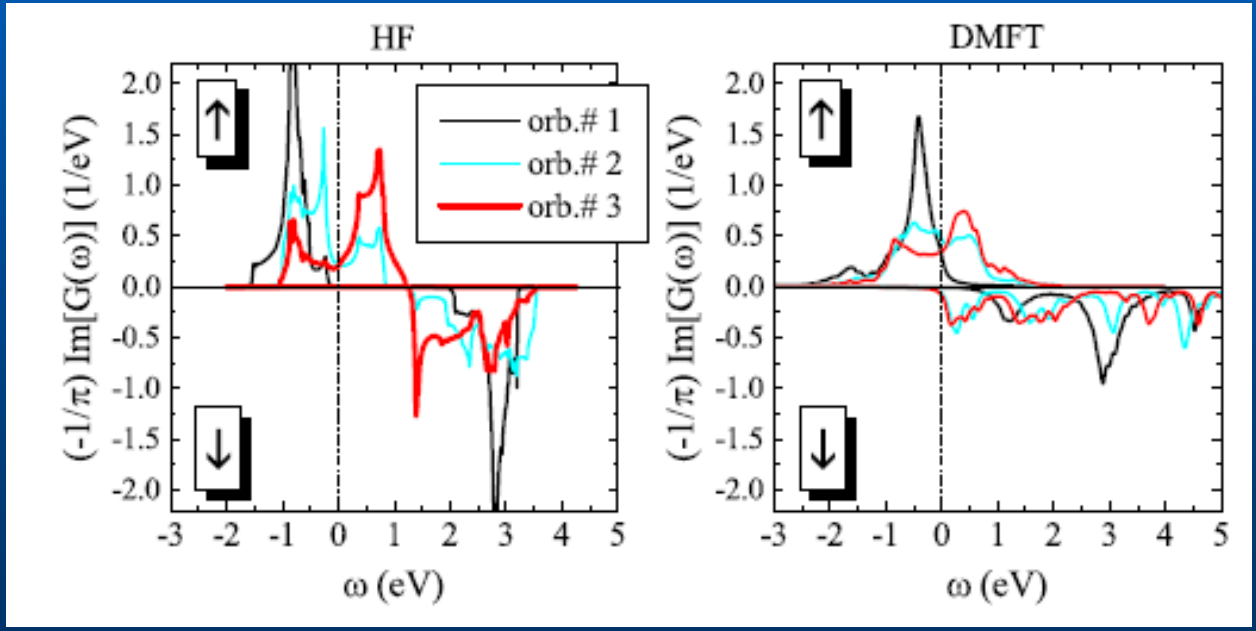
CrO_2 II

PHYSICAL REVIEW B **92**, 144407 (2015)

Mechanisms and origins of half-metallic ferromagnetism in CrO_2

I. V. Solovyev,[1,2,*] I. V. Kashin,[2] and V. V. Mazurenko[2]

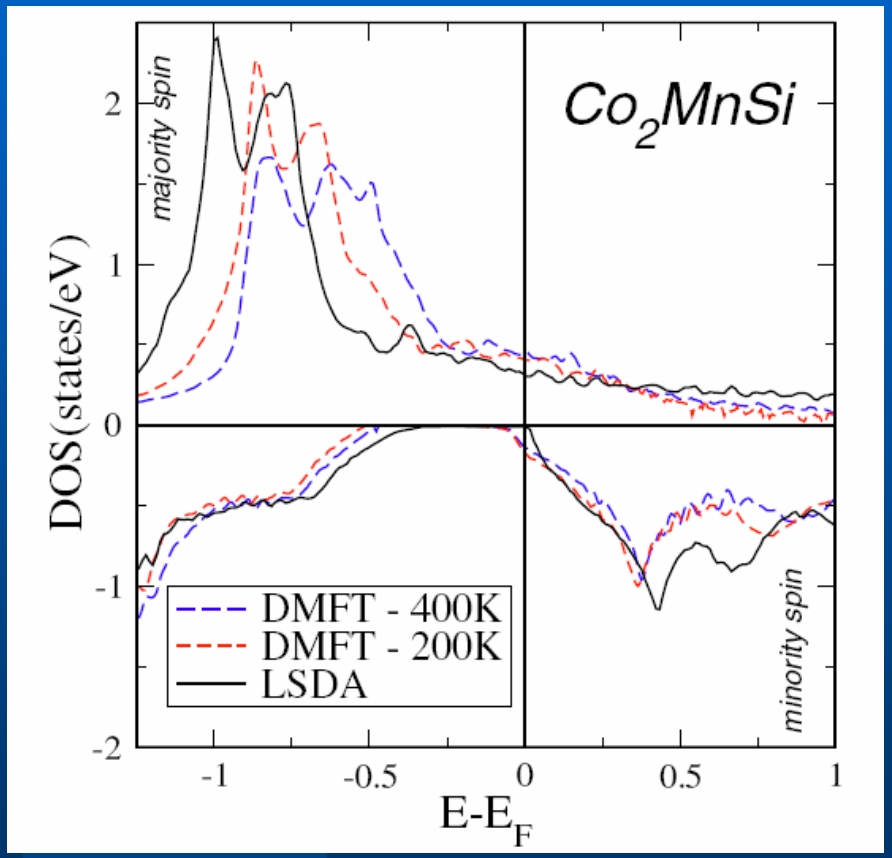
Half-metallic FM
DMFT shows
non-quasiparticle
states in the gap
MIK et al, RMP 80, 315 (2008)

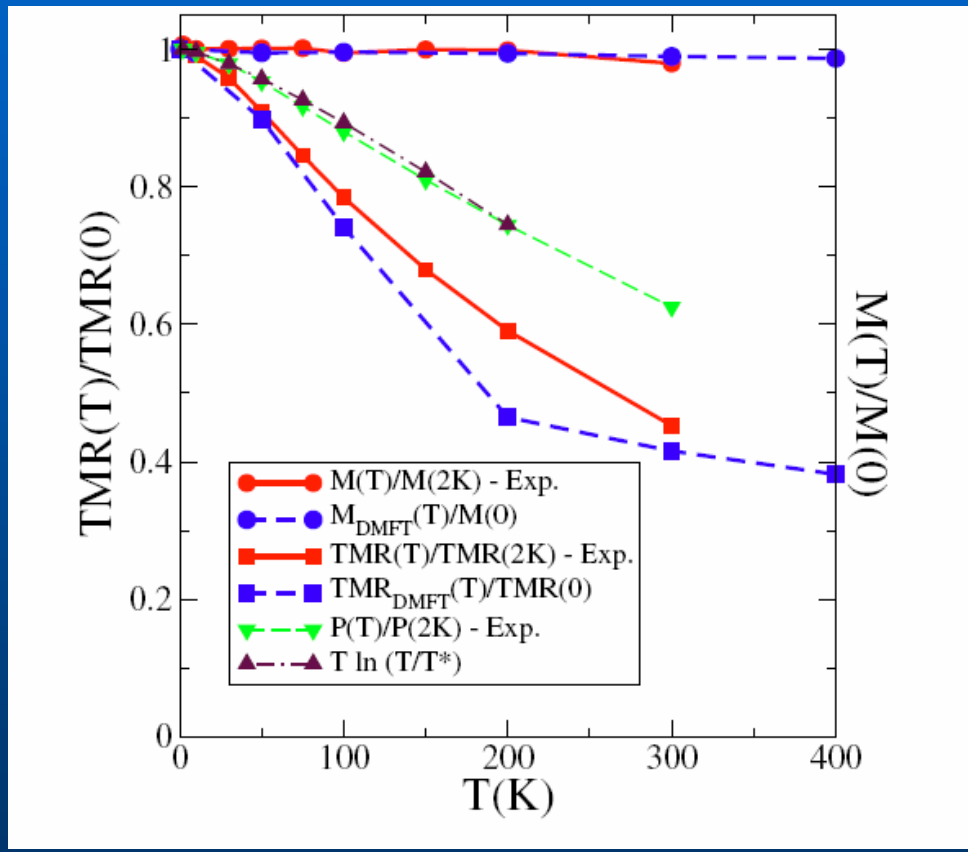


PRL 100, 086402 (2008) PHYSICAL REVIEW LETTERS week ending 29 FEBRUARY 2008

Nonquasiparticle States in Co_2MnSi Evidenced through Magnetic Tunnel Junction Spectroscopy Measurements

L. Chioncel,[1,2] Y. Sakuraba,[3] E. Arrigoni,[1] M. I. Katsnelson,[4] M. Oogane,[3] Y. Ando,[3] T. Miyazaki,[3] E. Burzo,[5] and A. I. Lichtenstein[6]





$$1 - P(T)/P(0) \propto T \ln T/T^*$$

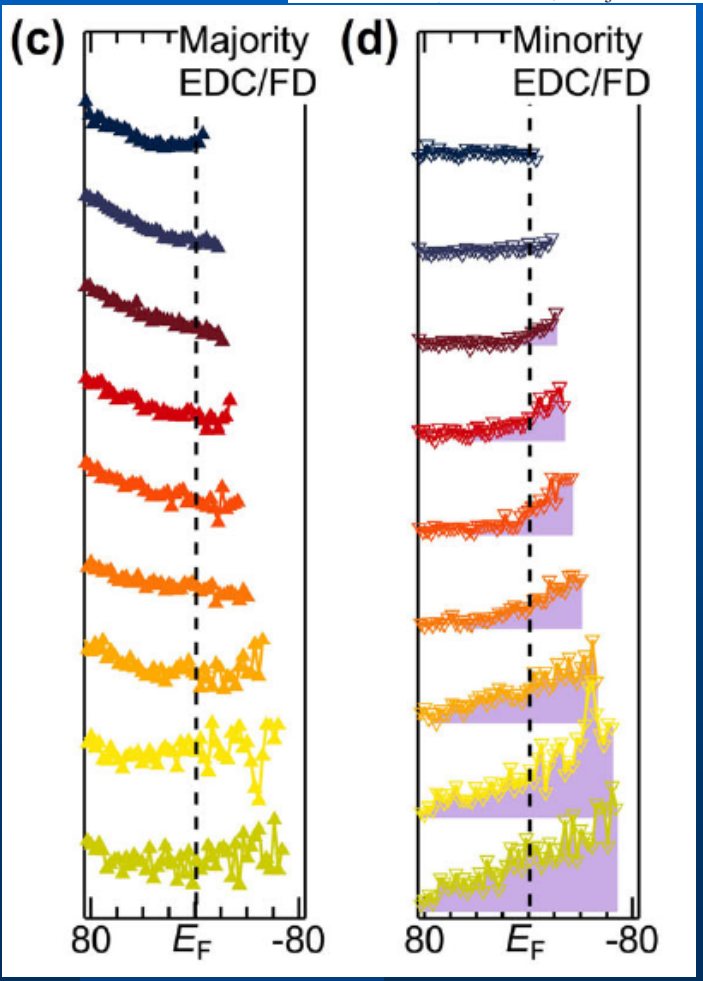
Irkhin, MIK PRB 2006

Direct experimental confirmation

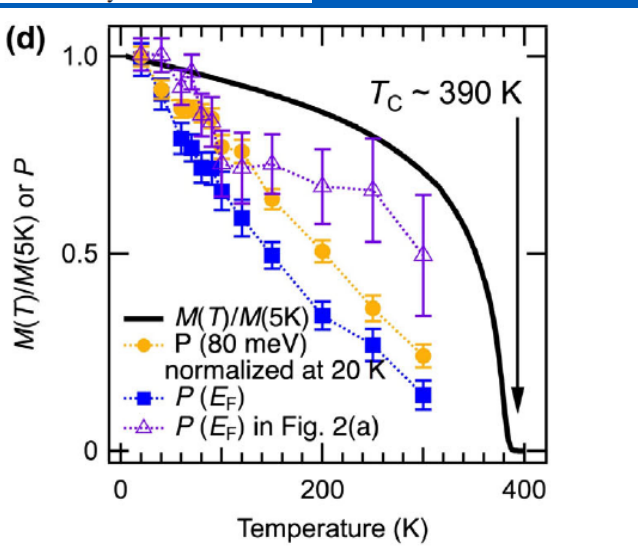
PHYSICAL REVIEW LETTERS **121,** 257201 (2018)

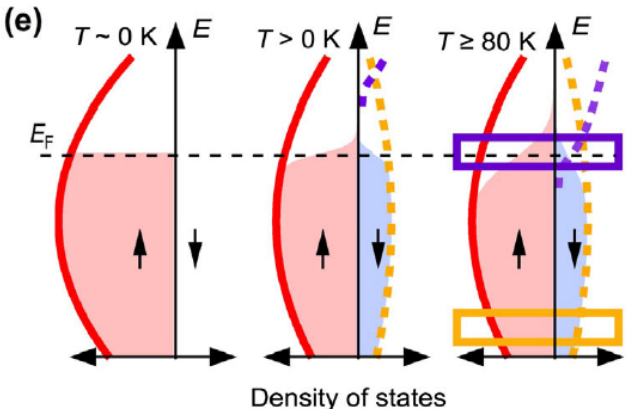
Origins of Thermal Spin Depolarization in Half-Metallic Ferromagnet CrO_2

Hirokazu Fujiwara,[1,*] Kensei Terashima,[2] Masanori Sunagawa,[1] Yuko Yano,[1] Takanobu Nagayama,[1] Tetsushi Fukura,[1] Fumiya Yoshii,[1] Yuka Matsuura,[1] Makoto Ogata,[1] Takanori Wakita,[2] Koichiro Yaji,[3] Ayumi Harasawa,[3] Kenta Kuroda,[3] Shik Shin,[3] Koji Horiba,[4] Hiroshi Kumigashira,[4,5] Yuji Muraoka,[1,2] and Takayoshi Yokoya[1,2]



NQP in spin-resolved photoemission





Beyond the talk

sp-electron magnetism

Ab initio spin dynamics for real systems

Spin and orbital magnetism

Nonequilibrium magnetism

And many, many specific applications to real materials

Collaboration

Recent:

A. Lichtenstein and S. Brener (Hamburg)
A. Secchi, E. Stepanov, and A. Rudenko (Nijmegen)
V. Mazurenko, Yu. Gornostuyrev, S. Okatov,
I. Razumov (Ekaterinburg)
Ya. Kvashnin and O. Eriksson (Uppsala)

and many other people involved in development of the formalism and calculations for specific materials in 1987-2013, esp. V. Antropov (Ames) and D. Boukhvalov (Nanjing)

Thank you for your attention