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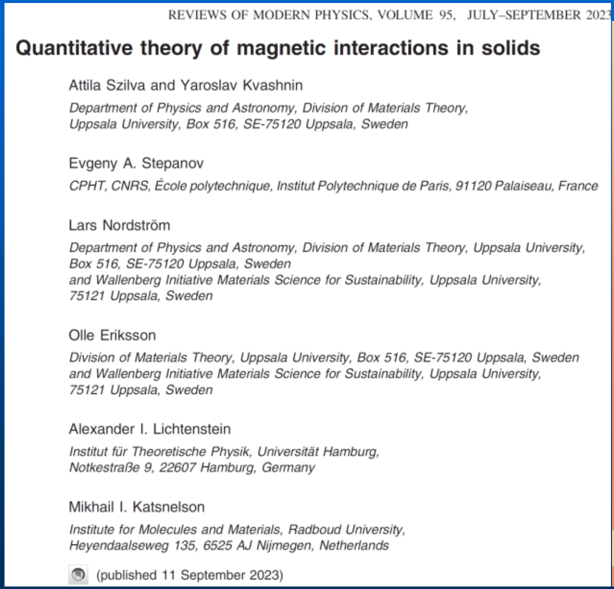
Quantitative theory of magnetic interactions in solids

Mikhail Katsnelson

For a general reference



REVIEWS OF MODERN PHYSICS, VOLUME 95, JULY–SEPTEMBER 2023

Quantitative theory of magnetic interactions in solids

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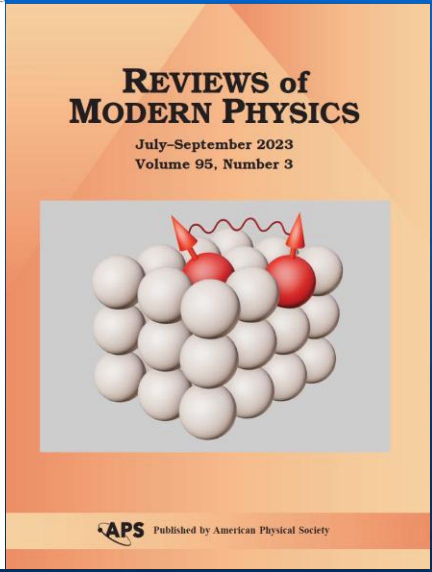
(published 11 September 2023)



REVIEWS of MODERN PHYSICS

July–September 2023
Volume 95, Number 3

APS Published by American Physical Society

Epigraphs

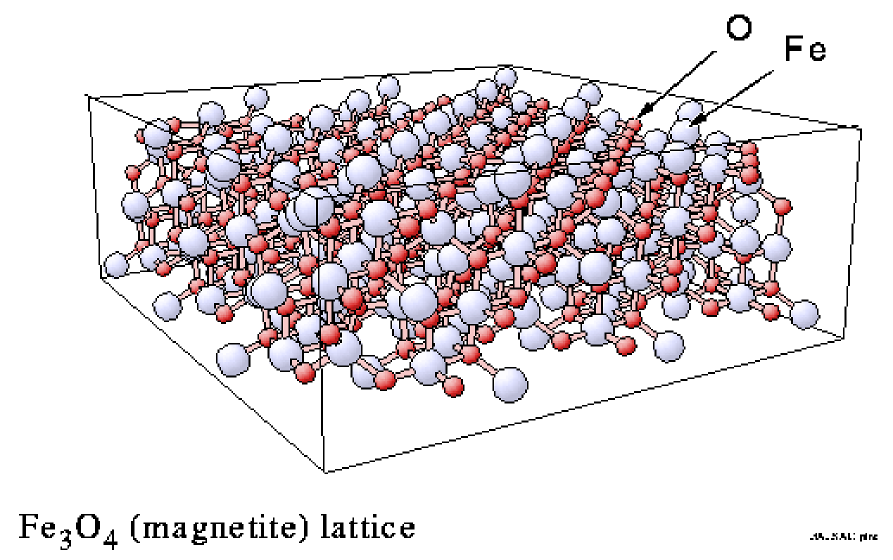
To the theoretical physicists, ferromagnetism presents a number of very interesting, unsolved and beautiful challenges. Our challenge is to understand why it exists at all.

(Feynman Lectures on Physics)

Make things as simple as possible but not simpler

(A. Einstein)

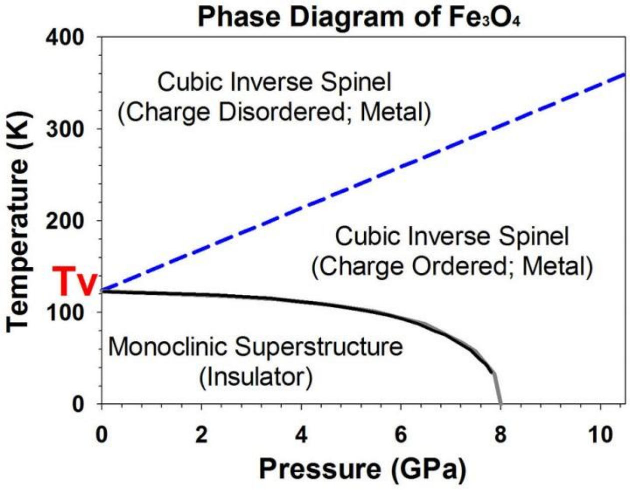
Magnetite – first known magnet



Fe_3O_4 (magnetite) lattice

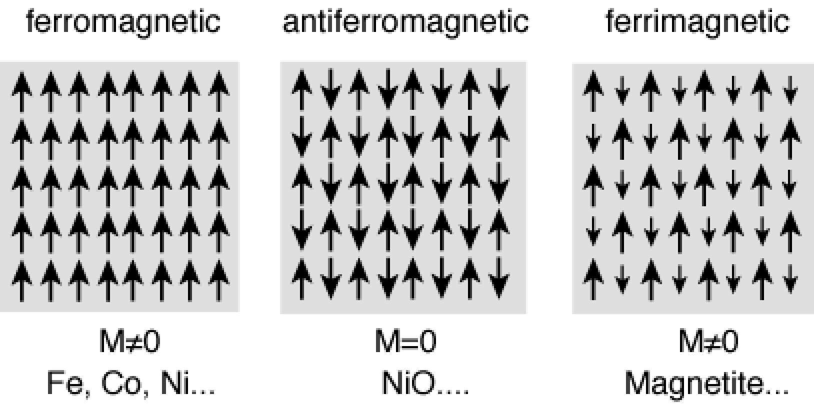
Very complicated structure, still a lot of open questions

Two types of Fe sites (tetra and octa);
Metal-insulator transition;
Charge ordering;
Role of orbital degrees of freedom;
Half-metallicity...



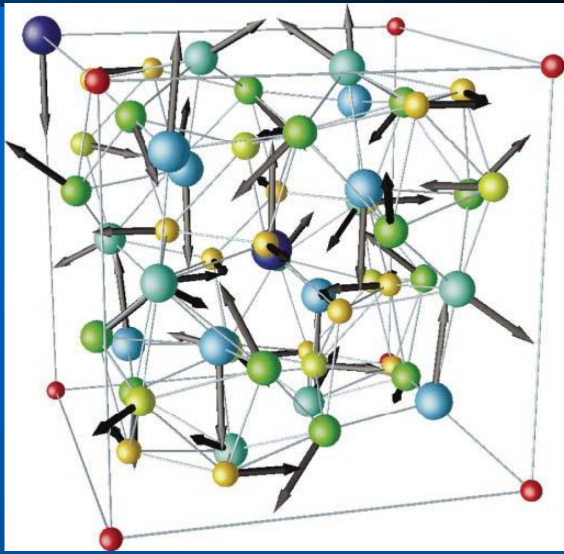
Types of magnetic ordering

Textbook wisdom

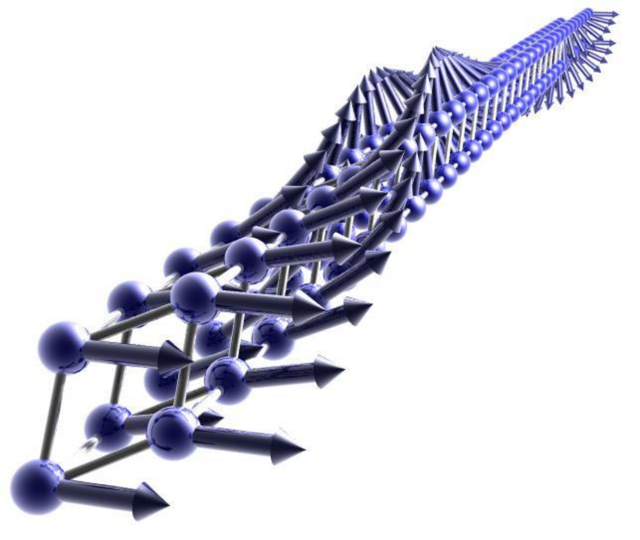


Sometimes very complicated

α-Mn

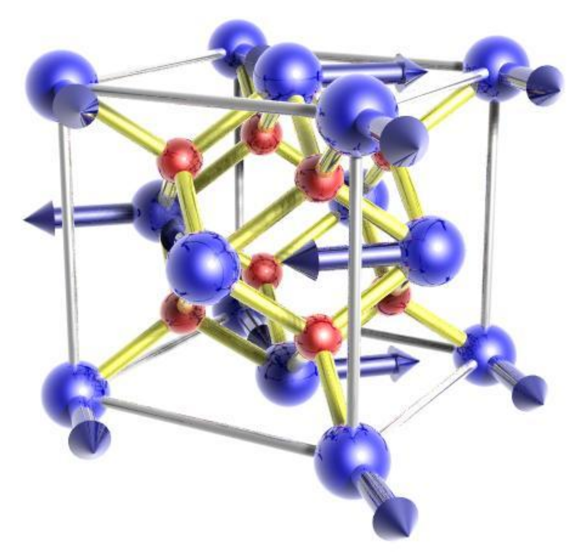


Spin spirals



γ-Fe

UO_2



Types of magnetic interactions

$$\hat{H} = \sum_{ij} J_{ij} \hat{\vec{S}}_i \hat{\vec{S}}_j + \sum_{i\mu\nu} \hat{S}_i^{\mu} A_i^{\mu\nu} \hat{S}_i^{\nu} + \sum_{ij} \vec{D}_{ij} [\hat{\vec{S}}_i \times \hat{\vec{S}}_j]$$

The first term: exchange interactions (Heisenberg model)
Quantum, nonrelativistic (Coulomb interaction plus Pauli principle).
Determine the type of magnetic ordering (mostly)

The second term: magnetic anisotropy
Quantum, relativistic (due to spin-orbit interaction). At least, second-order in SOC. Determine "practical" magnetism (hard and soft magnetic materials, hysteresis loop, etc.)

The third term: Dzyaloshinskii-Moriya interactions
Quantum, relativistic (due to spin-orbit interaction). First-order in SOC but require broken inversion symmetry. Responcible for weak FM, skyrmiones etc.

How to map fully microscopic description to magnetic Hamiltonians?

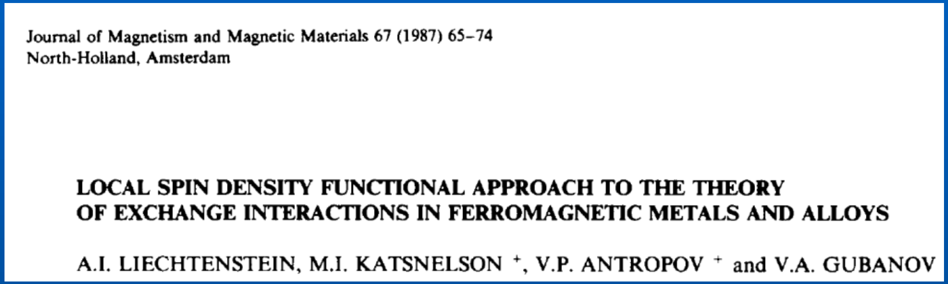
The talk is based on theory developed for about 40 years, first of all, with Sasha Lichtenstein, and with other friends and colleagues

J. Phys. F: Met. Phys. **14** (1984) L125–L128. Printed in Great Britain

LETTER TO THE EDITOR

Exchange interactions and spin-wave stiffness in ferromagnetic metals

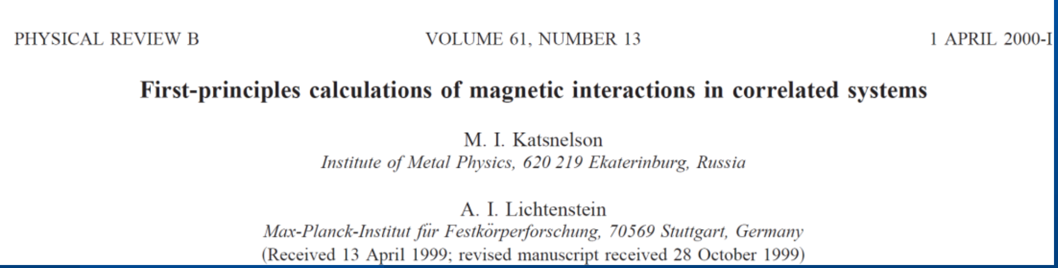
A I Liechtenstein†, M I Katsnelson‡ and V A Gubanov†



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



PHYSICAL REVIEW B VOLUME 61, NUMBER 13 1 APRIL 2000-I

First-principles calculations of magnetic interactions in correlated systems

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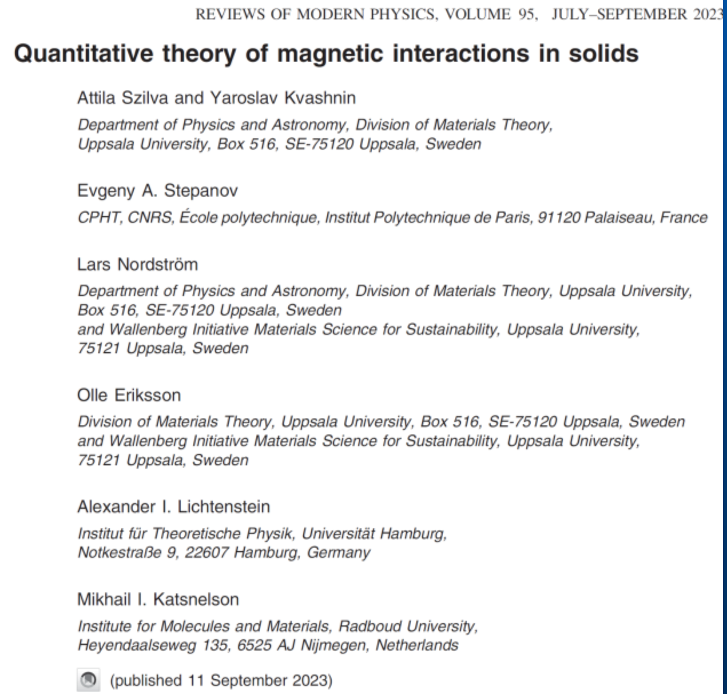
(Received 13 April 1999; revised manuscript received 28 October 1999)



REVIEWS OF MODERN PHYSICS, VOLUME 95, JULY–SEPTEMBER 202

Quantitative theory of magnetic interactions in solids

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(published 11 September 2023)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

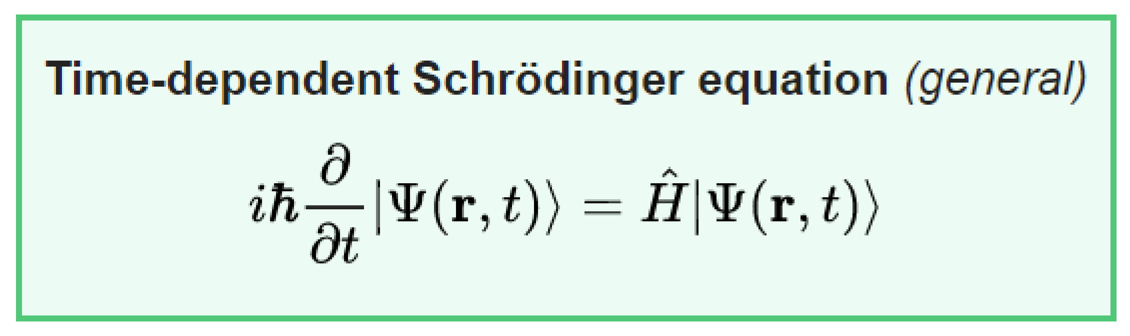
J. Phys.: Condens. Matter **16** (2004) 7439–7446 PII: S0953-8984(04)80755-0

Magnetic susceptibility, exchange interactions and spin-wave spectra in the local spin density approximation

M I Katsnelson[1,2] and A I Lichtenstein[2,3]

Quantum Hamiltonians: General

In condensed matter physics we know the basic laws, it is laws of quantum mechanics



Time-dependent Schrödinger equation *(general)*

$$i\hbar\frac{\partial}{\partial t}|\Psi(\mathbf{r},t)\rangle = \hat{H}|\Psi(\mathbf{r},t)\rangle$$

In solids/liquids/molecules/clusters...

$$\hat{H} = \hat{T}_n + V_{nn}\left(\vec{R}_l\right) + \hat{H}_e\left(\vec{R}_l\right)$$

$$\hat{T}_n = \sum_l \frac{\hat{\vec{P}}_l^2}{2M_l}$$

Kinetic energy of nuclei

$$V_{nn}\left(\vec{R}_l\right) = \frac{1}{2}\sum_{l\neq l'} \frac{Z_l Z_{l'} e^2}{\left|\vec{R}_l - \vec{R}_{l'}\right|}$$

Coulomb repulsion of nuclei

$$\hat{H}_e\left(\vec{R}_l\right) = \sum_i \frac{\hat{\vec{p}}_i^2}{2m} + \frac{1}{2}\sum_{i\neq j}\frac{e^2}{\left|\vec{r}_i - \vec{r}_j\right|} - \sum_{il}\frac{Z_l e^2}{\left|\vec{r}_i - \vec{R}_l\right|}$$

Electron Hamiltonian at a given position of nuclei

How do we work in solids?

(1) Separate motion of nuclei and electrons (adiabatic approximation) – well justified, small parameter

$$\kappa = \left(\frac{m}{M}\right)^{1/4}$$

(2) For electrons: density functional or Green’s function functional – formally exact but unavoidable approximations for the form of functionals

In both cases, interaction is important, energy is not the sum of energy of individual “quasiparticles” E_{sp} but “local force theorem”: *variation* of total energy can be expressed via variation of E_{sp}

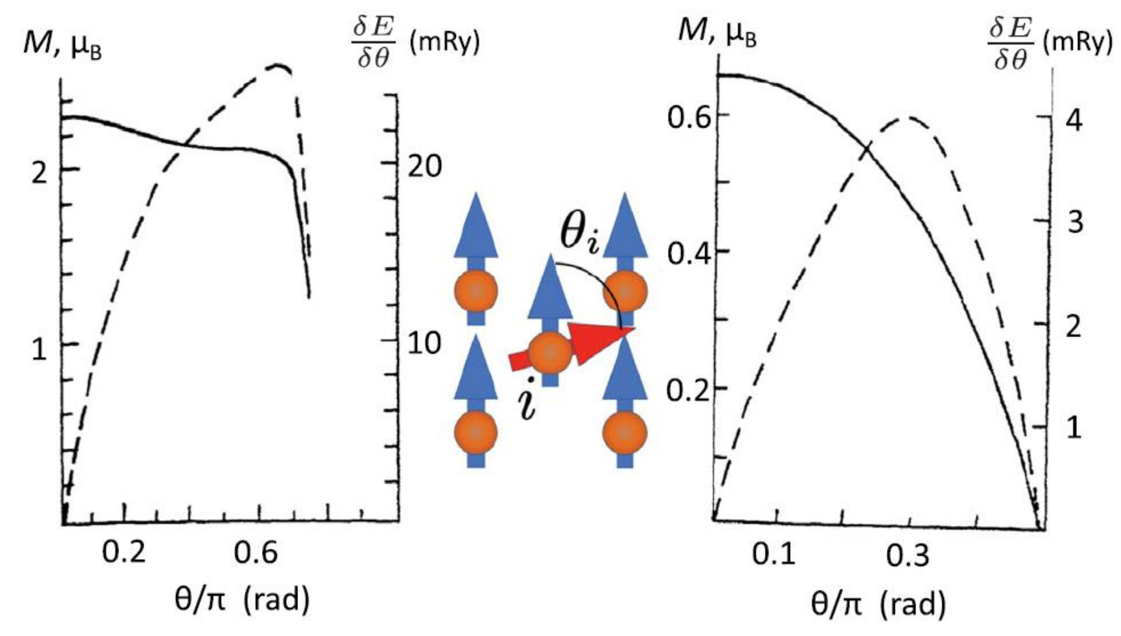
The idea: consider small rotations of spins with respect to a given magnetic configuration, use local force theorem – we come to explicit expression for torque and compare with model expression

The main conceptual results

1. *Mapping of interacting electrons onto effective spin Hamiltonians is possible only locally, near given equilibrium spin configuration; distinction of local and global spin models*
2. *Even locally, ambiguity in definition of exchange parameters: magnon energies (poles of dynamic susceptibility) vs energy of static magnetic configurations (static susceptibility)*
3. *In two cases the mapping is unambiguous: (3a) small wave vectors (spin-wave stiffness constant is unique) and (3b) well-localized magnetic moments (Stoner splitting is much larger than characteristic magnon energy)*

Non-Heisenberg exchange

Almost obvious for itinerant-electron magnets



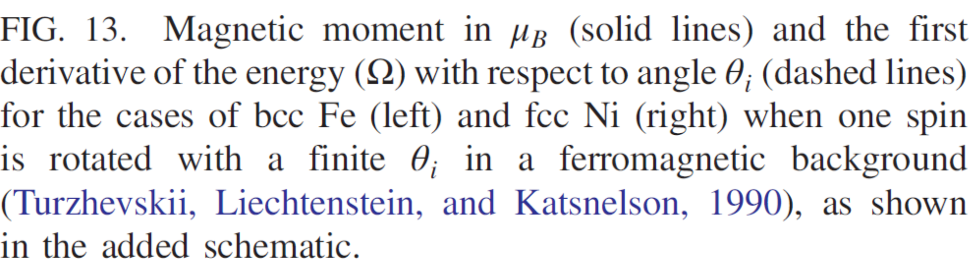
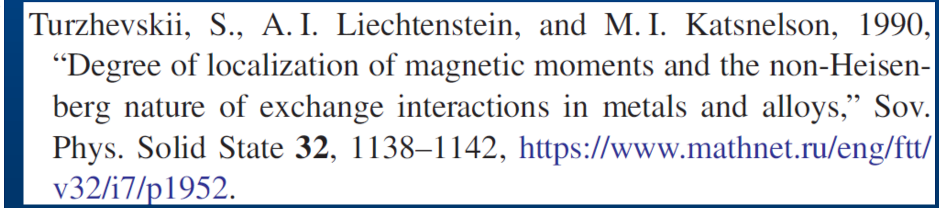


FIG. 13. Magnetic moment in μ_B (solid lines) and the first derivative of the energy (Ω) with respect to angle θ_i (dashed lines) for the cases of bcc Fe (left) and fcc Ni (right) when one spin is rotated with a finite θ_i in a ferromagnetic background (Turzhevskii, Liechtenstein, and Katsnelson, 1990), as shown in the added schematic.


Turzhevskii, S., A. I. Liechtenstein, and M. I. Katsnelson, 1990, "Degree of localization of magnetic moments and the non-Heisenberg nature of exchange interactions in metals and alloys," Sov. Phys. Solid State **32**, 1138–1142, https://www.mathnet.ru/eng/ftt/v32/i7/p1952.

Non-Heisenberg exchange II

Even for insulating metal-oxide compounds

J. Phys.: Condens. Matter **29** (2017) 335801 (9pp) https://doi.org/10.1088/1361-648X/aa7b00

Exchange interactions in transition metal oxides: the role of oxygen spin polarization

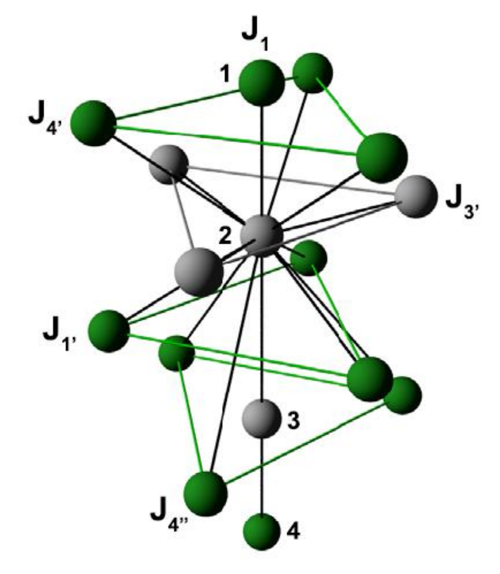
R Logemann, A N Rudenko, M I Katsnelson and A Kirilyuk

Nomenclature

$$H = -\sum_{i>j} 2J_{ij}\boldsymbol{s}_i \cdot \boldsymbol{s}_j$$

$\boldsymbol{s}_i$ ($\boldsymbol{s}_j$) is the unit vector

LDA+U calculations



Fe atoms in elementary cell of hematite; green spins down

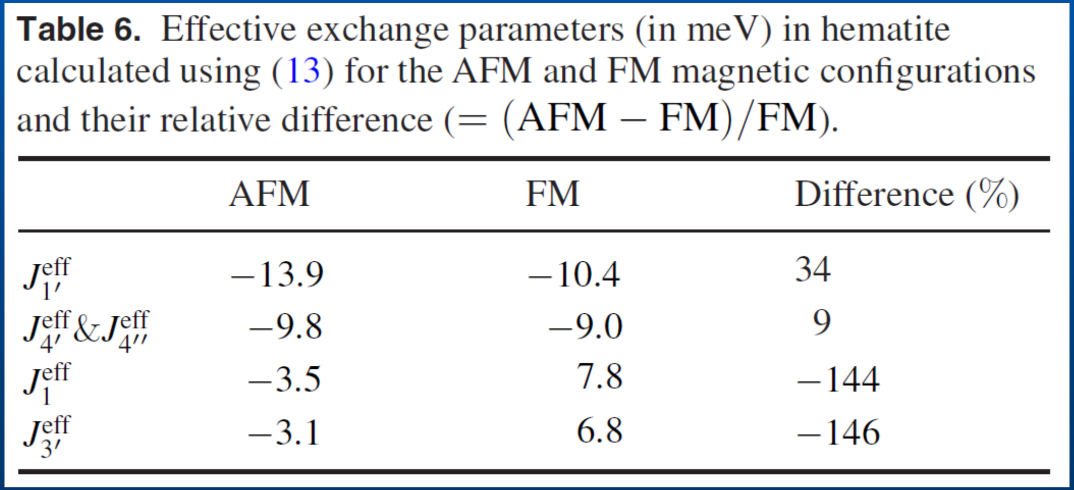
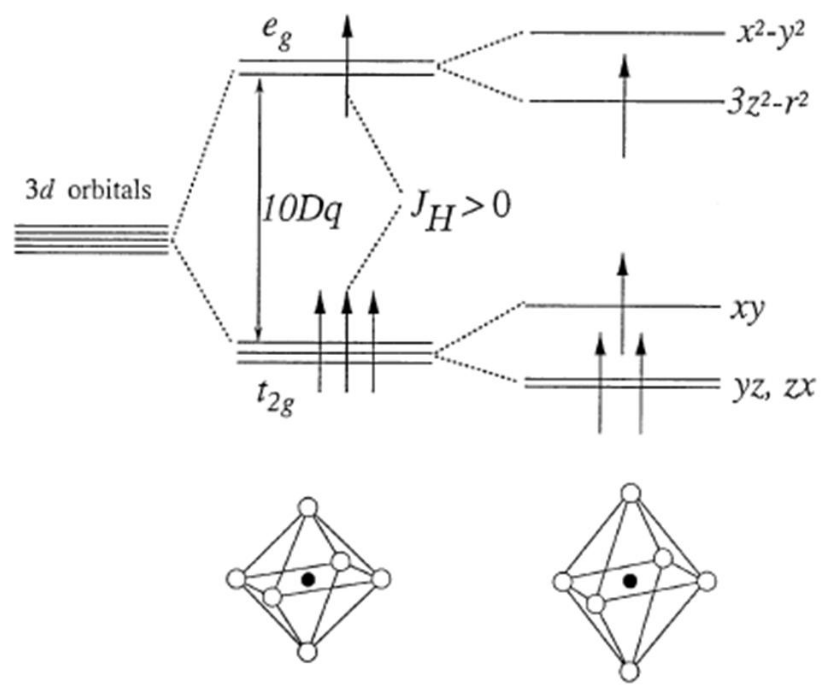


Table 6. Effective exchange parameters (in meV) in hematite calculated using (13) for the AFM and FM magnetic configurations and their relative difference (= (AFM − FM)/FM).

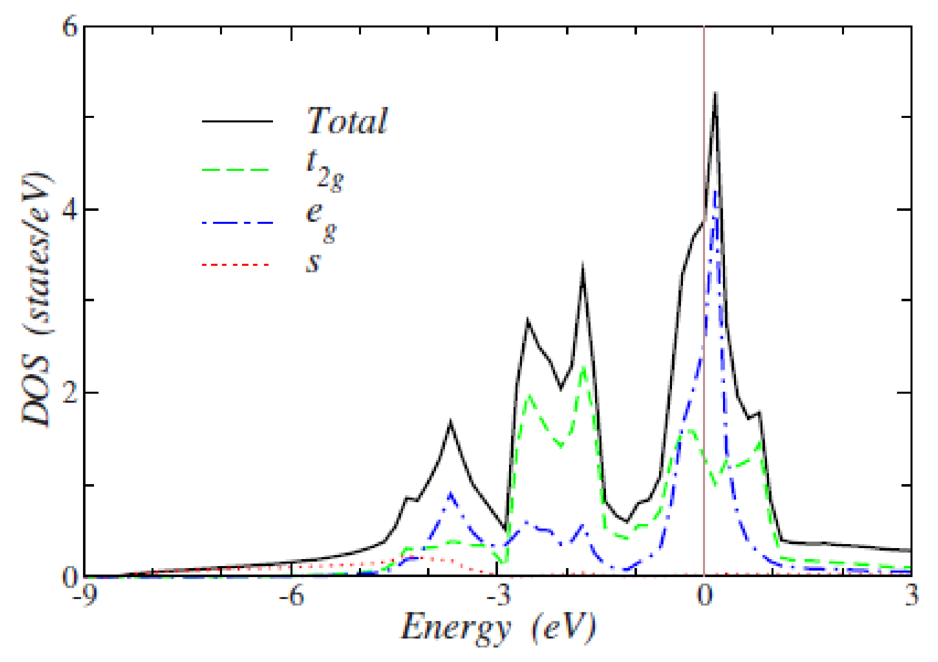
	AFM	FM	Difference (%)
$J_{1'}^{\mathrm{eff}}$	−13.9	−10.4	34
$J_{4'}^{\mathrm{eff}}$&$J_{4''}^{\mathrm{eff}}$	−9.8	−9.0	9
J_{1}^{eff}	−3.5	7.8	−144
$J_{3'}^{\mathrm{eff}}$	−3.1	6.8	−146

Polarization of oxygen effects essentially on superexchange

Iron: some details



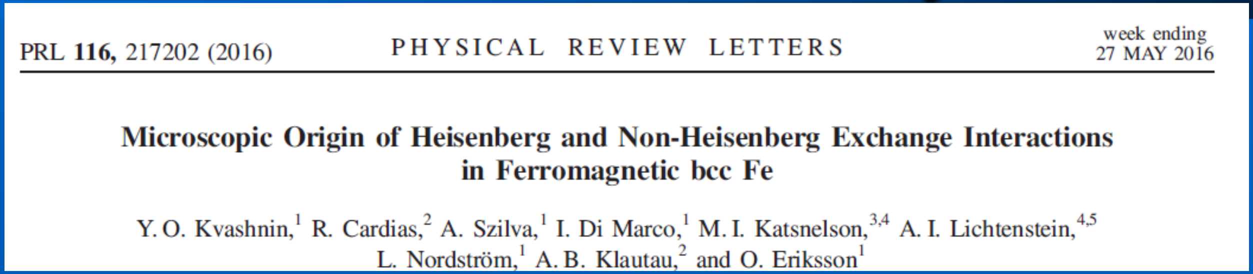
Crystal field splitting



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]

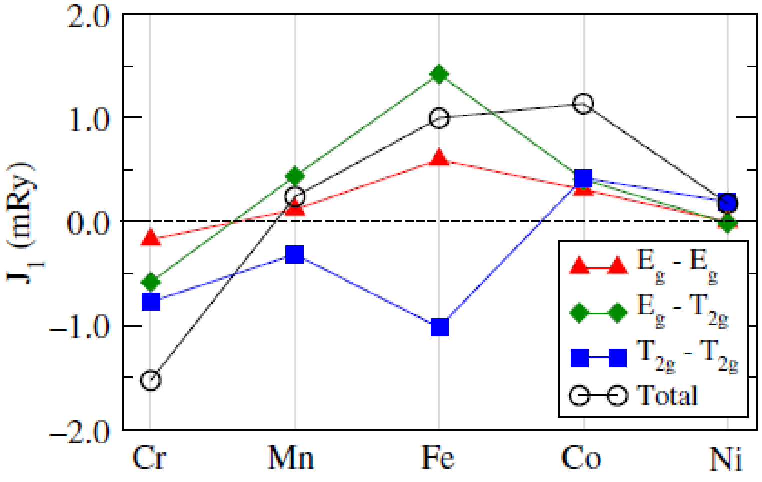
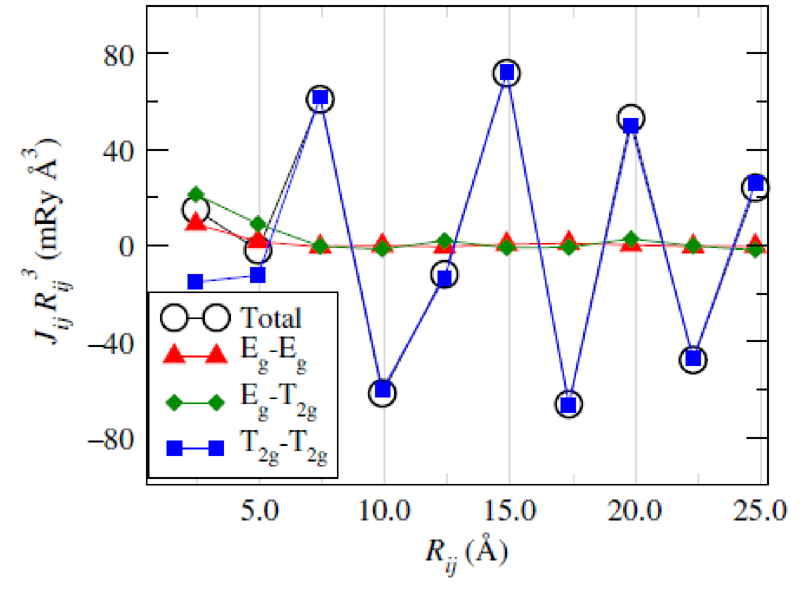


FIG. 1. Orbitally decomposed NN exchange interaction in elemental 3*d* metals in the bcc structure.



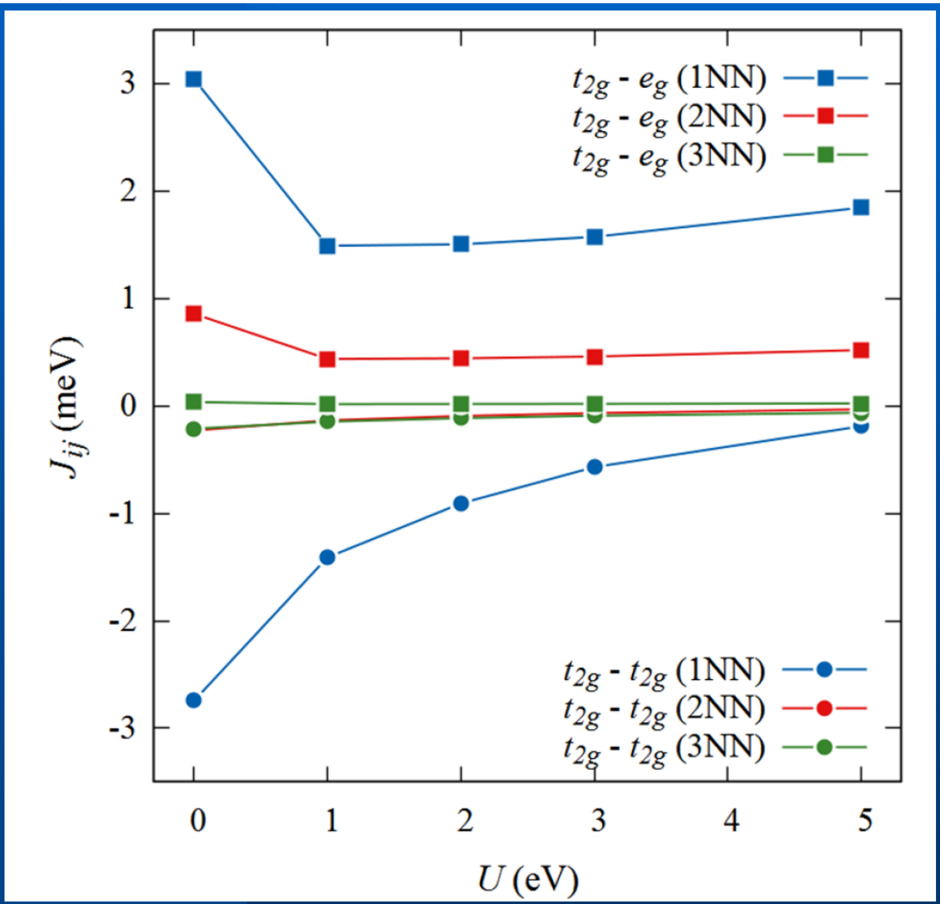
t_{2g} are itinerant electrons providing (Heisenberg-like) RKKY exchange with Friedel oscillations; e_g are more correlated providing (non-Heisenberg) “double exchange” typical for narrom-band systems

Applications: 2D magnets

Orbitally-resolved ferromagnetism of monolayer CrI_3

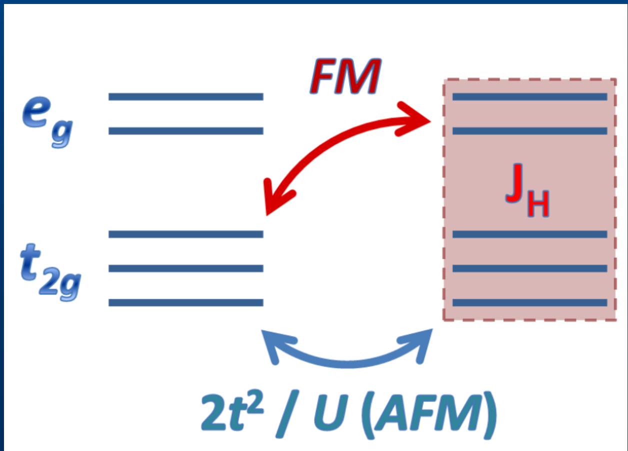
I V Kashin[1], V V Mazurenko[1], M I Katsnelson[1,2] and A N Rudenko[3,2,1]

2D Mater. **7** (2020) 025036



LDA+U results: competing FM and AFM contributions to superexchange

Qualitative explanation within Kugel-Khomskii model



Applications: Transition Metal Alloys

Invar problem

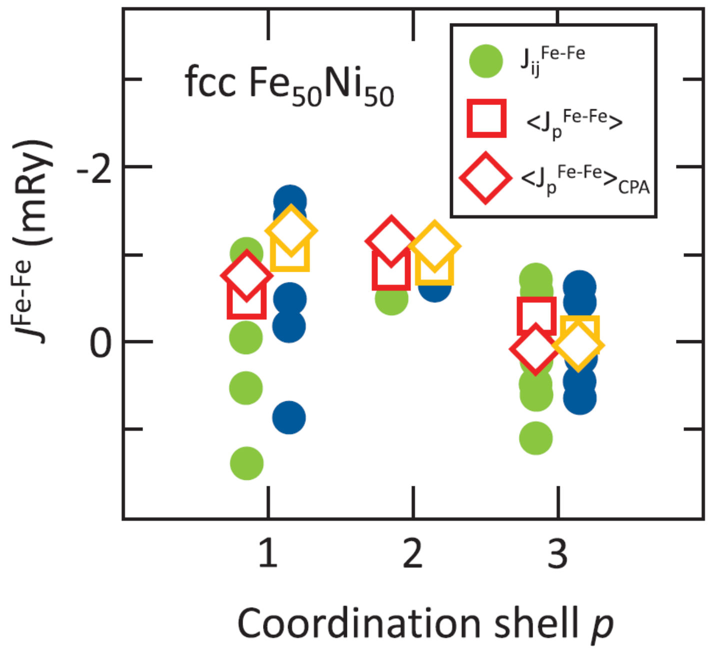


FIG. 15. Calculated Fe-Fe exchange interactions with first three coordination shells in fcc $Fe_{0.5}Ni_{0.5}$ for two different unit cell volumes (V) (Ruban *et al.*, 2005). The 16-atom supercell-based results for $V = 73.6$ a.u.^{3} and $V = 70.3$ a.u.^{3} are shown with blue (dark gray) and green (light gray) circles, respectively. Supercell- and CPA-averaged J_{ij}'s are shown for comparison.

Ruban, A. V., M. I. Katsnelson, W. Olovsson, S. I. Simak, and I. A. Abrikosov, 2005, "Origin of magnetic frustrations in Fe-Ni Invar alloys," Phys. Rev. B **71**, 054402.

Heussler alloys

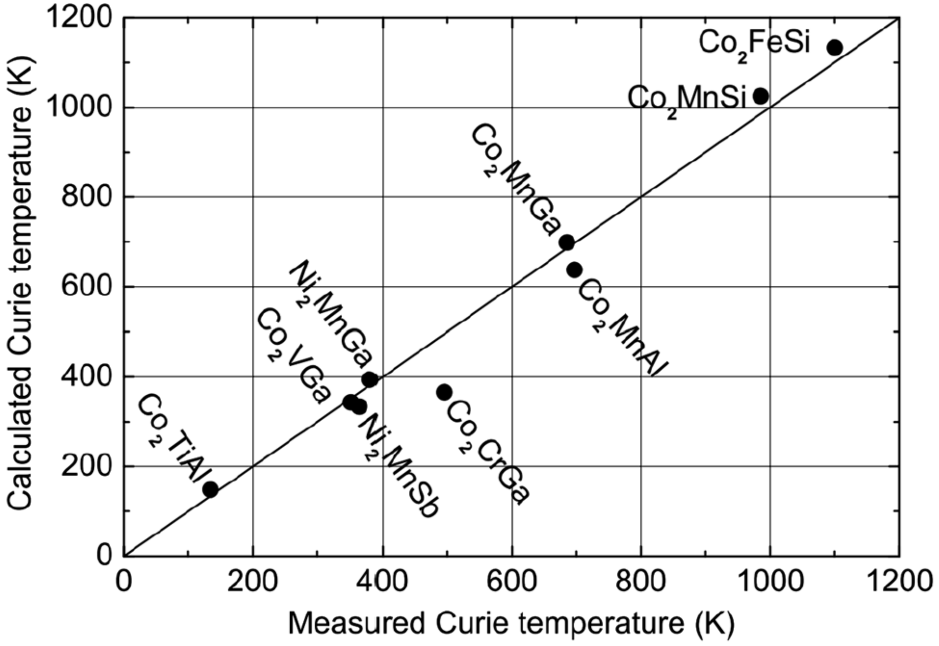


FIG. 16. Calculated vs measured T_c's in the series of $L2_1$ Heusler alloys. From Thoene *et al.*, 2009.

Thoene, Jan, Stanislav Chadov, Gerhard Fecher, Claudia Felser, and Jürgen Kübler, 2009, "Exchange energies, Curie temperatures and magnons in Heusler compounds," J. Phys. D **42**, 084013.

Mean-field estimate of Curie temperature

Applications: Magnetic monolayers

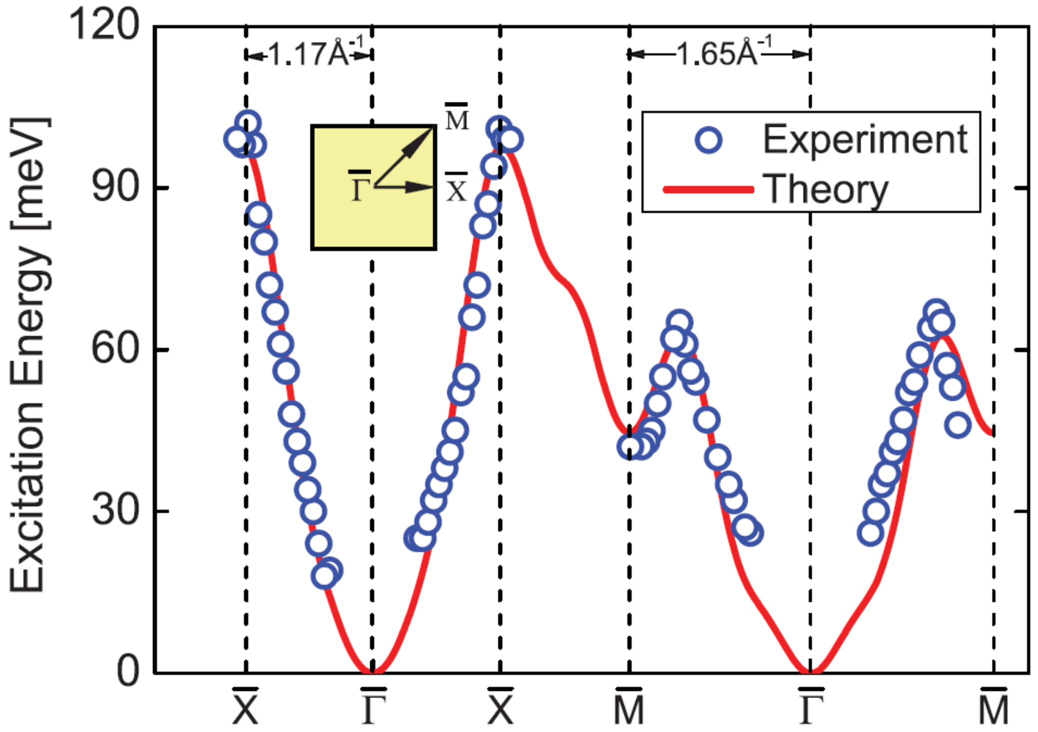
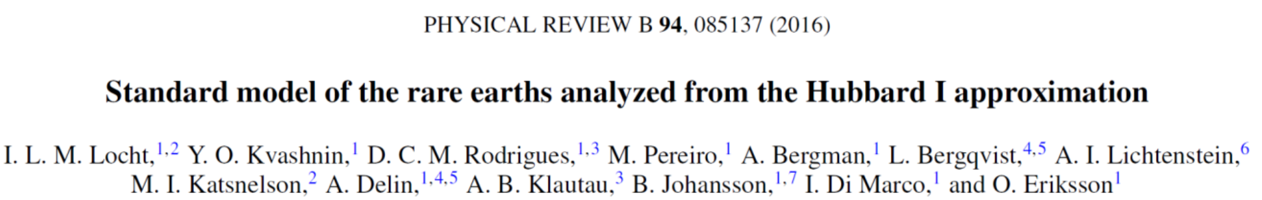


FIG. 19. Computed and measured acoustic magnon dispersions in Fe/Rh(001). Inset shows the parts of the Brillouin zone used in the plot. From Meng *et al.*, 2014.

Meng, Y., Kh. Zakeri, A. Ernst, T.-H. Chuang, H. J. Qin, Y.-J. Chen, and J. Kirschner, 2014, “Direct evidence of antiferromagnetic exchange interaction in Fe(001) films: Strong magnon softening at the high-symmetry $\bar{M}$ point,” Phys. Rev. B **90**, 174437.

Applications: rare-earth elements



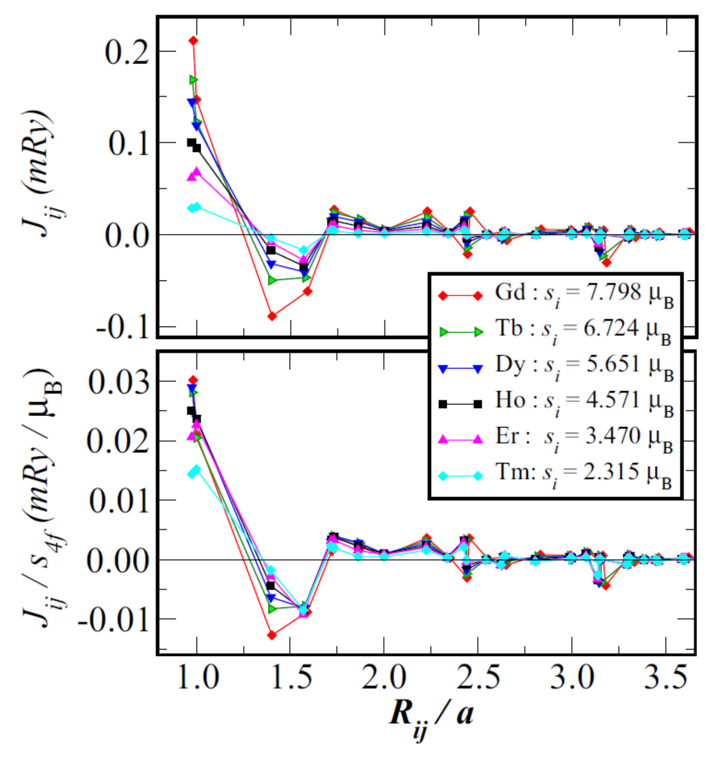
PHYSICAL REVIEW B **94**, 085137 (2016)

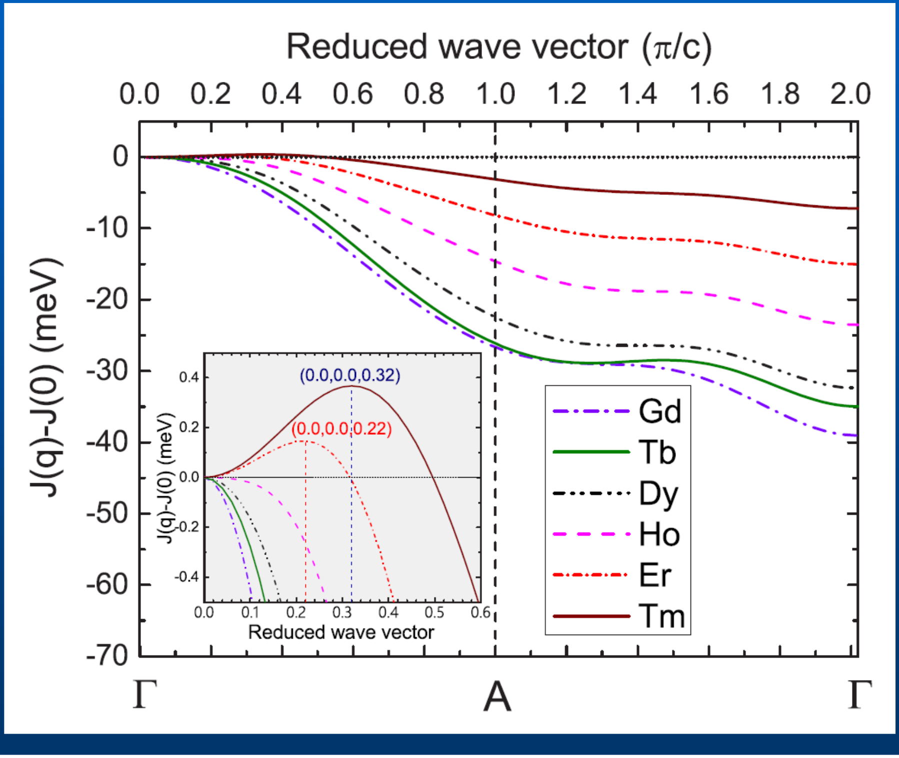
Standard model of the rare earths analyzed from the Hubbard I approximation

I. L. M. Locht,[1,2] Y. O. Kvashnin,[1] D. C. M. Rodrigues,[1,3] M. Pereiro,[1] A. Bergman,[1] L. Bergqvist,[4,5] A. I. Lichtenstein,[6]
M. I. Katsnelson,[2] A. Delin,[1,4,5] A. B. Klautau,[3] B. Johansson,[1,7] I. Di Marco,[1] and O. Eriksson[1]

Nomenclature

$$H = -\sum_{i \neq j} J_{ij}\, \mathbf{e}_i \cdot \mathbf{e}_j$$





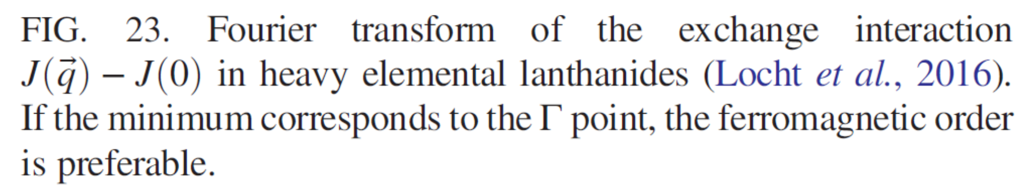
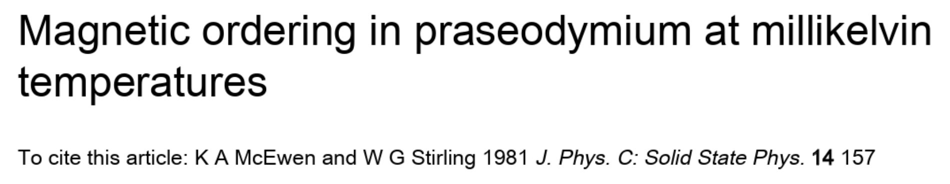


FIG. 23. Fourier transform of the exchange interaction $J(\vec{q}) - J(0)$ in heavy elemental lanthanides (Locht *et al.*, 2016). If the minimum corresponds to the Γ point, the ferromagnetic order is preferable.

Pr: nonmagnetic ground-state?!

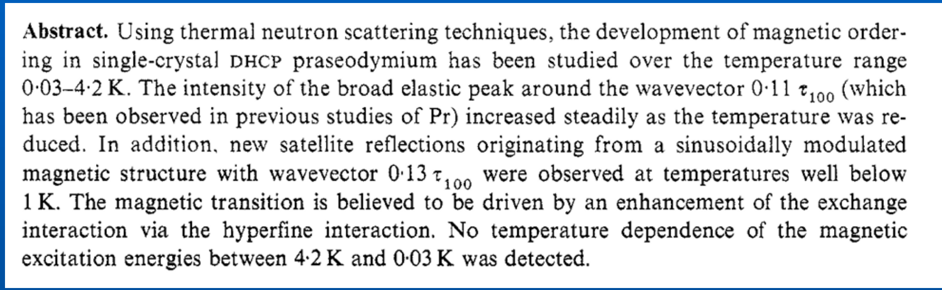
f^2 configuration of Pr^{3+} The ground state multiplet is S = 1, L = 5, J = 4

Experimentally: no magnetic ordering at "normal" temperatures and nuclear magnetic ordering at millikelvins!



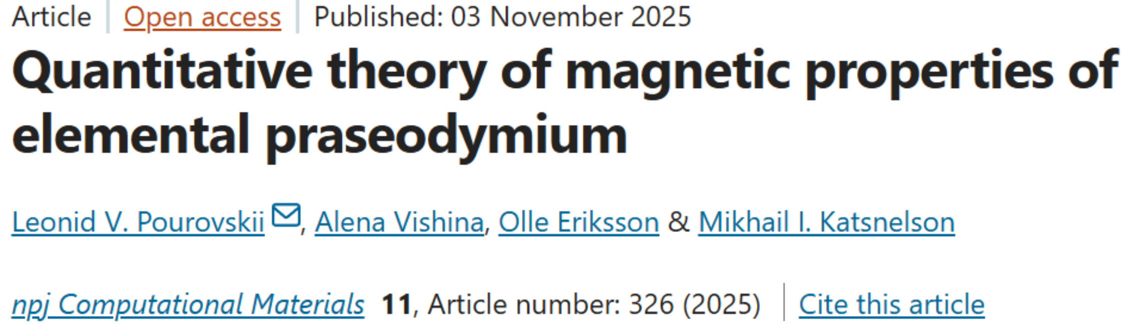
Magnetic ordering in praseodymium at millikelvin temperatures

To cite this article: K A McEwen and W G Stirling 1981 *J. Phys. C: Solid State Phys.* **14** 157



Abstract. Using thermal neutron scattering techniques, the development of magnetic ordering in single-crystal DHCP praseodymium has been studied over the temperature range 0·03–4·2 K. The intensity of the broad elastic peak around the wavevector 0·11 τ_{100} (which has been observed in previous studies of Pr) increased steadily as the temperature was reduced. In addition, new satellite reflections originating from a sinusoidally modulated magnetic structure with wavevector 0·13 τ_{100} were observed at temperatures well below 1 K. The magnetic transition is believed to be driven by an enhancement of the exchange interaction via the hyperfine interaction. No temperature dependence of the magnetic excitation energies between 4·2 K and 0·03 K was detected.

General explanation are known: crystal-field splitting of $^3H_4$ multiplet with singlet ground state but *(1) interionic interactions can change energetics making magnetic state favorable; (2) what is the role of various sites is unknown; (3) what is on the surface – neither theory nor experiment; (4) quantitative theory is absent*



Article | Open access | Published: 03 November 2025

Quantitative theory of magnetic properties of elemental praseodymium

Leonid V. Pourovskii, Alena Vishina, Olle Eriksson & Mikhail I. Katsnelson

npj Computational Materials **11**, Article number: 326 (2025) | Cite this article

In spirit of our "standard model"; Hubbard-I-like approach for crystal field and f-electron-in-the core calculations of exchange parameters

Crystal field splittings

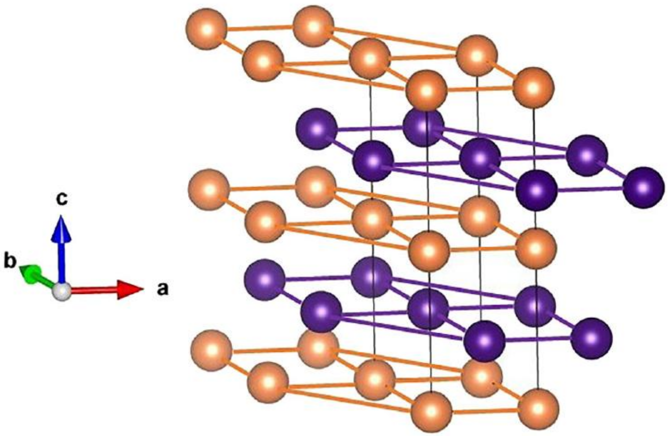


Fig. 1 | The crystal structure of dhcp Pr. The cubic (hexagonal) sites are depicted with orange (violet) spheres.

$$H^{\mathrm{CF}} = \sum_{kq} B_k^q O_k^q$$

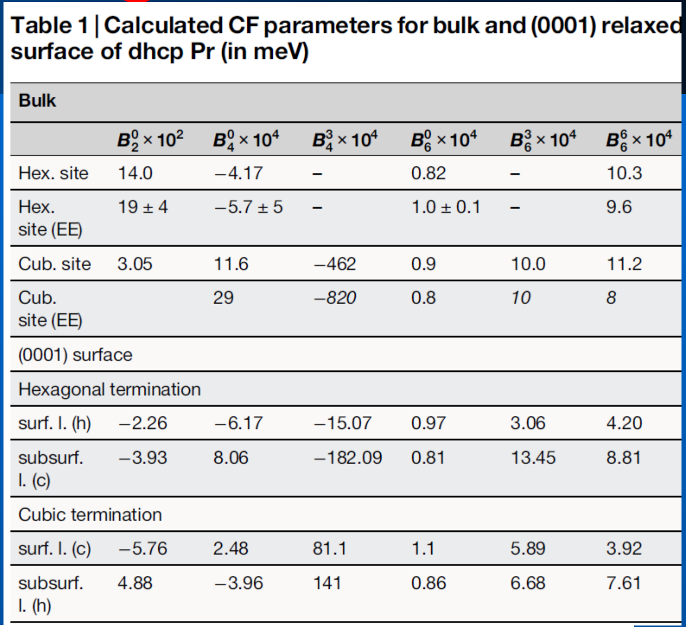


Table 1 | Calculated CF parameters for bulk and (0001) relaxed surface of dhcp Pr (in meV)

Bulk						
	$B_2^0\times10^2$	$B_4^0\times10^4$	$B_4^3\times10^4$	$B_6^0\times10^4$	$B_6^3\times10^4$	$B_6^6\times10^4$
Hex. site	14.0	−4.17	–	0.82	–	10.3
Hex. site (EE)	19 ± 4	−5.7 ± 5	–	1.0 ± 0.1	–	9.6
Cub. site	3.05	11.6	−462	0.9	10.0	11.2
Cub. site (EE)		29	*−820*	0.8	*10*	*8*
(0001) surface						
Hexagonal termination						
surf. l. (h)	−2.26	−6.17	−15.07	0.97	3.06	4.20
subsurf. l. (c)	−3.93	8.06	−182.09	0.81	13.45	8.81
Cubic termination						
surf. l. (c)	−5.76	2.48	81.1	1.1	5.89	3.92
subsurf. l. (h)	4.88	−3.96	141	0.86	6.68	7.61

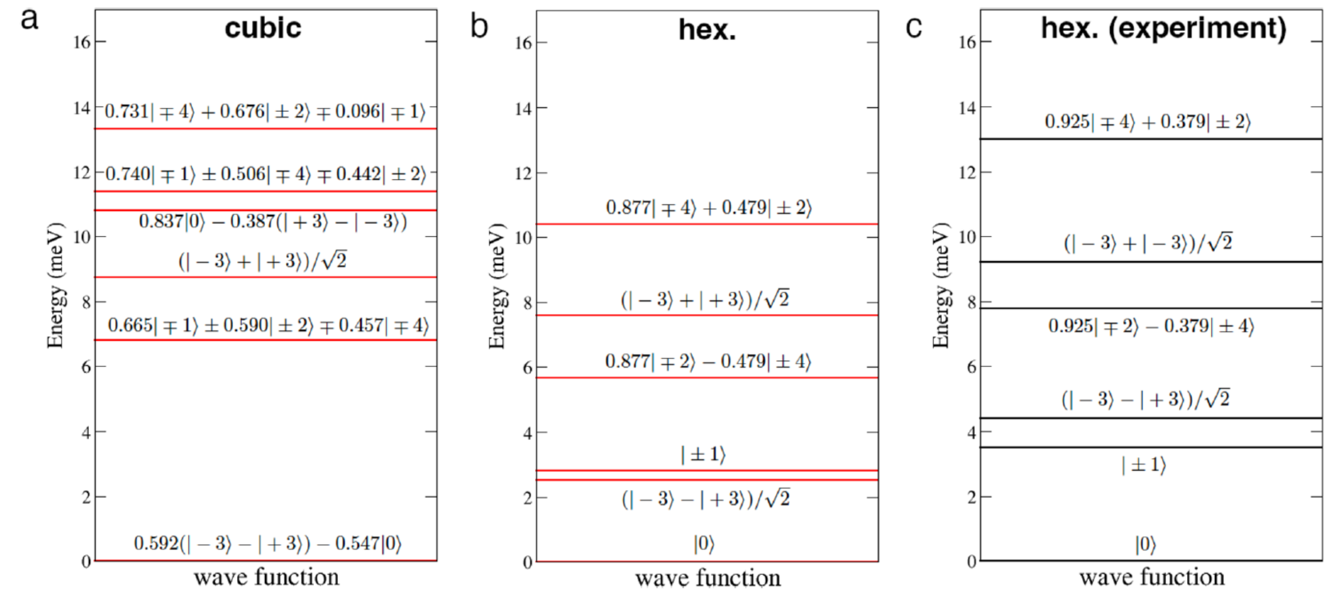


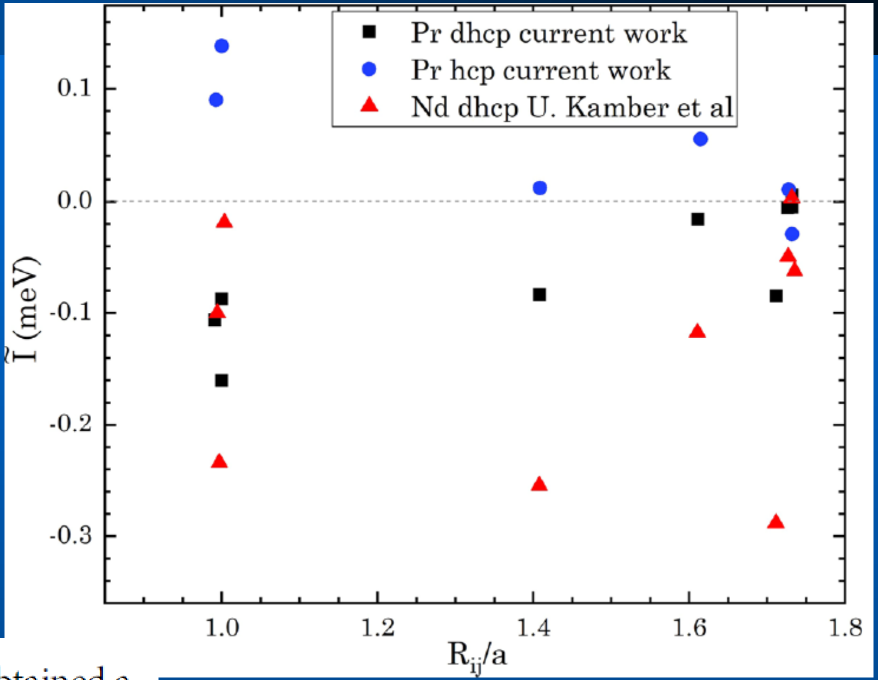
Fig. 2 | Calculated crystal-field splitting of the Pr $^3H_4$ configuration for the cubic (**a**) and hexagonal (**b**) site in bulk dhcp Pr. The CF wavefunctions are written in the $|M\rangle \equiv |J=4; M_J\rangle$ basis and are defined in the same coordination frame as the CFPs in Table 1. In panel (**c**), we reproduce the experimentally inferred CF level scheme of ref. 17 for the hexagonal site.

Exchange interactions in Pr

$$H_{\text{eff}} = \sum_i H_i^{\text{CF}} - \sum_{ij} I_{ij} \mathbf{J}_i \cdot \mathbf{J}_j,$$

$$\sum_{ij} I_{ij} \mathbf{J}_i \cdot \mathbf{J}_j \to \sum_{ij} I'_{ij} \mathbf{S}_i \cdot \mathbf{S}_j,$$

$$\sum_{ij} I'_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \to \sum_{ij} \tilde{I}_{ij} \mathbf{e}_i \cdot \mathbf{e}_j.$$



Solving $\hat{H}_{\text{eff}}$, Eq. (1), for the bulk dhcp phase we correctly obtained a nonmagnetic state, with both crystallographic sites having the same singlet ground state as shown in Fig. 2. It agrees with experimental observations and illustrates the competition between interatomic exchange, which favors a magnetically ordered state, and crystal field effects, which for Pr favor a non-magnetic, singlet state. Following the experimental observations, the singlet state has the lowest energy. It means that the energy gain that would come from a magnetically ordered state, as quantified by the second term of Eq. (1), is smaller than the gain of the singlet crystal field effect that arises due to the Coulombic interaction of the $J = 4$ state of Pr in the dhcp crystal structure. In the Supplementary Section 3, we analyze the magnetic contribution to the specific heat, and a Schottky anomaly that occurs due to the excited CF levels of Pr.

Exchange energies are smaller than CF splitting, the ground state of the crystal remains nonmagnetic (without nuclear spins)

Surface of Pr: prediction

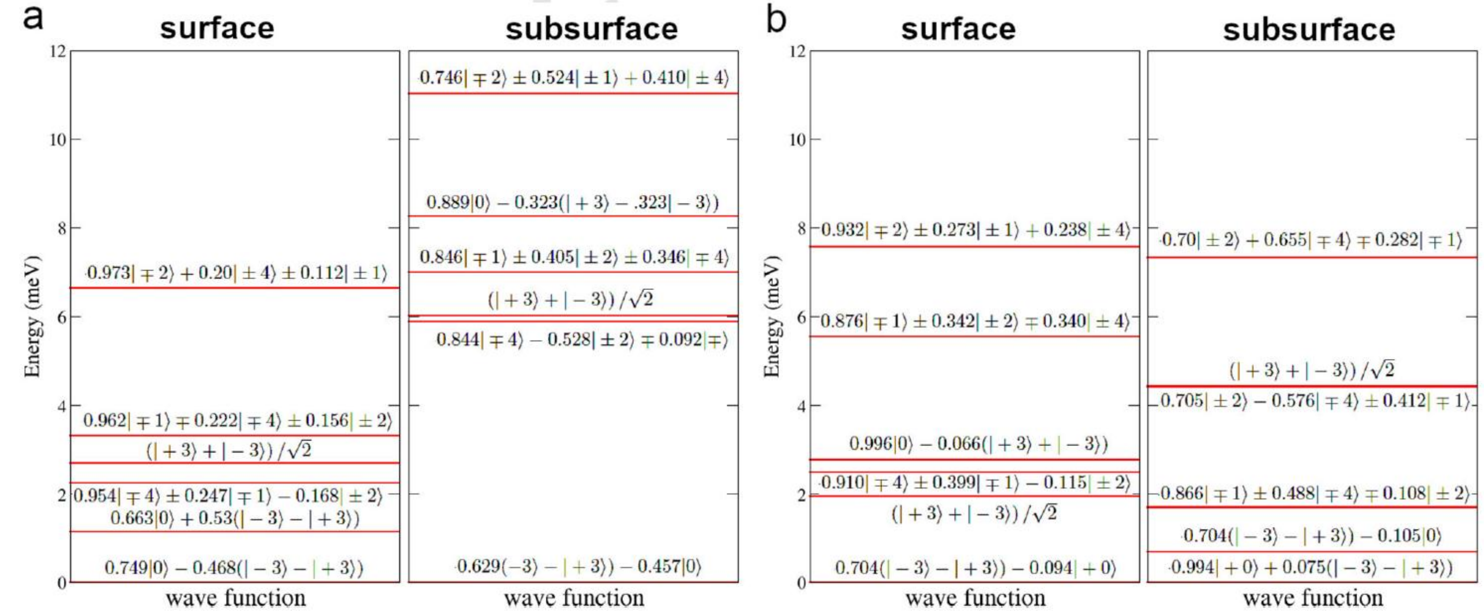


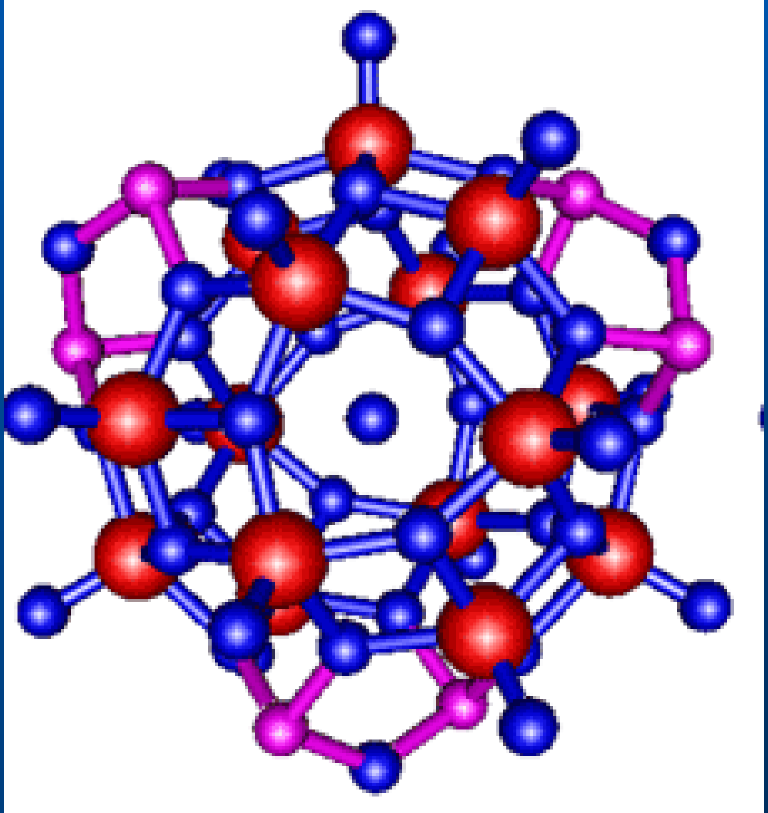
Fig. 5 | Calculated crystal-field level splitting of the Pr $^3H_4$ multiplet at the (0001) dhcp surfaces with hexagonal (**a**) and cubic (**b**) termination. The CF wavefunction representation and coordination frame are the same as in Fig. 2. For both cases, we show the levels for the surface and subsurface site. In the subsurface layer the site symmetries are reversed with respect to the surface one, becoming cubic in (**a**) and hexagonal in (**b**), respectively.

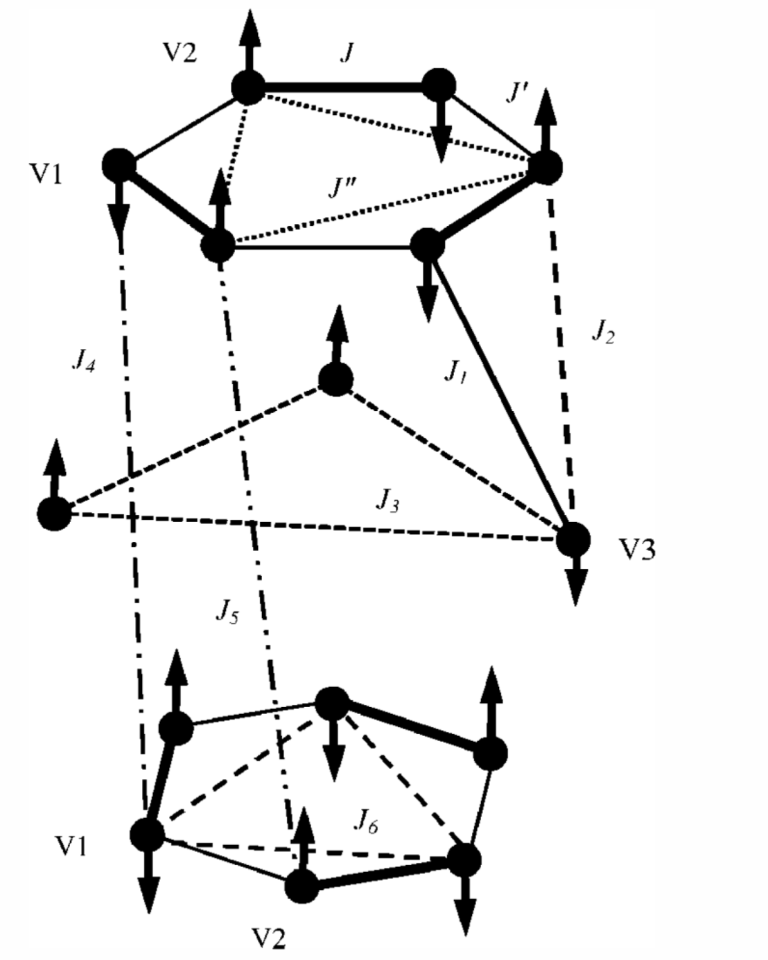
Crystal field splittings are smaller than in the bulk but still, singlet ground state wins, exchange interactions are not sufficient to change it, (0001) surface of Pr should be nonmagnetic

Molecular magnets

Example: V_{15} AFM ground state *S = 1/2*

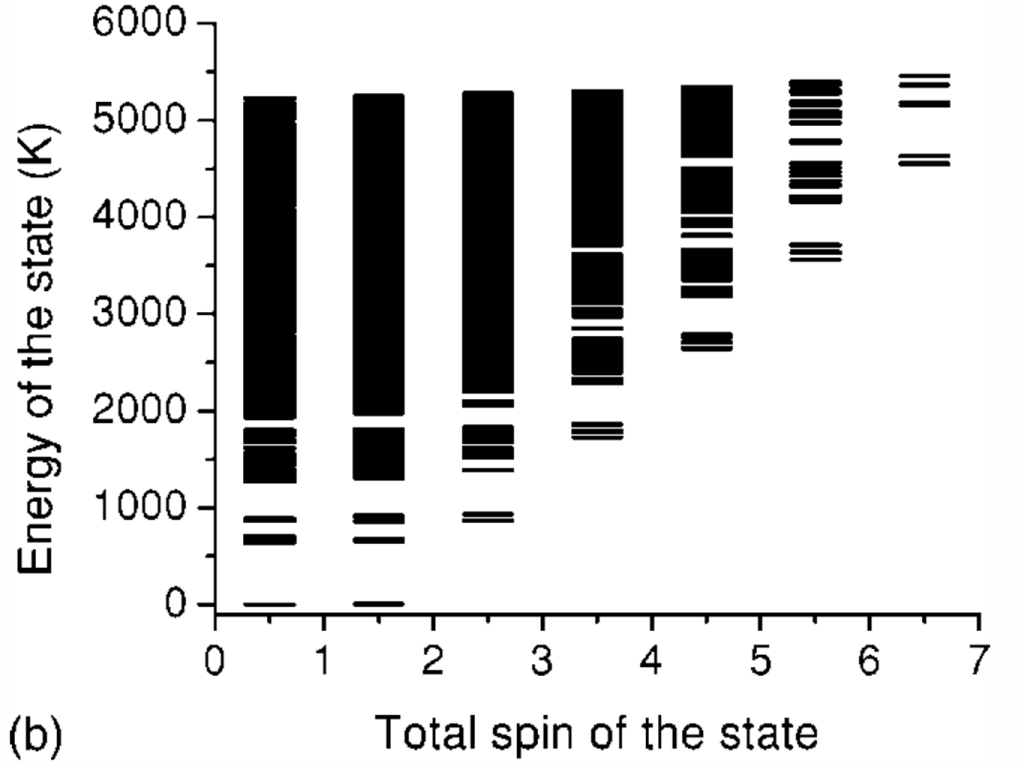
$V_{15}(K_6[V_{15}As_6O_{42}(H_2O)]\cdot 8H_2O)$

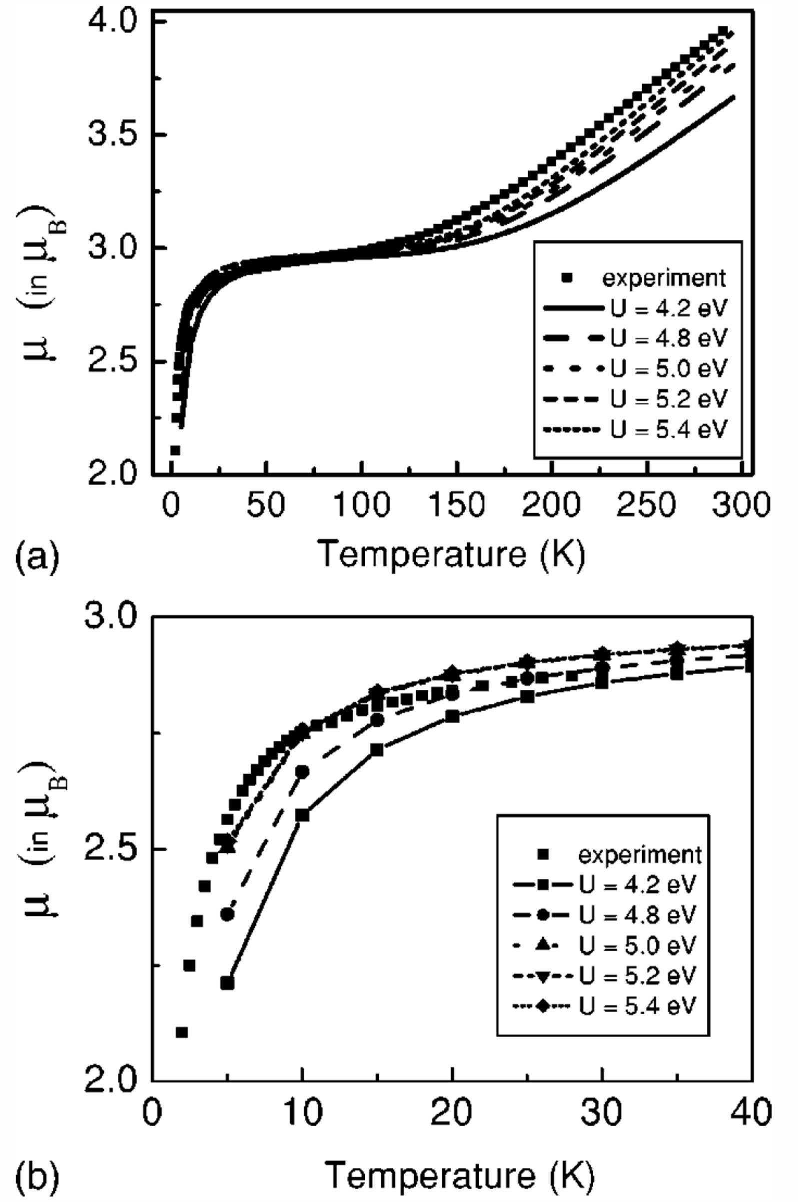




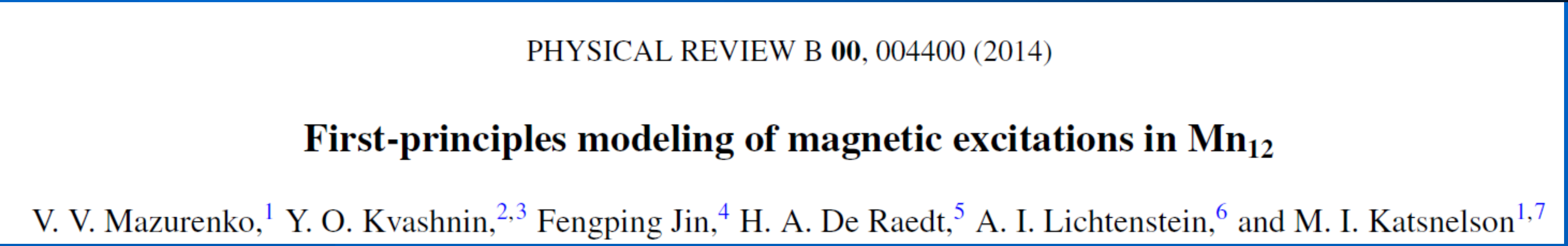
Microscopic calculations

Exact diagonalization for Heisenberg model





Mn_{12}: full calculations

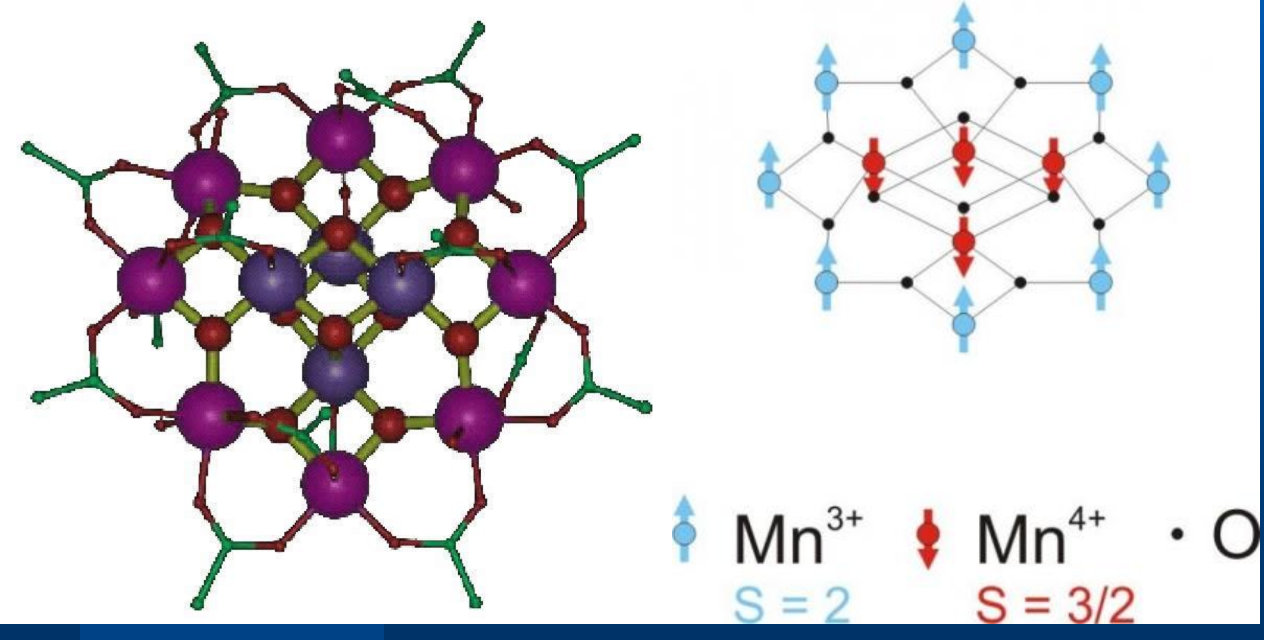


PHYSICAL REVIEW B **00**, 004400 (2014)

First-principles modeling of magnetic excitations in Mn_{12}

V. V. Mazurenko,[1] Y. O. Kvashnin,[2,3] Fengping Jin,[4] H. A. De Raedt,[5] A. I. Lichtenstein,[6] and M. I. Katsnelson[1,7]

Motivation



The prototype molecular magnet

Dimension of Hilbert space:

$(2\times2+1)^8(2\times3/2+1)^4=10^8$

A real challenge!

$[Mn_{12}O_{12}(CH_3COO)_{16}(H_2O)_4]\cdot 2CH_3COOH\cdot 4H_2O$

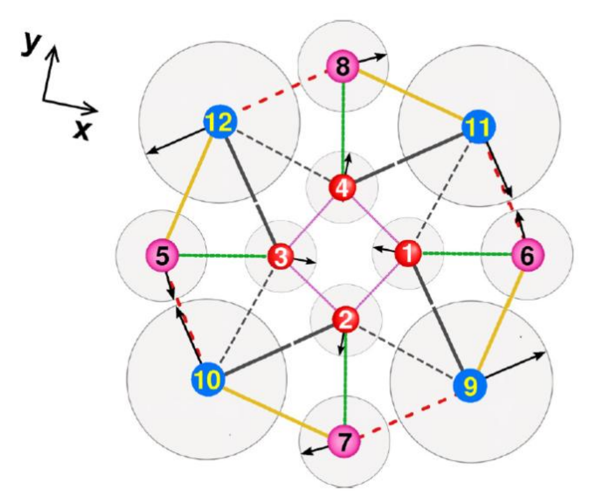
Mn_{12}: full calculations II

Inelastic netron scattering data: cannot be explained without strong DM interactions (MIK, Dobrovistki & Harmon, PRB 1999)

Eight-spin model: S = ½ dimers from S=2 and S=3/2
Dimensionality of Hilbert space decreases to 10^4
Cannot be justified quantitatively!

Full LDA+U calculations plus Lanczos ED

$$\hat{H} = \sum_{ij} J_{ij} \hat{\vec{S}}_i \hat{\vec{S}}_j + \sum_{i\mu\nu} \hat{S}_i^{\mu} A_i^{\mu\nu} \hat{S}_i^{\nu} + \sum_{ij} \vec{D}_{ij} [\hat{\vec{S}}_i \times \hat{\vec{S}}_j]$$



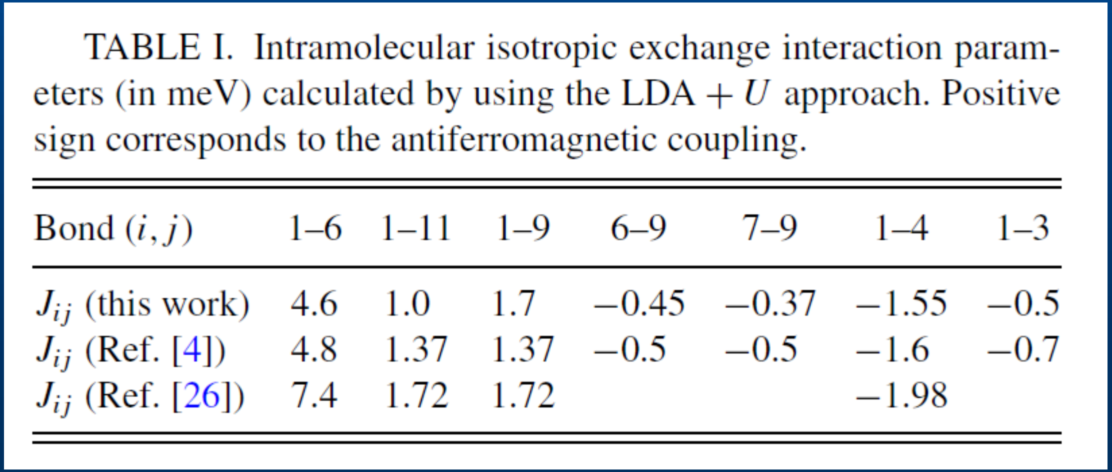


TABLE I. Intramolecular isotropic exchange interaction parameters (in meV) calculated by using the LDA + U approach. Positive sign corresponds to the antiferromagnetic coupling.

Bond (i, j)	1–6	1–11	1–9	6–9	7–9	1–4	1–3
J_{ij} (this work)	4.6	1.0	1.7	−0.45	−0.37	−1.55	−0.5
J_{ij} (Ref. [4])	4.8	1.37	1.37	−0.5	−0.5	−1.6	−0.7
J_{ij} (Ref. [26])	7.4	1.72	1.72			−1.98	

Mn$_{12}$: full calculations III

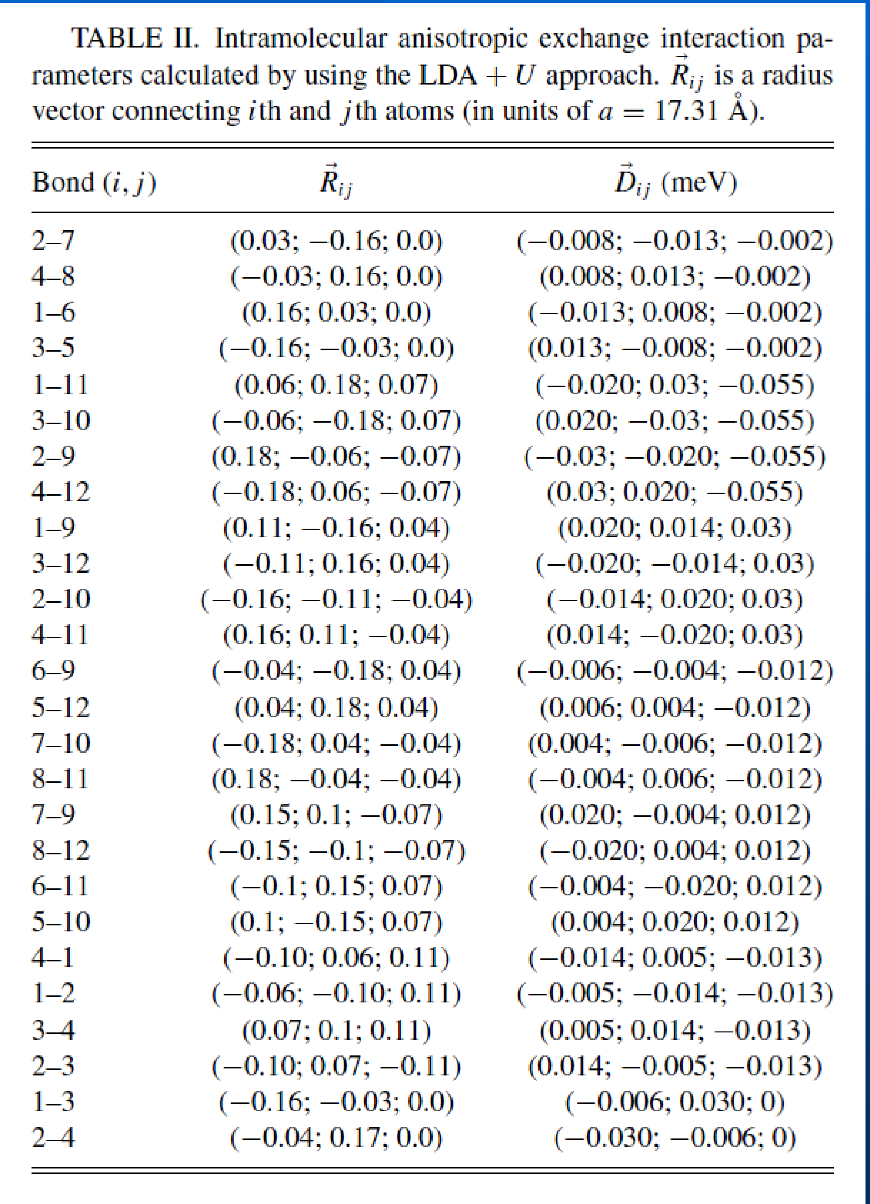


TABLE II. Intramolecular anisotropic exchange interaction parameters calculated by using the LDA + U approach. $\vec{R}_{ij}$ is a radius vector connecting ith and jth atoms (in units of $a = 17.31$ Å).

Bond (i, j)	$\vec{R}_{ij}$	$\vec{D}_{ij}$ (meV)
2–7	(0.03; −0.16; 0.0)	(−0.008; −0.013; −0.002)
4–8	(−0.03; 0.16; 0.0)	(0.008; 0.013; −0.002)
1–6	(0.16; 0.03; 0.0)	(−0.013; 0.008; −0.002)
3–5	(−0.16; −0.03; 0.0)	(0.013; −0.008; −0.002)
1–11	(0.06; 0.18; 0.07)	(−0.020; 0.03; −0.055)
3–10	(−0.06; −0.18; 0.07)	(0.020; −0.03; −0.055)
2–9	(0.18; −0.06; −0.07)	(−0.03; −0.020; −0.055)
4–12	(−0.18; 0.06; −0.07)	(0.03; 0.020; −0.055)
1–9	(0.11; −0.16; 0.04)	(0.020; 0.014; 0.03)
3–12	(−0.11; 0.16; 0.04)	(−0.020; −0.014; 0.03)
2–10	(−0.16; −0.11; −0.04)	(−0.014; 0.020; 0.03)
4–11	(0.16; 0.11; −0.04)	(0.014; −0.020; 0.03)
6–9	(−0.04; −0.18; 0.04)	(−0.006; −0.004; −0.012)
5–12	(0.04; 0.18; 0.04)	(0.006; 0.004; −0.012)
7–10	(−0.18; 0.04; −0.04)	(0.004; −0.006; −0.012)
8–11	(0.18; −0.04; −0.04)	(−0.004; 0.006; −0.012)
7–9	(0.15; 0.1; −0.07)	(0.020; −0.004; 0.012)
8–12	(−0.15; −0.1; −0.07)	(−0.020; 0.004; 0.012)
6–11	(−0.1; 0.15; 0.07)	(−0.004; −0.020; 0.012)
5–10	(0.1; −0.15; 0.07)	(0.004; 0.020; 0.012)
4–1	(−0.10; 0.06; 0.11)	(−0.014; 0.005; −0.013)
1–2	(−0.06; −0.10; 0.11)	(−0.005; −0.014; −0.013)
3–4	(0.07; 0.1; 0.11)	(0.005; 0.014; −0.013)
2–3	(−0.10; 0.07; −0.11)	(0.014; −0.005; −0.013)
1–3	(−0.16; −0.03; 0.0)	(−0.006; 0.030; 0)
2–4	(−0.04; 0.17; 0.0)	(−0.030; −0.006; 0)

Plus anisotropy tensors…

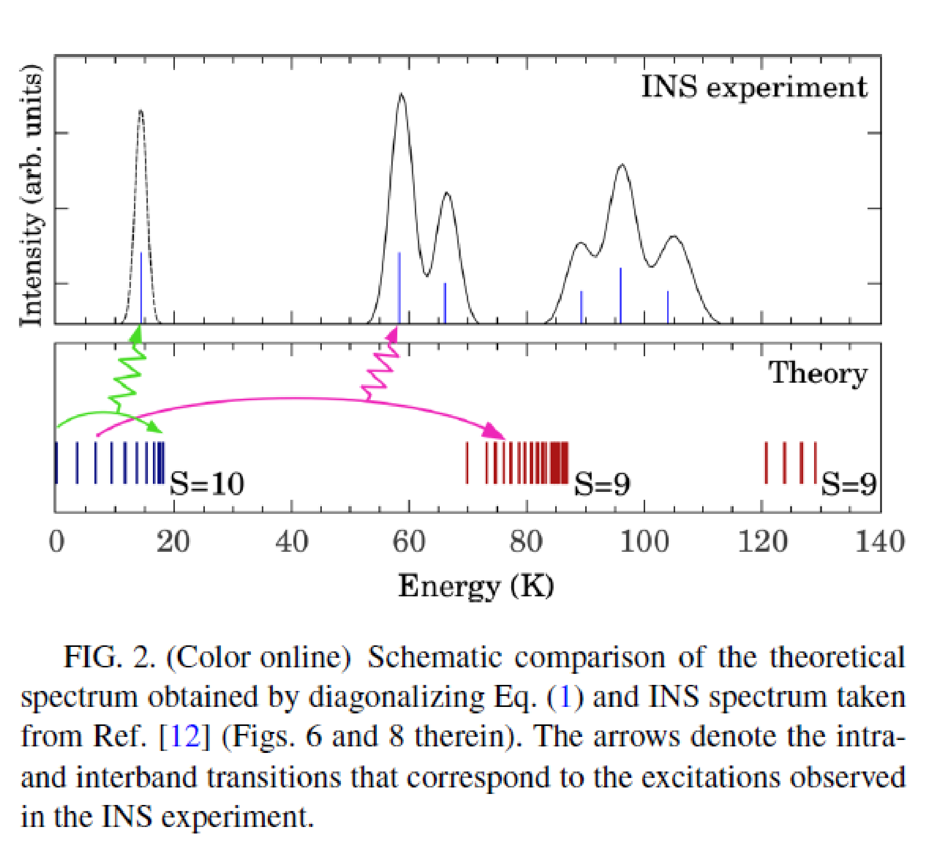
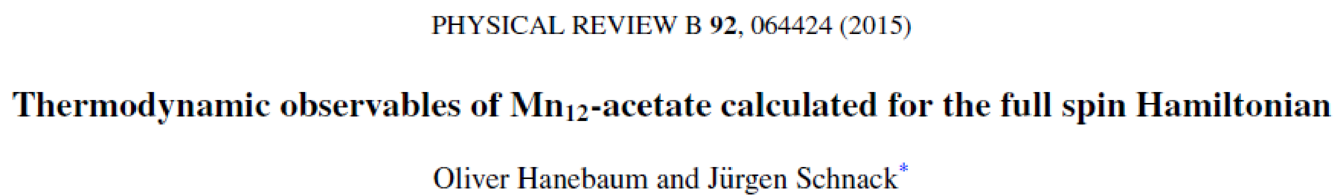


FIG. 2. (Color online) Schematic comparison of the theoretical spectrum obtained by diagonalizing Eq. (1) and INS spectrum taken from Ref. [12] (Figs. 6 and 8 therein). The arrows denote the intra- and interband transitions that correspond to the excitations observed in the INS experiment.

No fitting parameters at all – not so bad!

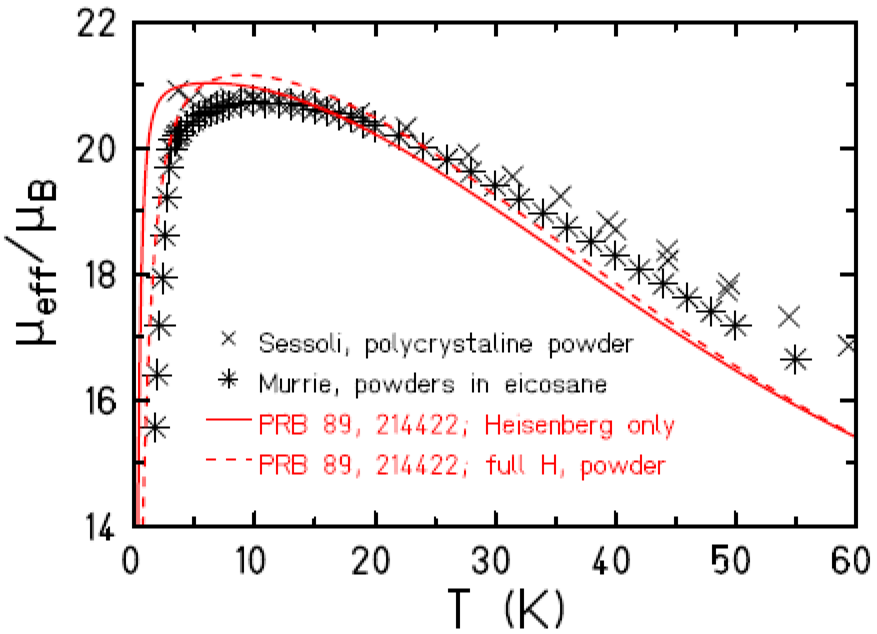
Mn_{12}: full calculations IV

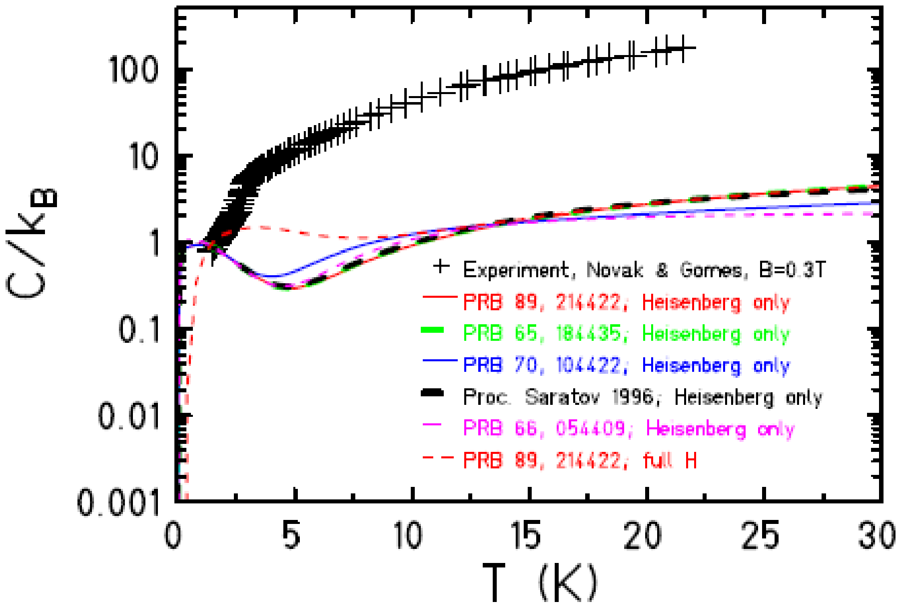


PHYSICAL REVIEW B **92**, 064424 (2015)

Thermodynamic observables of Mn_{12}-acetate calculated for the full spin Hamiltonian

Oliver Hanebaum and Jürgen Schnack*





Also, thermodynamic quantities can be calculated

To conclude

Starting from the laws of quantum mechanics, step by step, we can calculate successfully magnetic properties of real materials

Perspective: combining with novel machine learning based approaches one can use these data to search novel magnetic materials better than existing (e.g., without expensive rare earths)

MANY THANKS FOR YOU ATTENTION