

**ELECTRONIC STRUCTURE AND MAGNETISM IN
COMPLEX MATERIALS**

WASHINGTON, DC, USA

26 – 28 JULY 2000



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Conference on Electronic Structure and Magnetism in Complex Materials

Final Report

The Conference on Electronic Structure and Magnetism in Complex Materials was held on July 26-28, 2000, at Georgetown University. There were 85 participants from across the US, Asia, Europe, and South America. About 40 talks and 30 posters were presented on topics including magnetic semiconductors, oxides, half metallic materials, magnetic molecules, non-collinear magnetism, spin transport, and electronic correlation and magnetism. No proceedings were published. The book of abstracts distributed to participants is enclosed.

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Welcome to the First Washington Conference on Electronic
Structure of Complex Materials:

ELECTRONIC STRUCTURE AND MAGNETISM IN COMPLEX MATERIALS

WASHINGTON, DC, USA

26 – 28 JULY 2000

All activities are on the campus of Georgetown University:

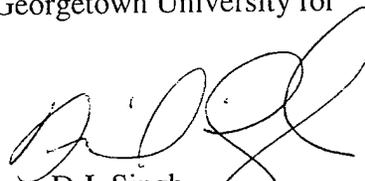
- Registration is in the lobby of the Reiss Science Building.
- Oral Sessions are in Reiss Science Building, Room 103.
- Poster Session and Reception, July 26 at 6:00 PM in the ICC Galleria, adjacent.
- Conference Dinner, July 27 at 6:45 PM in the ICC Galleria, followed by the Conference Lecture.
- Lunch is on the fifth floor of the Reiss Science Building.

July 25, 2000

Dear Participants,

We would like to welcome you to Washington D.C. and thank you for your participation in the 1st Washington Conference on Electronic Structure of Complex Materials (ESCM 2000). The conference is organized by the Center for Computational Materials Science of the Naval Research Laboratory in cooperation with the Physics Department of Georgetown University. This year's event focuses on the microscopic theory of magnetism. We hope that you will find the program interesting and your interactions with other participants fruitful. We wish to thank the members of the organizing and advisory committees and especially Georgetown University for offering their campus to host this event.


D.A. Papaconstantopoulos,
Co-Chair


D.J. Singh,
Co-Chair

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Wednesday, July 26, 2000

Time	Speaker	Title
08:30	Liu, Papaconstantopoulos, Serene, Singh	Welcome & Conference Opening
08:45	Session 1: S. Satpathy, Chair	
08:45	G.M. Stocks	Constrained local moment states for spin dynamics of itinerate magnets
09:30	I.V. Solovyev	Band theory of magnetic interactions in perovskite manganites
10:05	A. Moreo	Giant cluster coexistence in doped manganites: an explanation
10:40	Coffee Break	
11:00	Session 2: I. Solovyev, Chair	
11:00	T.A. Kaplan	Spin waves and non-Stoner continuum states in ferromagnetic-metal manganites
11:25	V. Antropov	Current problems in ab-initio description of properties of non-collinear magnets
11:50	S.V. Halilov	Low-lying magnetic excitations on the basis of density functional theory
12:15	Lunch Break	
13:30	Session 3: O.K. Andersen, Chair	
13:30	L. Nordstrom	Calculations of spin wave spectra within an unconstrained magnetization functional method
14:05	H. Eschrig	Density functional theory of low temperature phase diagrams: magnetism in the $[\text{Fe}(\text{Mn})]_{(1-x)}\text{Al}_x$ system
14:40	Poster Preview	2 minute poster previews
15:25	Coffee Break	
15:45	Session 4: A.J. Freeman, Chair	
15:45	H.J.F. Jansen	Calculation of magnetocrystalline anisotropy in transition metals
16:20	L.M. Sandratskii	Noncollinear spin and orbital magnetism in Uranium compounds
16:45	B.R. Cooper	Dependence of the magnetic properties of trivalent uranium on chemical environment: from spatially-random to periodic-random to periodic-magnetic-lattice magnetic ordering
17:10	T. Oguchi	Electron theory of magnetic properties of uranium chalcogenides
17:35	Break	
18:00	Poster Session and Reception	

ID #	Poster Authors	Poster Title
P1	C. Ashman, J. Kortus, M.R. Pederson and S.N. Khanna	Magnetic properties of mixed transition metal clusters
P2	Y.H. Chang and C.H. Park	First-principles study of compensation in p-type DMS GaMnAs
P3	L. Didukh, V. Didukh, Yu. Skorenkyy and O. Kramar	Ferromagnetism and antiferromagnetism in narrow-band model: taking into consideration interatomic interactions and correlated hopping
P4	L. Didukh, V. Hankevych, Yu. Skorenkyy and Yu. Dovhopyaty	Metal-insulator transition in antiferromagnetic narrow-band materials
P5	M. Eisenbach and B.L. Gyorffy	States of orientation along a magnetically inhomogeneous nano wire
P6	J. Enkovaara, A. Ayuela, R.M. Nieminen and L. Nordstrom	First principles calculation of magnetic anisotropy in Ni ₂ MnGa
P7	M.J. Graf and A.V. Balatsky	Identifying the pairing state of Sr ₂ RuO ₄
P8	M. Guerrero and R.M. Noack	Ground state ferromagnetism in the one-dimensional d-p and periodic Anderson models
P9	D.W. Hess	Density functional theory for lattice models and exchange-correlation potentials for spin-polarized systems
P10	H. Kaiju, T. Komine and K. Shiiki	Study of spin tunneling magnetoresistive effect by first principles band calculation
P11	M.V. Kapustyany, V.B. Kapustyanyk, E.N. Khatsko, M.I. Kobets, V.A. Pashchenko and A.I. Kaplienko	Phase transitions in the low-dimensional magnet NH ₂ (CH ₃) ₂ MnCl ₃ X2H ₂ O
P12	K. Knopfle, L.M. Sandratskii and J. Kubler	Spinspiral groundstate of gamma-iron
P13	J. Kortus and M.R. Pederson	Magnetic and vibrational properties of the uniaxial Fe ₁₃ O ₈ cluster
P14	J. Kortus and M.R. Pederson	Electronic and magnetic structure of the V ₁₅ molecular magnet
P15	P.M. Marcus and S.L. Qiu	Antiferromagnetism in Chromium
P16	N. Marzari and D.J. Singh	Electronic structure and transport in ferromagnetic La _{1+x} Sr _{2-x} Mn ₂ O ₇
P17	I.I. Mazin and D.J. Singh	Magnetism and superconductivity in ruthenates
P18	N.Y. Moghadam, G.M. Stocks, M. Kowalewski and W.H. Butler	Magnetic structure of Ni-rich Ni-Ta and Ni _{0.8} Fe _{0.2} -Ta alloys
P19	S. Mukherjee and R.E. Cohen	Non-collinear spins in FCC and HCP Fe
P20	N. Noginova, A.A. Vevkin, G.B. Loutts and E. Gillman	Hopping conductivity and high electric field transport phenomena in manganese oxide single crystals and CMR films
P21	D.A. Papaconstantopoulos, M.J. Mehl, I.I. Mazin, N.C. Bacalis, M. Lach-hab and W.E. Pickett	Precise tight-binding description of ferromagnetic and paramagnetic cobalt, nickel and iron
P22	J.E. Pask and D.J. Singh	Structural, electronic and magnetic properties of MnO
P23	V. Perebeinos and P.B. Allen	Self-trapped hole and excitons in LaMnO ₃ : Frank-Condon vibrational broadening of optical and photoemission spectra
P24	S. Satpathy, H. Meskine and H. Konig	Orbital ordering and exchange interaction in the manganites
P25	K. Sengupta	Spin/Charge quantum Hall effect in superconducting Sr ₂ RuO ₄
P26	A.K. Setty, B.R. Cooper and D.L. Price	Theoretical and computational studies of structural phase transitions in elemental plutonium
P27	A.I. Shick, W.E. Pickett and A.I. Liechtenstein	Ground state and excitations in gamma-Ce from correlated band theory
P28	D.J. Singh, I.I. Mazin, P. Blaha and K. Schwarz	Electronic structure of NaCo ₂ O ₄ and heavy Fermion LiV ₂ O ₄
P29	J. Xie and S.P. Chen	First principles calculation of As diffusion in Si
P30	I. Zutic, S. Das Sarma and O.T. Valls	Spin-polarized transport in conventional and unconventional superconductors

Thursday, July 27, 2000

Time	Speaker	Title
08:30	Session 5: B. Harmon, Chair	
08:30	H. Ohno	Ferromagnetism and heterostructures of magnetic III-V semiconductors
09:15	T.C. Schulthess	On the ferromagnetic interactions in Mn doped III-V semiconductors
09:40	A.H. MacDonald	Theory of $\text{III}_{1-x}\text{Mn}_x\text{V}$ semiconductor ferromagnetism
10:15	Coffee Break	
10:35	Session 6: B.M. Klein, Chair	
10:35	M. van Schilfgaarde	Exchange interactions in Mn-doped GaN and GaAs
11:00	C.S. Hellberg	Correlation induced magnetism in the Sn/Ge surface
11:35	R.E. Cohen	Metal-insulator transitions and energetics of FeO and CoO at high pressures within LDA+U
12:00	Lunch Break	
13:15	Session 7: J. Serene, Chair	
13:15	A.I. Lichtenstein	Electronic structure and magnetism of correlated systems: beyond the LDA
13:50	M. Jarrell	The dynamical cluster approximation
14:15	S. Savrasov	Electronic structure calculations with DMFT
14:40	N. Kioussis	Development of magnetism in strongly correlated electron systems: non-Kondo mechanism for moment collapse
15:05	Coffee Break	
15:30	Session 8: P.B. Allen, Chair	
15:30	M.R. Pederson	Anisotropy barriers and spin-tunneling fields of nanoscale magnets
16:05	G.T. Yee	Molecule-based ferromagnets, ferrimagnets, metamagnets and spin-glasses
16:30	A.J. Epstein	Organic magnets - chemistry and physics
16:55	S.N. Khanna	Measuring cluster magnetic moments without magnetic experiments
17:20	S. Blugel	Magnetism of two-dimensional itinerant antiferromagnets on a triangular lattice
17:45	T. Momoi	Magnetization plateaus of two dimensional frustrated antiferromagnets
18:10	Break	
18:45	Conference Dinner	
20:00	G.A. Prinz	Conference Lecture

Friday, July 28, 2000

Time	Speaker	Title
08:30	Session 9: J. Freericks, Chair	
08:30	W.E. Pickett	Coexisting superconductivity and magnetism: the novel case of $\text{RuSr}_2\text{GdCu}_2\text{O}_8$
09:15	I.I. Mazin	Fermiology and spin-polarized tunneling
09:50	W.H. Butler	Spin dependent tunneling conductance of Fe MgO Fe sandwiches
10:15	Coffee Break	
10:35	Session 10: K. Hathaway, Chair	
10:35	L. Szunyogh	Theoretical investigation of magnetotransport of Co and $\text{Ni}_x\text{Fe}_{1-x}$ related spin valves
11:00	B. Nadgorny	Spin dependent transport in real systems
11:25	S. Cottenier	Hyperfine fields and local relaxations for impurities in bcc Fe an FLAPW study
11:40	S.L. Qiu	Magnetic phases of Mn and Fe and the epitaxial Bain path
12:05	Lunch Break	
13:20	Session 11: C. Park, Chair	
13:20	V.V. Dobrovitski	Statistical coarse-graining as an approach to multiscale problems in magnetism
13:45	R.F. Sabiryanov	Magnetic properties of Co clusters embedded in Cu matrix
14:10	A. Ayuela	Electronic properties in magnetic Heusler alloys: Ni_2MnGa
14:35	Coffee Break	
14:50	Session 12: D. Papaconstantopoulos, Chair	
14:50	O.K. Andersen	3rd generation muffin tin orbitals of arbitrary order
15:20	D. Hobbs	Fully unconstrained noncollinear magnetism within the projector augmented wave method
15:45	O. Heinonen	A fully parallelized pseudopotential code for noncollinear magnetic systems
16:10	O.N. Mryasov	Magnetic interactions in the vicinity of extended lattice defects: examples of calculations for para, soft and hard magnets
16:35		Conference Closing

Wednesday, July 26

Oral Sessions

Reiss Science Building
Room 103

- | | |
|-------|--|
| 08:30 | Conference Opening |
| 08:45 | Session 1: Stocks, Solovyev, Moreo |
| 11:00 | Session 2: Kaplan, Antropov, Halilov |
| 13:30 | Session 3: Nordstrom, Eschrig, Poster Preview |
| 15:45 | Session 4: Jansen, Sandratskii, Cooper, Oguchi |

Constrained Local Moment States for Spin Dynamics of Itinerant Magnets

G.M. Stocks
Oak Ridge National Laboratory

Abstract not available.

Band theory of magnetic interactions in perovskite manganites

I. V. Solovyev

JRCAT - Angstrom Technology Partnership,
1-1-4 Higashi, Tsukuba, Ibaraki 305-0046, Japan;

Institute of Metal Physics, Russian Academy of Sciences,
Ekaterinburg GSP-170, Russia

I will discuss the main trends in the behavior of magnetic interactions in colossal magnetoresistive perovskite manganites $R_{1-x}D_x\text{MnO}_3$, using both the first-principles band structure calculations in the local-spin-density approximation and the simplified tight-binding analysis for the e_g electrons. In a number of cases, the tight-binding model can be treated analytically, that provides a clear physical picture underlying the calculations. Particularly, I will emphasize the importance of the double-exchange physics and the two-fold degeneracy of the e_g levels.

I will consider the following problems.

(i) Magnetic interactions in the homogeneous ferromagnetic state of the cubic manganites: the nearest-neighbor double-exchange and superexchange contributions; the longer-range interactions and the characteristic shape of the low-temperature spin-wave dispersion; the volume-dependence of magnetic interactions [1].

(ii) The anisotropy of double-exchange interactions induced by the antiferromagnetic spin ordering: the origin of the A- and C-type antiferromagnetic states; the canted spin states; the doping-dependence of magnetic interactions and the phase diagram [2].

(iii) The ferromagnetic zigzag chains and properties of the so-called "charge ordered" state in half-doped manganites [3]. I will argue that many low-temperature properties of these compounds can be readily explained from the viewpoint of a peculiar zigzag antiferromagnetic ordering. Particularly, the anisotropy of magnetic interactions in the double-exchange limit explains the local stability of the antiferromagnetic state. The two-fold degeneracy of e_g levels plays a very important role in the problem and is responsible for the insulating behavior, as well as for the appearance of the orbital ordering in the double-exchange picture.

I am grateful to K. Terakura, Z. Fang and P. Mahadevan for their contribution to this work.

The work is partly supported by NEDO.

[1] I. V. Solovyev and K. Terakura, Phys. Rev. Lett. **82**, 2959 (1999).

[2] Z. Fang, I. V. Solovyev, and K. Terakura, Phys. Rev. Lett. **84**, 3169 (2000).

[3] I. V. Solovyev and K. Terakura, Phys. Rev. Lett. **83**, 2825 (1999).

Giant cluster coexistence in doped manganites: an Explanation

Adriana Moreo, Department of Physics
Florida State University
Tallahassee, FL 32306, U.S.A.

Computational studies of models for manganese-oxides show the generation of large coexisting metallic and insulating clusters with *equal* electronic density, in agreement with the recently discovered micrometer-size inhomogeneities in manganites. The clusters are induced by disorder on exchange and hopping amplitudes near first-order transitions of the non-disordered strongly-coupled system. The random-field Ising model illustrates the qualitative aspects of these results. Percolative characteristics associated with large variations in resistivity are natural in this context. The conclusions are general and apply to a variety of compounds.[1] The mixed phase state observed here complements the electronic phase separation proposed before.[2] Together these results illustrate the key role of intrinsic inhomogeneities in manganites.

[1] A. Moreo et al., cond-mat/9911448, to appear in PRL.

[2] A. Moreo, S. Yunoki and E. Dagotto, Science, Vol.283, page 2034-2040 (1999).

Spin Waves and Non-Stoner Continuum States in Ferromagnetic-metal Manganites

T. A. Kaplan, S. D. Mahanti and Yen-Sheng Su
Michigan State University
East Lansing, MI 48824

Early theories of ferromagnetic metals like Fe, Ni, yielded a picture of the magnetic elementary excitations, namely spin waves (or magnons) and Stoner continuum states. The latter were called "single-particle" excitations, and were commonly plotted along with the magnons, both involving a single spin flip from the ferromagnetic ground state. The energy vs. translational quantum number (k) plot shows a low-lying single branch (spin wave) that begins at zero energy at $k = 0$, rising as k^2 at small k . At $k = 0$ there is also a positive energy, E_s , which broadens into a continuum with increasing k (Stoner states). E_s is essentially the splitting between the up- and down-spin bands. At large enough k , the spin wave branch crosses into the continuum, acquiring a finite lifetime. A closely related picture of the ferromagnetic-metal *manganites* has been presented recently.¹ The essential difference is that the conduction electron bandwidth is much narrower than that in the early theories, leading to a very large splitting of the up-spin and down-spin bands, and in fact to the half-metallic state. (The splitting in the standard double exchange (DE) model is proportional to the Hund's rule exchange, strength j). Then the Stoner continuum lies high above the complete magnon branch out to the Brillouin zone boundary, implying that there is no magnon damping in such a purely electronic model.¹

While the large splitting of the up- and down-spin bands is correct, the picture of an isolated magnon branch with no continuum nearby is fundamentally incorrect for the manganites. Exact calculations² on finite systems within the DE model in the single-spin-flip channel, where $j \rightarrow \infty$ (and therefore the energies of the Stoner states $\rightarrow \infty$), reveal not only spin wave states, but also a quasi-continuum of states which have *finite* energy (thus the term "non-Stoner"). Although for the finite systems studied, the bottom of this continuum lies somewhat above the magnon energies, extrapolation suggests that in the thermodynamic limit the continuum will overlap the magnon energies. This gives the possibility that spin waves will show damping within this purely electronic model.² Variational studies³ also found finite-energy continuum states, but their energies do not overlap the spin waves. A physical picture of these new non-Stoner states, formed from consideration of various correlation functions, will be presented, addressing in particular the question of how they differ from the magnon wave functions.

Concerning the shape of the spin wave dispersion, our calculations² showed that the DE model could not explain the softening observed⁴ at large k in various low-Curie-temperature materials. Further, there is recent strong experimental evidence that the softening is due to magnon-phonon interactions.⁴ In this connection, we are studying spin waves in modified DE models which consider orbital degeneracy and phonons, including the Jahn-Teller effect, and will report the results.

¹N. Furukawa in *Physics of Manganites*, edited by T. A. Kaplan and S. D. Mahanti, Kluwer Academic/Plenum Press, New York, 1999, pg.1.

²T. A. Kaplan and S. D. Mahanti, in *Physics of Manganites* (see ref. 1), pg. 135.

³T. Okabe, *Prog. Theor. Phys. (Japan)* 97, 21 (1997).

⁴P. Dai et al, cond-mat/99044372, 26 Apr 1999; to appear in *Phys. Rev. B*, April 1, 2000.

Current problems in ab-initio description of properties of non-collinear magnets

Vladimir Antropov, Ames Lab
Ames, IA, USA

I will discuss the current problems in area of electronic structure description of magnets with general non-collinear orderings. These problems can be classified in three groups: search for non-collinear ground state, physics of domain and domain walls and thermal and dynamic effects. In spite of great success of density functional approximation there many cases when it fails to describe both ground state and excited state properties. In many recent publications these difficulties have been ignored leading to the controversial results. I will show several possible ways to avoid these difficulties. At the end the first results for the electronic structure and magnetic properties of domain walls in hard magnets including defects will be discussed. The way how to connect electronic structure and model simulations of magnetization processes in materials with domain walls in case of different strong magnets (CoPt, Nd-Fe-B, R-Co) will be demonstrated.

Low-lying magnetic excitations on the basis of Density Functional Theory

Halilov S.V.

NIST, Gaithersburg, MD, and School of Physics, Georgia Institute of Technology, Atlanta, GA
Electron Physics Group, 100 Bureau Dr Stop 8412, NIST, Gaithersburg 20899-8412

Perlov A.Y.

Max Planck Institute for Physics of Complex Systems, D-01187 Dresden, Germany

Eschrig H.

Institute for Solid State and Materials Research, D-01171 Dresden, Germany

The adiabatic theory of low-lying magnetic excitations, which are driving for thermodynamics at low temperatures, is developed on the basis of spin density functional theory (SDFT)[1]. The central assumption considers a fast electronic and a slow magnetic time-scale, and postulates negligible correlation of the fast motion between different ionic sites, which allows to introduce the concept of adiabatic magnetic moments formed by the itinerant electrons and to construct effective adiabatic spin Hamiltonian suitable for generally non-Heisenberg systems. The wavenumber dependent exchange force constants are obtained from SDFT calculations with constrained moment directions, what is similar to determination of the *static* spin susceptibility.

The parameter-free calculated magnon spectra for Fe, Co, and Ni show a very close conformity to the experimental data available only at low magnon energies. In the case of Fe, they show strong Kohn anomalies, especially at higher energies, where however only limited experimental evidence (because of poor resolution) could be established. Using Planck statistics at low temperature, the temperature dependence of the = magnetization is well described up to half the Curie temperature. It is conjectured = that correlated local moment clusters survive the Curie transition.

The treatment of magnon dynamics in heavy rare earth (RE) metals Gd through Tm rests on a pseudocore description of the Russel-Saunders state of the local open $4f$ shell [2]. This state sets up a spin and orbital polarization of the f shell and a spin-orbit coupling between both. The f -orbital polarization couples to the crystal field, which introduces anisotropy. The f spin-polarization exchange couples to the conduction-electron spin.

It is shown that the account of the on-site coupling, that is a possible noncollinearity of conduction electron and f spins at the same site, have strong influence on magnon spectra. The magnon energies get remarkably softer, especially at the upper part of the spectra, where the f spin moments do not follow the fast motion of the conduction-electron site spin moments anymore.

The obtained magnon spectra are in semi-quantitative agreement with experimental data, where the latter are available. Main sources of discrepancy might be incomplete knowledge of the crystal field parameters and the neglect of intersite correlations of the fast conduction electron motion. Essential part of these problems might be solved within an all-electron approach.

- [1] S.V.Halilov, H.Eschrig, A.Y.Perlov, and P.M.Oppeneer, Adiabatic spin dynamics from spin density functional theory: Application to Fe, Co, and Ni, Phys. Rev. B, **58**, 293 (1998)
- [2] A.Y.Perlov, S.V.Halilov, and H.Eschrig, Rare earth magnetism and adiabatic magnon spectra, Phys. Rev. B **61**, 4070 (2000)

Calculations of Spin Wave Spectra within an Unconstrained Magnetization Functional Method

L. Nordstrom

Physics Department, Uppsala University
75105 Uppsala, Sweden

Based on spin density functional theory in combination with an adiabatic approximation for the spin dynamics, spin wave spectra have been calculated for various ferromagnets. Since our calculational scheme, in contrast to standard non-collinear methods, treats the magnetization density as a vector field which is free to change both in magnitude as well as direction throughout space, the calculated resonance energies have a natural spread. This distribution of the magnon excitations is in accordance with the broadened magnon peaks found in neutron scattering experiments. The obtained results will be analyzed in terms of Stoner excitations as well as Kohn anomalies, and compared to experiments and other calculations. As examples, the calculated spectra from weak and strong ferromagnets will be compared and the differences analyzed with help of the calculated electronic structure.

**Density functional theory of low temperature phase diagrams:
Magnetism in the $[\text{Fe}(\text{Mn})]_{(1-x)}\text{Al}_x$ system**

Helmut Eschrig

IFW Dresden, P.O.Box 27 00 16, D-01171 Dresden, Germany

Klaus Koepnik

Max Planck Institute CPFS, D-01187 Dresden, Germany

The full-potential nonorthogonal local-orbital minimum-basis band-structure scheme (FPLO) [1] is very well fit to combine with the generalized Blackman-Esterling-Berk coherent-potential approximation (CPA) [2] into a highly precise charge and spin self-consistent approach to total energies of substitutional alloys with taking into account effects of short-range order. The main features of this approach are shortly outlined. Its FPLO part yields a precise representation of the electronic structure in terms of optimally localized (by means of total energy minimalization) orbitals, and the CPA part uses a pseudo-spin technique to cast the tight-binding CPA into a scattering formulation largely equivalent to the single-site Korringa-Kohn-Rostoker CPA, but very flexible with respect to structures and short-range correlations.

The approach is applied to a number of phases of the Al-Fe and the Al-Fe-Mn phase diagram, for which total energies are calculated as functions of concentrations and of magnetic order. By adding the entropy of static disorder rudimentary low temperature phase diagrams are calculated, which reproduce a number of features of the experimental phase diagrams quite well. The interplay of magnetic order and chemical short-range correlations can be understood on the basis of these results.

[1] K. Koepnik and H. Eschrig, *Phys. Rev.* **B59**, 1743 (1999).

[2] K. Koepnik, B. Velický, R. Hayn, and H. Eschrig, *Phys. Rev.* **B55**, 5717 (1997); **B58**, 6944 (1998).

Calculation of Magnetocrystalline Anisotropy in Transition Metals

Henri J.F. Jansen
Oregon State University
Dept. of Physics, Corvallis, OR 97331

Magnetocrystalline anisotropy of magnetic materials is an important property. Magnetic multilayers with perpendicular anisotropy are important materials with applications in data storage. The fabrication of these complex materials is not straightforward, and guidance by theory would be useful. The problem is, however, that even for the basic transition metals iron, nickel, and cobalt the physical origin of magnetocrystalline anisotropy is not well understood. The numerical calculation of the small energy difference between crystals magnetized along the easy and hard axis is very demanding. The convergence properties of the k -space integrals are different compared with the case of the calculation of structural energies. Given sufficient integration points, however, all methods converge to the same result, as we have shown using a realistic tight-binding model. The results of standard local density calculations do not agree with experiment, and additional correlation effects have to be considered. We have also studied the sensitivity of the magnetocrystalline anisotropy with respect to changes in the parameters in the tight-binding Hamiltonian, in order to simulate changes in the chemical environment. The surprising result is that for certain changes in tight-binding parameters large changes in the anisotropy energy are observed, without any visible change in the band structure. Almost all of k -space contributes to the change in energy, showing that magnetocrystalline anisotropy should really be described in a real space manner. The convergence in real space, however, is also slow because of the oscillations caused by the discontinuity in k -space at the Fermi surface.

Noncollinear Spin and Orbital Magnetism in Uranium Compounds

L.M. Sandratskii

Institut für Festkörperphysik, Technische Universität
D-64289 Darmstadt, Germany

Numerous Uranium compounds possess a noncollinear magnetic structure. The physical interactions responsible for the noncollinearity of are analyzed on the basis of the first-principles calculations and symmetry arguments. The noncollinear ferromagnets U_3X_4 ($X=P,As,Sb$) and UFe_4Al_8 and noncollinear antiferromagnets U_2Pd_2Sn , $UPdSn$ and $UPtGe$ are considered. Special attention is given to the UFe_4Al_8 where two different types of the noncollinearity are obtained both experimentally and theoretically. Possibility of the formation of a spiral structure in a strongly relativistic systems is discussed by the example of the unique magnetic structure of $UPtGe$.

It is shown that the spin-orbit coupling is crucial for the appearance of the noncollinearity of the magnetic structure. Additionally it is shown that the hybridization of the U states and the states of other atoms is essential for the noncollinearity of the magnetic structure in a number of compounds. The last property allows to use the noncollinearity of the magnetic structure as indirect measure of the hybridization of the U 5f and other electron states.

An unusual physical mechanism of the magnetic anisotropy is suggested to explain the magnetic anisotropy in UFe_4Al_8 . It is based on the dependence of the induced magnetic moments on the direction of the atomic moments in the magnetic sublattice.

Close connection between the crystal structure and magnetic noncollinearity is shown. A criterion of the noncollinearity of the spin and orbital moments of the same atom is formulated.

Symmetry principles governing the formation of the magnetic structures within the density functional theory are related to the symmetry principles governing the formation of the magnetic structures within the Landau theory of phase transitions.

Dependence of the Magnetic Properties of Trivalent Uranium on Chemical Environment: From Spatially-Random to Periodic-Magnetic-Lattice Magnetic Ordering

B.R. Cooper, Dept. of Physics, West Virginia U.,
Morgantown, WV 26506-6315, U.S.A.

O. Vogt, J. Lohle, and K. Mattenberger, Lab. Fur Festkorperphysik,
ETH, CH 8093, Zurich, Switzerland

The magnetic properties of actinide compounds are intermediate between rare earth-like localized-moment and transition-metal-like itinerant-electron magnetism. These properties are of great fundamental and technological interest. Fundamentally, studying the variation of magnetic behavior of uranium in varying chemical environment, especially in comparison with cerium in the same range of chemical environments, provides a unique, systematic way to gain understanding of the development of transition-shell magnetic properties, i.e. the heart of magnetism. Technologically, these properties, and their change in time, provide valuable diagnostic information on the physical and chemical state and environment of nuclear fuels and wastes. Use of the experimental variation of behavior, in comparison with predictive theory, for the series of monpnictides and monochalcogenides provides an experimentally and conceptually elegant way systematically to study a very wide range of chemical environments and magnetic consequences in a crystallographically simple isostructural (NaCl-structure) sequence. The monpnictides $UX(X=N,P,As,Sb,Bi)$ and monochalcogenides $UY(Y=S,Se,Te)$ all provide U-U spacing above the Hill limit so that the magnetic ordering is basically localized-moment behavior, but differs significantly from being truly atomistic, i.e. heavy rare-earth-like, because of remaining weak, but significant, band (ligand)- f hybridization. The pnictides, X, are trivalent and the chalcogens, Y are always divalent, so we have the following bonding, $U^{3+}X^{3-}$ and $U^{3+}Y^{2-}+e^-$. The behavior and the influence of the excess unbound electron, is of special interest. The number of such unbound electrons can be systematically varied by forming the pseudobinaries $UX_{1-x}Y_x$, or by partially replacing the trivalent uranium by tetravalent thorium (for the pnictides, each thorium introduces one excess electron). By replacing U with nonmagnetic La or Y we obtain magnetic dilution; the band electron hybridization per uranium $5f$ electron is increased, but no extra electrons are introduced. Our ab-initio-based calculations predict a range of behavior from spatially-random localized-moment magnetic ordering at the relatively-most-hybridizing US end to conventional periodic-magnetic-lattice behavior with almost the full trivalent moment at the least-hybridizing UBi end. (In pure US, we predict that only half the sites, randomly located, have localized trivalent moments.) Comparison with the experimental ordered moments strongly supports this systematic progression across the combined monpnictide-monochalcogenide series. The theoretical model is further supported by the prediction and validating observation of a high-temperature susceptibility of modified Curie-Weiss form $\chi=C/(T-\theta) + \chi_0$, where as predicted, the temperature-independent χ_0 is very low for the pnictides and high for the chalcogenides.

Electron Theory of Magnetic Properties of Uranium Chalcogenides

Tamio Oguchi and Tatsuya Shishidou*

Hiroshima University, ADSM

1-3-1 Kagamiyama, Higashihiroshima 739-8526, Japan

Magnetic properties of cubic uranium mono-chalcogenides, UX ($X=S, Se$ and Te), are studied by means of fully-relativistic electronic structure calculations. Our theory is based on the local spin-density approximation to the density functional theory. One-electron Kohn-Sham equations are solved self-consistently by using the Full-potential Linear Augmented Plane Wave method with inclusion of the spin-orbit coupling as the second variation. Calculated spin and orbital magnetic moments are compared with experimental data available. It is found that the orbital moments are underestimated while the spin counterparts are slightly overestimated, resulting to underestimation of the total moments. It is shown that a Hartree-Fock type exchange potential in which spin off-diagonal elements are included in a self-consistent manner is crucial to realize the size of the orbital magnetic moments [1].

Magnetic anisotropy energy is estimated from the total energies with different magnetization directions [2]. Calculated easy and hard axes for the chalcogenides are [111] and [100], respectively, being in excellent agreement with experiment. Mechanism of the anisotropy energy is interpreted in terms of pseudo-gap formation near the Fermi energy and angular distribution of $5f$ electrons around the U atom. Systematic trends seen in the properties are discussed in detail.

* Present address: Department of Physics and Astronomy, Northwestern University, Evanston, Illinois 60208-3112.

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Wednesday, July 26

Poster Session and Reception

ICC Galleria

18:00 Poster Session

Magnetic Properties of Mixed Transition Metal Clusters

C. Ashman,¹ J. Kortus², M. R. Pederson², and S. N. Khanna¹

¹*Department of Physics, Virginia Commonwealth University, Richmond, VA 23284-2000*

²*Complex Systems Theory Branch - 6692, Naval Research Laboratory, Washington, D. C.*

20375-5000

Abstract

Atomic clusters containing two to few hundred atoms have been found to display novel magnetic properties. Clusters of ferromagnetic solids exhibit superparamagnetic relaxations while clusters of non-magnetic solids are magnetic. While these developments have generated excitement, the ab-initio theoretical studies on clusters have focussed on the magnetic moments. Actual applications involving magnetic clusters however require an understanding of the magnetic anisotropy which determines the energy barrier protecting the magnetic moment from orienting in any random direction.

Using a recently proposed approach^a to incorporate spin-orbit coupling, we shall present the ab-initio calculations of the magnetic anisotropy in pure and mixed transition metal clusters. The new approach is based on a simplified exact method to calculate spin-orbit coupling in multicenter systems. It is free of shape approximations, is independent of the choice of basis sets, and can be applied to periodic or finite systems. Using this, we shall provide the first density functional calculations of the magnetic anisotropy energy in pure Fe_n , Co_n and Fe_nCo_m clusters containing up to 6 atoms. The studies will highlight the role of size, shape and composition on this important quantity.

^aM.R. Pederson and S.N. Khanna, Phys. Rev. B **60**, 9566 (1999).

First-principles study of compensation in p-type DMS GaMnAs

Y. H. Chang and C. H. Park

Department of Physics and RCDAMP, Pusan National University
Pusan, South Korea, 609-735

During recent years much interest was focused on diluted magnetic semiconductors (DMS) based on III-V compounds such as GaMnAs and InMnAs. The reason for this interest was the fact that DMS bridge the physics of semiconductors and the physics of magnetics and bring to light a new class of magnetic materials, namely, carrier-controllable magnetic semiconductors. Moreover, (Ga,Mn)As reveals ferromagnetic behavior, not observed in bulk II-VI DMS. With the increase of hole concentrations, the III-V DMS becomes ferromagnetic. In the talk, we will discuss the electronic structure of the semiconductors and discuss what leads to the ferromagnetic transition and also compensation mechanism to the Mn-acceptor doping through first-principles pseudopotential local spin density approximation calculations.

For the calculations, we used the norm-conserving nonlocal pseudopotentials, using the approach of Troullier and Martins and Kleinman-Bylander type of fully separable pseudopotentials. The Ceperly-Alder correlation as parametrized by Perdew and Zunger is used. For simulating the alloy ratio x of the $\text{Ga}_{1-x}\text{Mn}_x\text{As}$, we tested several supercell with 8, 16 and 32 atoms supercell. We compared the total energies of the antiferromagnetic and ferromagnetic phase of GaMnAs within local spin density approximation calculations. We calculate that the ferromagnetic state of GaMnAs becomes more stable than the antiferromagnetic state by the hole carriers. We find that the d-orbitals of majority spin of Mn atoms are significantly affected by the increase of hole carrier density and the d-orbitals becomes strongly localized with the reduction of the Fermi-energy level. The hybridization between Mn-d-orbitals and As-p-orbitals are found to be significantly changed by hole carriers. We will discuss the role of Mn-interstitial defect in the compensation leading to the low doping efficiency of 15 %.

Ferromagnetism and Antiferromagnetism in Narrow-Band Model: Taking into Consideration Interatomic Interactions and Correlated Hopping

L. Didukh, V. Didukh, Yu. Skorenkyy, O. Kramar

Ternopil State Technical University

Department of Physics, 56 Rus'ka Str., Ternopil UA-46001, Ukraine

In the present work magnetic and antiferromagnetic orderings in the Hubbard model generalized by taking into account the interatomic exchange interaction, interatomic Coulomb interaction and correlated hopping in partially filled narrow band are considered. Expressions for the magnetization, Curie and Neel temperatures as functions of model parameters and deviation from half-filling are obtained. Conditions of ferromagnetic state realization are found. The obtained results indicate the important role of correlated hopping.

The expressions for Curie temperature as functions of model parameters are found for the cases of strong and weak intra-atomic Coulomb interaction. In the case of strong intra-atomic Coulomb interaction correlated hopping is shown to be the factor favouring ferromagnetism in more than half-filled band. In the case of weak intra-atomic Coulomb interaction the role of correlated hopping is considered. In less than half-filled band correlated hopping leads to the stabilization of ferromagnetism as well as inter-atomic exchange interaction and intra-atomic Coulomb interaction. If band is more than half-filled correlated hopping can lead to the destabilization of ferromagnetism. On the basis of obtained results experimental data on $\text{Fe}_x\text{Co}_{1-x}\text{S}_2$ where electron concentration in doubly degenerate e_g -band of $3d$ -electrons changes from 0 to 1 and $\text{Co}_x\text{Ni}_{1-x}\text{S}_2$ where this concentration changes from 1 to 2 can be explained, in particular, we explain the unusual dependence of Curie temperature on concentration of localized magnetic moments $\text{Fe}_x\text{Co}_{1-x}\text{S}_2$ at $0.75 < x < 1$.

The possibility of coexistence of antiferromagnetically ordered and charge-ordered phases in narrow-band model is considered (this situation is observed in Magneli phases of vanadium). Expression for Neel temperature at partial filling dependent on energy parameters and band filling is calculated. The obtained results can explain the observed Neel temperature of Magneli phases of vanadium in charge-ordered state.

Metal-Insulator Transition in Antiferromagnetic Narrow-Band Materials

L. Didukh, V. Hankevych, Yu. Skorenkyy, Yu. Dovhopyaty

Ternopil State Technical University

Department of Physics, 56 Rus'ka Str., Ternopil UA-46001, Ukraine

In the present work we study metal-insulator transition in the systems $\text{NiS}_{2-x}\text{Se}_x$ and $(\text{V}_{1-x}\text{Cr}_x)_2\text{O}_3$. Narrow $3d$ -band of these compounds is considered within frames of a generalized Hubbard model with correlated hopping at half-filling by means of two-pole approximation [1]. The quasiparticle energy spectrum and width of energy gap as functions of the model parameters and temperature are calculated. The conditions for metallic and insulating states realisation are found. In particular, at zero temperature in a paramagnetic phase we find the condition of vanishing of energy gap as a function of $w = z|t|$, $\tilde{w} = z|\tilde{w}|$, $\tilde{t} = t + 2T$; z is the number of nearest-neighbors to a site, t is the hopping integral, T is the correlated hopping integral. The energy gap increases with increasing temperature, i.e. the system can undergo transition from a metallic state to an insulating one. We show that in generalized Hubbard model with correlated hopping metal-insulator transition occurs at smaller temperatures than in the Hubbard model. The obtained results indicate the important role of correlated hopping.

The approach which allows to describe transition from paramagnetic metallic to anti-ferromagnetic insulating state is discussed. It is shown that taking into account correlated hopping which leads to the narrowing of subbands have essential influence on this transition.

On the basis of the obtained results experimental data on metal-insulator transition of magnetic systems $\text{NiS}_{2-x}\text{Se}_x$ and $(\text{V}_{1-x}\text{Cr}_x)_2\text{O}_3$ can be satisfactory explained. In particular, the phase diagram (pressure-temperature) of the model in a paramagnetic state is in good agreement with the experimentally found one for NiS_2 .

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States of orientation along a magnetically inhomogeneous nano wire

M. Eisenbach, B. L. Györfly
H H Wills Physics Laboratory
University of Bristol

We investigate the magnetic states of nano wires (diameter 50 – 500 Å) which consist of disc shaped magnetic segments separated by non-magnetic spacers. To describe this system we propose a simple classical one dimensional spin model and study its consequences. In particular we examine the ground state and thermal behaviour as function of both anisotropy of the ferromagnetic discs and thickness of the non magnetic spacer. We find a rich structure of possible ground states and a temperature driven reorientation of the magnetic moments in various regions of the parameter space.

We shall also report on our investigation of the above system in terms of an itinerant model based on mobile electrons and their spins. The Hubbard like model investigated here incorporates the dipolar interaction between the magnetic moments at different sites, and we are able to calculate the shape anisotropy of a disc in the Hartee-Fock approximation of our itinerant model. For increasing strength of the dipolar interaction we see a deviation of the total energy of these discs from the behaviour predicted by a fixed moment classical Heisenberg like model.

First Principles Calculation of Magnetic Anisotropy in Ni₂MnGa

J. Enkovaara, A. Ayuela, R. M. Nieminen

Laboratory of Physics, Helsinki University of Technology

P.O.B. 1100, FIN-02015 HUT, Finland

L. Nordström

Condensed Matter Theory, Uppsala University

P.O. Box 530, S-751 21 Uppsala, Sweden

Magnetic shape memory (MSM) alloys are materials which can undergo deformations of several percents upon application of an external magnetic field. Compared to the conventional shape memory effect, where the deformations are obtained by heating and cooling, magnetic control offers greater speed and efficiency. One key property in MSM materials is the magnetocrystalline anisotropy energy (MAE). In this work, the MAE is studied theoretically for the prototype MSM alloy Ni₂MnGa, which has the cubic L2₁ structure and undergoes a martensitic transformation to a tetragonal structure [1].

The calculations are done within the density functional theory using the full potential linearized augmented plane wave (FLAPW) method [2]. The spin-orbit interaction is included in the second variational step. According to the force theorem [3], the MAE can be calculated as a difference in the sum of the single particle energies when the magnetization is in the (001) and (110) directions. The MAE is calculated in the tetragonal structure with different ratios of the c and a lattice constants. The correct easy axis is found for the experimental c/a . As the MAE and orbital moment anisotropy are related [4], the contribution of different atoms to the MAE is discussed through the orbital moment decomposition into the atomic spheres.

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Identifying the pairing state of Sr_2RuO_4

M.J. Graf and A.V. Balatsky
Los Alamos National Lab.
Mail stop: B262
Los Alamos, New Mexico 87545

We have analyzed heat capacity and thermal conductivity measurements of Sr_2RuO_4 in the normal and superconducting state and come to the conclusion that an order parameter with nodal lines on the Fermi surface is required to account for the observed low-temperature behavior. A gapped order parameter is inconsistent with the reported thermodynamic and transport data. Guided by a strongly peaked dynamical susceptibility along the diagonals of the Brillouin zone in neutron scattering data, we suggest a spin-fluctuation mechanism that would favor the pairing state with the gap maxima along the zone diagonals (such as for a d_{xy} gap). The most plausible candidates are an odd parity, spin-triplet, f -wave pairing state, or an even parity, spin-singlet, d -wave state. Based on our analysis of possible pairing functions we propose measurements of the ultrasound attenuation and thermal conductivity in the magnetic field to further constrain the list of possible pairing states.

Ground state ferromagnetism in the one-dimensional d - p and periodic Anderson models

M. Guerrero

Theoretical Division, Los Alamos National Laboratory
Los Alamos, NM 87545

R. M. Noack

Institut de Physique Théorique, Université de Fribourg
CH-1700 Fribourg, Switzerland

Using the Density Matrix Renormalization Group, we study metallic ferromagnetism in a one-dimensional copper-oxide model which contains one oxygen p -orbital and one copper d -orbital. The parameters for the d - p model can be chosen so that it is similar to the one-dimensional periodic Anderson model. For equivalent parameters, we compare the ground-state phase diagram of the d - p model with that of the Anderson model. We find a ferromagnetic region analogous to the one found in the Anderson model, but which is pushed to somewhat higher densities and interaction strengths. In both models, we find a regime with phase separation in which there is a ferromagnetic domain separated from a region with antiferromagnetic correlations. An interpretation of the origin of this phase based on an estimation of competing energy scales is provided. We also choose a set of parameter values appropriate for copper-oxide materials and explore the ground-state phase diagram as a function of the oxygen-oxygen hopping strength and the electron density. We find three disconnected regions of metallic ferromagnetism and give physical pictures of the three different mechanisms for ferromagnetism in these phases.

Density Functional Theory for Lattice Models and Exchange-Correlation Potentials for Spin-Polarized Systems

Daryl W. Hess

Center for Computational Materials Science
Naval Research Laboratory, Washington, DC

The challenge to predict low-energy properties of materials with strong electronic correlations from first principles has inspired hybrid schemes based on a combination of ab initio density-functional theory calculations and lattice models for strongly correlated systems. A method for determining the bare interaction parameters of the lattice model is to require that both models agree on electronic properties calculated using the same theoretical approximation. Using a two-band Hubbard model, I explore an exact density-functional theory and the density-functional theory with a local approximation for the exchange-correlation potential. Calculations of exchange-correlation potentials in a corresponding local approximation are presented and compared for paramagnetic and spin polarized systems. Unlike continuum ab initio calculations for which LDA eigenvalues often provide a good approximation for true quasiparticle energies, the eigenvalues for lattice models are in significantly poorer agreement with true quasiparticle energies. The eigenvalues of exact density-functional theory are generally in much better agreement. The difference may reflect the rapid variation of density on nearest-neighbor lattice sites and the likely greater importance of the frequency dependence (relative to momentum dependence) of the self-energy for lattice as compared with that for continuum models.

Study of spin tunneling magnetoresistive effect by first-principle band calculation

Hideo Kaiju, Takashi Komine, and Kazuo Shiiki
Department of Applied Physics and Physico-Informatics,
Faculty of Science and Technology, Keio University,
3-14-1 Hiyoshi, Kohoku, Yokohama 223-8522, Japan

Spin tunneling magnetoresistive (TMR) effects in ferromagnetic metal / insulator / ferromagnetic metal tunnel junctions have attracted much attention. Although a great progress has been made in experiences, there remain some unsolved problems: the tunnel conductance was estimated using the density of states (DOS) at the Fermi level for bulk ferromagnetic metal and the transmission coefficient based on the free-electron model. In our study, first-principle band structure calculation of Fe / insulator / Fe has been performed by using the LMTO-ASA method in order to elucidate the TMR effect. The calculated system of supercell consists of Fe₅ / insulator₂ / Fe₅ /vacancy₄ with the bcc(001) deposited, where vacancy means an atom sphere which has no atomic nucleus and the insulator is assumed to be a vacancy atom with varying barrier height. The transmission coefficient has been evaluated as a ratio of total charge at Fermi level between the insulator and the interfacial Fe atom. The tunnel conductance can be evaluated as the products of the transmission coefficient and the DOS at the Fermi level for each spin channel for both of interfacial Fe atoms. Our calculations show that the DOS for the interfacial Fe atom is different from that for the bulk Fe. An important feature of the spin-polarized DOS of the interfacial Fe atom is that since the up-spin d-bands are filled but the down-spin d-bands are not filled, the DOS at the Fermi level for the down-spin electrons is much larger compared to the up-spin electrons. As a result, the tunnel conductance increases with increasing barrier height because the DOS at the Fermi level for the down-spin electrons of the interfacial Fe atom increases. Also, magnetic moment of the interfacial Fe atom decreases with increasing barrier height. The transmission coefficient for each spin is different and decreases with increasing barrier height. In conclusion, it has been found that the TMR ratio in Fe / insulator / Fe increases with increasing barrier height, which is consistent with experimental results.

Phase transitions in the low-dimensional magnet $\text{NH}_2(\text{CH}_3)_2\text{MnCl}_3 \times 2\text{H}_2\text{O}$

M.V. Kapustyanyk, V.B. Kapustyanyk
Lviv Franko National University
Lviv, UA-79005, Ukraine

E.N. Khatsko, M.I. Kobets, V.A. Pashchenko and A.I. Kaplienکو
B.I. Verkin Physicotechnical Institute of Low Temperatures
Kharkiv, UA-310164, Ukraine

Considerable interest has been aroused in recent years by low-dimensional organometallic compounds of transitional metals having a number of unusual magnetic properties. In this work we present the results of study of phase transitions (PTs) in the crystals of $\text{NH}_2(\text{CH}_3)_2\text{MnCl}_3 \times 2\text{H}_2\text{O}$ (DMA- MnCl_3). It is shown that this compound belongs to the space group $C2/c$. The manganese atom in the crystal has an octahedral surrounding consisting of four chlorine atoms and two oxygen atoms from the water molecules. The octahedron is considerably distorted due to different types of atoms surrounding Mn. The manganese ions form zigzag chains through common Cl(1) atoms along the c -axis. The octahedral chains form the layers (100). The chlorine atoms Cl(2) and Cl(3) from adjoining octahedral chains in the layer are "joined" through H -bonds of the protonized aminogroup. The interaction between adjacent layers is due to Van der Waals contacts between the methyl groups of dimethylamine. Such a layered structure is reflected in magnetic properties.

The magnetic susceptibility $\chi(T)$ was measured by the Faraday method in the temperature range 2-300 K. It has been found that lowering of temperature leads to a PT in the magnetically ordered state and to a susceptibility anisotropy characteristic of an antiferromagnet. The magnetic ordering temperature, determined from the point of inflection on the $\chi_a(T)$ curve, is $T_N = 7 \pm 0.5$ K. A comparison with the theoretical models indicates that the experimental results are in better agreement for a chain than for a square lattice. Therefore, one can conclude that DMA- MnCl_3 has a one-dimensional magnetic structure. Such a conclusion is in agreement with the crystal structure. Preliminary measurements at $T = 0.7$ K show that for a magnetic field orientation parallel to the a -axis, the magnetization undergoes a jump at $H_{sf} = 14$ kOe due to spin-flip transition, while no $M(H)$ anomalies are observed along the other two axes. An estimate of the exchange interaction field from the slope of the curve $M(H)$ above the spin-flop transition gives the value $2H_e = 354$ kOe, which is in good accord with the value $J/k = -2.4$ K obtained from the measurement of static magnetic susceptibility. Experiments carried out on the magnetization and magnetic susceptibility fail to provide vital information on weak interactions between layers or chains in DMA- MnCl_3 . Consequently, antiferromagnetic resonance (AFMR) measurements were carried out. The frequency-field dependence of AFMR is reconstructed at $T = 4.2$ K, and effective fields of exchange interaction and anisotropy are determined; a subthreshold two-magnon absorption is detected.

On the basis of dielectric, dilatometric and spectral investigations of DMA- MnCl_3 the structural changes and lattice dynamics at higher temperatures were analyzed. It was shown that this crystal undergoes the PTs at $T = 300, 235$ and 180 K.

Spinspiral groundstate of γ -iron

K. Knöpfle, L.M. Sandratskii and J. Kübler

Institut für Festkörperphysik, Technische Universität, D-64289 Darmstadt, Germany

Using density functional theory we calculate the magnetic groundstate properties of γ -Fe for a large set of spiral vectors and lattice constants. The effective single-particle equations are solved by means of an advanced version of the augmented spherical waves (ASW) method which takes into account the full-shape potential and the intra-atomic noncollinearity of the magnetization. Together with the generalized gradient approximation (GGA) the experimentally determined spiral magnetic groundstate is, for the first time, reproduced successfully. Symmetry properties of the intra-atomic noncollinearity of the magnetization are analyzed and illustrated for spiral magnetic structures. We conclude that γ -Fe is an itinerant electron system possessing well defined atomic moments.

Electronic and magnetic structure of the V_{15} molecular magnet

Jens Kortus and Mark R. Pederson

Center for Computational Materials Science

Naval Research Laboratory, Washington, DC 20375

The system $K_6[V_{15}As_6O_{42}(H_2O)] \cdot 8H_2O$ has a crystallographically imposed trigonal symmetry with three sets of nonequivalent vanadium atoms. The three sets of the vanadium atoms define two hexagons separated by a triangle of vanadiums. Due to the layered structure the V_{15} cluster shows interesting magnetic properties. We report density-functional based studies of the electronic structure and magnetic anisotropy energy in dependence of different magnetic couplings between the vanadium atoms. The state with spin $S=3/2$ is found to have the lowest total energy. The magnetic anisotropy barrier is small with only 1.5K. The total energy of the V_{15} cluster with spin $S=1/2$ is nearly degenerate with the spin $S=3/2$ state, which is only 8 meV lower in energy. In case of the $9/2$ spin configuration we found the total energy 0.784 eV higher than the spin $3/2$ state. The magnetic anisotropy barrier is still small with 1.6K. For the ferromagnetic state ($S = 15/2$) we obtain for all V atoms local moments of $1 \mu_B$ within a sphere of 1.32 \AA radius. The anisotropy barrier changed only slightly to 1.85K. This state is also higher in energy than the $3/2$ spin state by 0.72 eV.

Magnetic and vibrational properties of the uniaxial Fe_{13}O_8 cluster

Jens Kortus and Mark R. Pederson
Center for Computational Materials Science
Naval Research Laboratory, Washington, DC 20375

We present all-electron density-functional-based calculations on a recently synthesized iron oxide Fe_{13}O_8 cluster. The Fe_{13}O_8 cluster shows a complicated magnetic structure, with several magnetically stable ferro-, ferri- and antiferromagnetic states. The most stable state is a ferromagnetic state with a total moment of $32 \mu_B$ per cluster. We report a systematic investigation of the electronic and magnetic structure of different magnetic states. For the most stable ferromagnetic state we calculate the magnetic anisotropy barrier and the complete vibrational spectra including IR and Raman intensities calculated from density functional theory.

Antiferromagnetism in Chromium

P. M. Marcus, IBM Research, Yorktown Hgts., NY 10598
S. L. Qiu, Florida Atlantic University, Boca Raton, FL 33431

Chromium has a weak antiferromagnetic (AF) ground state of unusual structure. This ground state is a consequence of two special features of the Cr electronic structure. The first feature, which has long been known, is a sensitivity to periodic potentials of particular direction and long wavelength determined by the nesting properties of the Cr Fermi surface. The second feature, which has become known from recent first-principles total-energy calculations¹, is an unusual nearness of the volume at which a second-order transition to a bcc AF phase takes place to the volume of the nonmagnetic (NM) lowest energy bcc state. The two special features combine to produce an AF ground state with a strained bcc atomic cell and a magnetic cell about 20 lattice constants long in which the weak AF moments are modulated at the wavelength corresponding to the nesting. The basic mechanism of this unusual ground state is expansion of the lattice to make the lowest energy bcc state an AF state, and modulation of the AF moments at the nesting wavelength to lower the energy and more than compensate the strain energy of the expansion. This spin density wave (SDW) ground state, balanced between volume strain and moment modulation, makes Cr volume sensitive, which explains many properties of Cr that are puzzling without the second feature. Thus the weakness of the AF moment is due to the rapid rise of strain energy at larger moments, which cannot be compensated by the SDW. The strong effect of pressure in reducing the Néel temperature is due to rapid reduction of the AF moment as volume is reduced. However, the persistence of the SDW at high pressures is due to the rise in the bulk modulus as the transition volume of the second-order transition is approached. The negative thermal expansion at low temperatures is explained by the existence of two energy minima, the SDW ground state and a lower-volume higher-energy minimum in the NM unstrained state. The decrease in volume on rising through the Néel temperature and loss of all atomic moments is explained by a return to the lower-volume NM state when the SDW is broken up. The effect of increasing electron density by adding Mn impurity, which produces a commensurate bcc AF phase, is explained by the shift of the transition volume to the AF phase to below the volume of the NM minimum. However, decreasing the electron density by adding V shifts the transition to larger volumes with more strain energy, which the SDW cannot compensate and Cr becomes NM. Similarly, although Mo has a Fermi surface with nesting properties like Cr, it remains NM because the transition to an AF phase occurs at large volume and high strain energy, which cannot be compensated by an SDW.

¹P. M. Marcus, S. L. Qiu and V. L. Moruzzi, *J. Phys.: Condens. Matter* **29**, 6541 (1998)

Electronic structure and transport in ferromagnetic $\text{La}_{1+x}\text{Sr}_{2-x}\text{Mn}_2\text{O}_7$

Nicola Marzari

Department of Chemistry, Princeton University
Princeton, NJ 08544

David J. Singh

Center for Computational Materials Science, Naval Research Laboratory
Washington, D.C. 20375-5345

Density functional calculations are used to investigate the magnetic order, electronic structure and from these transport coefficients as a function of doping for the layered manganites, $\text{La}_{1+y}\text{Sr}_{2-y}\text{Mn}_2\text{O}_7$ with an emphasis on the ferromagnetic magnetoresistive phases near $y = 0.2$. The electronic ground state for the ferromagnetic state is close to half-metallic, with small, probably localized, minority spin pockets analagous to those found in previous studies of perovskite colossal magnetoresistive manganites. The effects of variations in the doping level and La-Sr cation disorder are addressed using virtual crystal and rigid band models from which transport functions are calculated. These results are discussed in relation to transport and photoelectron spectroscopic measurements.

Magnetism and Superconductivity in Ruthenates

I.I. Mazin and D.J. Singh
Center for Computational Materials Science
Naval Research Laboratory
Washington, D.C. 20375

Ru based perovskites are known to have variegated magnetic properties. Both 3D and 2D subfamilies include ferromagnetic (FM), antiferromagnetic (AFM), and nonmagnetic compounds (NM), some of them being metallic and insulating. Superconductivity was found in one member of the 2D family, Sr_2RuO_4 . It is believed to be triplet, and induced by FM spin fluctuations. A popular interpretation of the magnetism in ruthenates uses the same concept as in cuprates, namely Hubbard-type strong Coulomb correlations. In this concept, the ground state of a ruthenate is defined by the competition between the hopping t and the Hubbard U . This interpretation, however, has difficulty explaining ferromagnetism in such materials as SrRuO_3 , and the fact that an extremely 2D Sr_2RuO_4 appears to be one of the least correlated. A litmus paper for the strong correlations always was failure of the mean-field LDA calculations to provide accurate descriptions of the corresponding material, as for instance in cuprates. However, for ruthenates, including AFM and insulators, LDA seems to work about as well as for typical conventional material (An interesting case of Ca_2RuO_4 , which occurs in several different structures with different properties, is somewhat different from other ruthenates, and will be discussed separately). In particular, it does yield AFM solutions for the two AFM ruthenates where the crystal structure is sufficiently well known. The reason for magnetism appears to be typical Stoner. Tendency to FM is due to the role of oxygen, and is stronger in 3D than in 2D, and the tendency to AFM appears due to a Fermi surface nesting. Numerical estimates give for Sr_2RuO_4 AFM spin fluctuation at $q \approx (2\pi/3, 2\pi/3)$ (recently confirmed by neutron scattering) comparable to, or even stronger than, the FM ones. This fact has important implications for superconductivity: there are *two* competing superconducting states, p -wave, and d -wave. The former, being gapped everywhere, enjoys a larger range of stability in the parameter space than the latter, and current experiments do indeed point to a p -wave state.

* Supported by the Office of Naval Research

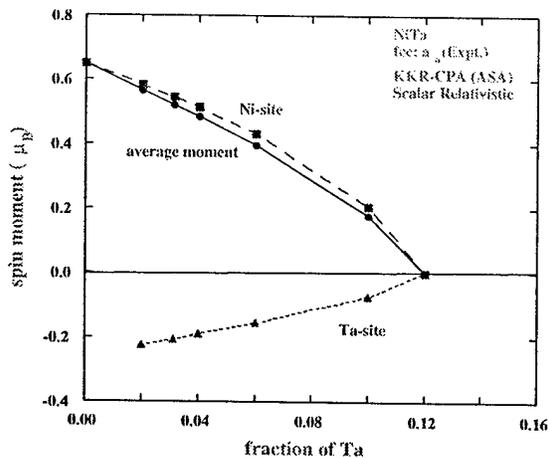
Magnetic structure of Ni-rich Ni-Ta and Ni_{0.8}Fe_{0.2}-Ta alloys

Nassrin Y. Moghadam, G. M. Stocks, M. Kowalewski, W. H. Butler

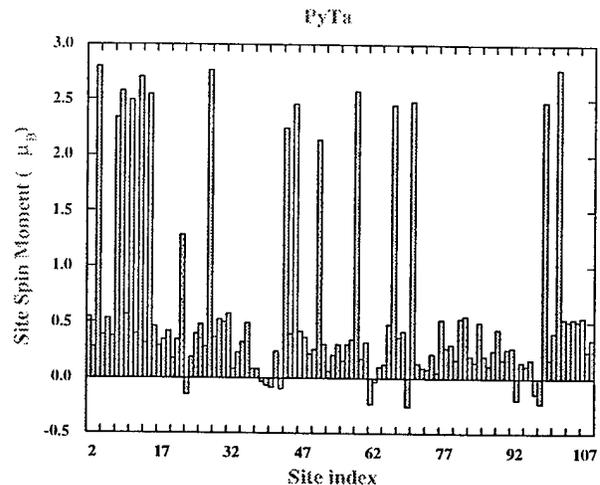
Metals & Ceramics Division

Oak Ridge National Laboratory, Oak Ridge, TN 37831-6114

Tantalum is widely used as seed and cap layers in Magnetic Random Access Memory (MRAM) devices. The magnetic part is typically thin layers of permalloy, an alloy of 80% Ni and 20% Fe. Tantalum is used to promote the growth of the Giant Magneto Resistance (GMR) layers and also to prevent damage to the substrate during the patterning of the memory cells. However, Ta has deleterious effects on the magnetic properties. Measurements of the magnetic moment of Ta/permalloy/Ta films carried out by Kowalewski et al (J. of Appl. Phys., **87**, 15 Apr., 2000) show that Ta is primarily responsible for the magnetic dead layers observed in MRAM devices. Theoretical studies of Ni-rich Ni-Ta alloys using the KKR-CPA method show that the average magnetic moment vanishes at 12% Ta. Similar studies of the effects of Ta on moment formation in permalloy using supercell models show large fluctuations and suppression of moments on Ni sites. Suppression is larger on Ni sites close to Tantalum. The moments on Fe sites are less suppressed and the fluctuations are smaller.



Spin moment as a function of concentration of Ta in Ni-Ta alloy. The average magnetic moment vanishes at 12% Ta.



Site spin moment for Ni_{0.8}Fe_{0.2}-Ta alloy using a supercell containing 108 atoms. Moments on Ni sites show significant fluctuation and reduction in their magnitude. Moments on Fe sites are reduced less. A negative moment is induced on Ta sites.

Non-collinear Spins in FCC and HCP Fe

Sonali Mukherjee and R.E. Cohen
Carnegie Institution Of Washington
Washington DC 20015-1305

Although the equilibrium crystal structure of Fe is Ferromagnetic BCC, at higher temperatures it is known that there is a phase transition to FCC Fe. The magnetic properties of FCC Fe has been studied intensely for the understanding of its stability and also because it shows complex magnetic behavior depending on its volume including the anti-Invar effects. Previous electronic structure calculations with collinear spins have shown that AFM states become more stable as compared to the FM states as the volume is reduced (C.S. Wang, B.M. Klein, and H. Krakauer, Phys. Rev. Lett. 1852(1985)). Experiments also reported the coexistence of low-spin antiferromagnetic and high-spin ferromagnetic states (D. Pescia et al, Phys. Rev. Lett. 2126(1987)). But recent experiments (Y. Tsunoda, J.Phys.: Condens. Matter 1, 10427 (1989)) and LDA based electronic structure calculations (M. Uhl et al, Phys. Rev. B 291 (1994), O.N. Mryasov et al, Phys. Rev. B 12330 (1992)), are providing evidence of the existence of non-collinear spins in FCC Fe. A clear picture is emerging where there is a gradual transition in FCC Fe from a low volume non-magnetic state to a high volume collinear Ferromagnetic state with the intermediate state being non-collinear with the magnetic moments increasing continuously throughout the transition. Our aim is to capture the magnetic correlations in FCC Fe and its variation with the volume using a tight-binding model. The parameters of the non-magnetic part of the model are obtained from the tight-binding model developed by Cohen, Mehl and Papaconstantopoulos (R.E. Cohen et al, Phys. Rev. B 8575 (1997)), which has an accuracy comparable to self-consistent calculations and has been able to reproduce correctly the compression, electronic structure, phase relations in Fe. The spin dependent part of the hamiltonian is modeled by a Stoner like approach. We find that our model exhibits the gradual transition from a non-magnetic state at a low volume to a collinear Ferromagnetic state at a high volume, with the intermediate states being non-collinear. In future we plan to extend our studies to finite-temperatures using tight-binding Molecular-dynamics. Moreover we would like to study the role of non-collinear spins for HCP Fe. At pressures around 13GPa BCC Fe undergoes phase transition to HCP Fe. Theoretical calculations have shown that magnetism plays an important role in stabilizing the HCP phase, (Gerd Steinle-Neumann et al, Phys. Rev. B 791 (1999)). Though antiferromagnetism brings the values of equilibrium volume and bulk modulus close to the experimental volume, as compared to non-magnetic HCP Fe, theoretical values of AFM FE are still 27 % off. We want to study if non-collinear spins are the underlying cause of HCP Fe.

Hopping conductivity and high electric field transport phenomena in manganese oxide single crystals and CMR films.

N. Noginova, A.A. Verevkin*, G. B. Loutts, E. Gillman,
Center for Materials Research, Norfolk State University, VA
*Yale University, New Haven, CT

Comparative study of electric charge transport was performed in CMR films of $\text{La}_{0.75}\text{Sr}_{0.25}\text{MnO}_3$ and $\text{LaGa}_{1-x}\text{Mn}_x\text{O}_3$ single crystals, with the relative concentration of Mn ions varying from 0% to 50%. Temperature dependence of the resistivity in steady state can be described adequately by the hopping model with the values of the activation energy and the resistivity coefficient strongly dependent on the concentration of Mn ions. Current-voltage (I-V) curves demonstrated strong nonlinearity with increase of the current. Non-monotonous I-V characteristics with switching to the low resistivity state at high currents were observed in $\text{LaGa}_{1-x}\text{Mn}_x\text{O}_3$ crystals. In contrast, IV of epitaxial CMR film, showed saturation of the voltage with increase of the electric current. We demonstrate quantitative agreement of the results with the small polaron hopping model taking into account heating processes as well as percolation effects, and evaluate the charge transfer parameters.

Precise Tight-Binding Description of Ferromagnetic and Paramagnetic Cobalt, Nickel, and Iron

Dimitrios A. Papaconstantopoulos, Michael J. Mehl, and Igor I. Mazin

Center for Computational Materials Science

Naval Research Laboratory, Washington, DC 20375

Naoum C. Bacalis

Theoretical and Physical Chemistry Institute

National Hellenic Research Foundation, Athens, Greece

Mohammed Lach-hab

George Mason University, Fairfax Virginia

Warren E. Pickett

Physics Department, University of California, Davis, California

We construct transferable tight-binding parameters for ferromagnetic and paramagnetic cobalt, nickel, and iron by fitting the total energy and the electronic band structures for three crystal structures (para- and ferromagnetic bcc and paramagnetic fcc) calculated using the Linearized Augmented Plane Wave (LAPW) method using the Generalized Gradient (GGA) exchange-correlation. We use these parameters to calculate the total energy and other properties of each element in various other crystal structures. Comparisons with independent LAPW results for the structures not in the fit are excellent, suggesting that the tight-binding parameters provide a realistic physical description for any structure of the group VIII magnetic metals. We then use this Hamiltonian to describe non-collinear magnetic systems.

Structural, Electronic, and Magnetic Properties of MnO

J.E. Pask and D.J. Singh

Center for Computational Materials Science, Naval Research Laboratory
Washington, DC

We have applied the full-potential linearized augmented planewave method to the study of the structural, electronic, and magnetic properties of MnO. Using a generalized gradient approximation to exchange and correlation within the framework of density functional theory, we find the ground state to be insulating, antiferromagnetic, and of rhombohedrally distorted B1 structure with compression along the $[1,1,1]$ direction; in agreement with experiment and recent pseudopotential-based calculations. We discuss the reasons for this ground state in terms of band formation associated with the interaction of Mn and O orbitals.

**Self-Trapped holes and excitons in LaMnO₃:
Franck-Condon Vibrational Broadening of Optical and Photoemission Spectra**

Vasili Perebeinos and Philip B. Allen
SUNY at Stony Brook

Department of Physics and Astronomy
State University of New York, Stony Brook, New York 11794-3800

The ground state of LaMnO₃ has a cooperative Jahn-Teller order (orbital ordering below 750 K) and magnetic order (ferromagnetic layers coupled antiferromagnetically below 140 K). There is a very natural Hamiltonian, where only the partly filled E_g subshell of the Mn d-electrons is explicitly included. The onsite Coulomb interaction U is large and included restricting to singly occupied E_g subshells (infinite U approximation). The important terms in the Hamiltonian are hopping to nearest neighbors if spin orientation allows (the "double-exchange" Hamiltonian), and coupling of E_g electrons to oxygen displacements (the Jahn-Teller term). This Hamiltonian successfully explains both the orbital and magnetic ordering.

The Hamiltonian also makes many interesting predictions about the nature of doped-in holes and about the low-lying electronic excitations of the system. The lowest electronic excitation is a flipped orbital which traps by oxygen un-distortion, forming a self-trapped exciton. The optical spectrum should show a Franck-Condon series, a Gaussian envelope of vibrational sidebands. Existing optical measurements are given a natural reinterpretation. The sudden photohole created in the photoemission process is also a vibrationally excited state of the polaron. Therefore the photoemission spectrum in LaMnO₃ is predicted to have multiple Franck-Condon vibrational sidebands. This generates an intrinsic line broadening ≈ 0.5 eV. We find dispersion of the hole by diagonalizing in a truncated subspace, which consists of a hole on each site coupled to the vibrations of the six surrounding oxygens. Although the eigenstates have band-widths narrowed by the Huang-Rhys factor $e^{-S} \approx 10^{-3}$, nevertheless the photoemission spectral function has two peaks whose central energies ϵ_{k1} , ϵ_{k2} disperse with band width ≈ 0.4 eV. Signatures of these phenomena are predicted to appear in angle-resolved photoemission spectra. The angle-integrated spectrum is predicted to have a width of 0.9 eV, which is consistent with existing data although higher resolution data are needed to test the theory.

Orbital ordering and exchange interaction in the manganites

S. Satpathy, H. Meskine and H. König

Department of Physics & Astronomy, University of Missouri-Columbia
Columbia, MO 65211

The nature of the magnetic exchange in the manganites is clarified by examining a simple electronic model Hamiltonian for the $Mn - O - Mn$ triad. It is shown that the magnetic structure of $La_{1-x}Ca_xMnO_3$ is correctly described within an electronic mechanism involving the hopping of the $Mn(e_g)$ and $O(p)$ electrons alone, taking into account the degeneracy of the e_g orbitals and the static Jahn-Teller distortion at the Mn sites. Electron hopping involving the $Mn(t_{2g})$ orbitals is unimportant for the most part, except in situations where it can induce a ferromagnetic-to-antiferromagnet transition, for instance, as a function of the $Mn - O - Mn$ bond angle θ . Specifically, for the case of $Mn^{3+} - O - Mn^{3+}$ we find such a transition at a crossover θ_c whose magnitude depends on the Hamiltonian parameters. Contrary to the belief by some that the t_{2g} hopping should produce an AF superexchange like in the Hubbard model, we show that it is in fact ferromagnetic. Rather, the antiferromagnetism in $CaMnO_3$ originates because the antiferromagnetic arrangement favors electron hopping between the e_g and the $O(p)$ electrons and not due to the hopping of the t_{2g} electrons. All these results are obtained by exact diagonalization of the model Hamiltonian, either by direct diagonalization or by diagonalization using the Lanczos method, if the Hamiltonian is too big, and are rationalized using results of the fourth-order perturbation theory. The magnetic structures of the end members $LaMnO_3$ and $CaMnO_3$ as well as of $La_{1/2}Ca_{1/2}MnO_3$ are all described correctly within the model.

Spin/Charge quantum Hall effect in superconducting Sr_2RuO_4

K. Sengupta, H-J. Kwon, and Victor. M. Yakovenko

Department of Physics, University of Maryland, College Park, MD 20742, U.S.A.

We explore the possibility of spin/charge quantum Hall effect in unconventional superconductors like Sr_2RuO_4 with triplet p-wave pairing with broken time-reversal symmetry. The role of screening in this context is pointed out. We show that as a natural consequence of time-reversal symmetry breaking and triplet pairing, these superconductors have chiral spin-current carrying edge states. The novel spin structure of these edge states makes them distinct from their singlet d+id counterparts. We also discuss possible experiments to probe the absence/presence of bulk /edge Hall currents.

Theoretical and Computational Studies of Structural Phase Transitions in Elemental Plutonium

A.K. Setty, B.R. Cooper
(West Virginia University)

Dept. of Physics, P.O. Box 6315, Morgantown, WV 26506-6315

D. L. Price
(University of Memphis)

Department of Physics, Campus Box 526670, Memphis, TN 38152-6670

Elemental plutonium exhibits unusual sequential phase transitions and other interesting properties including an anomalously low melting point. We seek to explain this behavior in light of a novel, self-induced-disorder localization mechanism¹. The model proposes the existence of an entropy-of-disorder-driven transition from a uniformly delocalized low temperature alpha phase to a high temperature delta phase characterized by a disordered distribution of two kinds of atomic sites. These sites are associated, with equal probability, with either a localized, or a fluctuating configuration of $5f$ electrons. The existence of sites with a fluctuating configuration, and the time-varying disordered distribution of such sites and those with a localized configuration, is due to the singlet $5f$ component of the two electron site-centered ground state, which is randomly driven by hybridization to itinerancy. The existence of this form of Anderson localization has been established in earlier studies in uranium-based systems.

Several computational approaches are being followed to examine the applicability of the above picture to plutonium. By carrying out LDA and SIC-LDA full-potential LMTO calculations for both the alpha and delta phases, we have established that a delocalized alpha phase is indeed the ground state, and that there is partial delocalization in the delta phase. The equilibrium atomic volume of delta plutonium is significantly improved by the SIC-LDA calculation as compared to the LDA calculation. As orthogonality of neighboring localized states is enforced by a potential barrier in the interstitial region, the total energy in this scheme² represents an upper bound, thereby establishing the onset of localization. Refinements such as explicit orthogonalization in a supercell geometry, or using a resonant localized state³ approach are in development to eliminate an observed dependence on the barrier height. A comparison of progress in these studies, and future objectives will be presented.

1. B. R. Cooper et al, *Phil. Mag.* B 79, 683 (1999).
2. D. L. Price, *Phys. Rev. B* 60, 10588 (1999).
3. J. M. Wills and B. R. Cooper, *Phys. Rev. B* 36, 3809 (1987).

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Ground State and Excitations in γ -Ce from Correlated Band Theory

Alexander B. Shick and Warren E. Pickett
Department of Physics, University of California
Davis CA 95616

Alexander I. Liechtenstein
Department of Physics, University of Nijmegen
the Netherlands

Multiple energy minima of the LDA+U energy functional are obtained for γ -Ce when it is implemented in a full potential, rotationally invariant scheme including spin-orbit coupling, and different starting local configurations are chosen. The lowest energy solution leads to a fully spin polarized 4f state and the lattice constant of γ -Ce. We show that the higher energy local minima of the LDA+U energy functional (additional self-consistent solutions) are strongly indicative of crystal electric field and multiplet excitations.

Work supported by National Science Foundation Grant DMR-9802076, and by NSF Grant PHY-94-07194.

Electronic Structure of NaCo_2O_4 and Heavy Fermion LiV_2O_4

David J. Singh and Igor I. Mazin
Center for Computational Materials Science
Naval Research Laboratory
Washington, D.C. 20375

P. Blaha and K. Schwarz
Institut für Physik und Theoretische Chemie,
TU Wien, A-1060 Wien, Austria

Spinel structure LiV_2O_4 was recently found to be an oxide heavy Fermion metal with properties consistent in all respects with those seen in the most renormalized rare earth compounds of this type. NaCo_2O_4 , which is a layered compound having a 2D triangular lattice, also shows heavy band masses and an upturn in specific heat at low temperature, though not nearly of the magnitude seen in LiV_2O_4 . Here we report electronic structure studies of these two compounds and discuss scenarios for their properties.

LiV_2O_4 is found to be a metal with local moment magnetic character and antiferromagnetic interactions. The moments are formed from the a_g component of the V t_{2g} manifold. The remainder of the V t_{2g} orbitals participate in itinerant lighter mass bands. NaCo_2O_4 also shows magnetic instabilities in LSDA calculations, in this case of an itinerant ferromagnetic type. However, although the ground state appears to be ferromagnetic, NaCo_2O_4 also shows a large space of nearly degenerate antiferromagnetic solutions.

* Supported by the Office of Naval Research

First-principles Calculation on As Diffusion in Silicon

Jianjun Xie and S.P. Chen

Theoretical Division, Mail Stop B262

Los Alamos National Laboratory, Los Alamos, NM 87545

We present a first-principles investigation of As diffusion in silicon. Both the vacancy-assisted and self-interstitial-assisted mechanisms are studied. A new diffusion mechanism is provided based on our *ab initio* density-functional theory calculations. The effects of the Fermi level position and the elastic stress on the diffusion behavior of As with different charged states have been discussed. We explained some experimental observations based on our theoretical calculations.

Spin-polarized Transport in Conventional and Unconventional Superconductors

Igor Žutić, S. Das Sarma

Department of Physics, University of Maryland
College Park, MD 20742

Oriol T. Valls

Department of Physics, University of Minnesota
Minneapolis, MN 55455

Recent advances in fabricating techniques have made it possible to grow heterostructures incorporating superconductors together with different classes of magnetic materials, ranging from manganite perovskites to Mn-doped GaAs ferromagnetic semiconductors. Spin-polarized transport in such systems provides means to study the interplay of magnetism and superconductivity as well as to employ superconductivity as a tool to examine the spin-dependent electronic properties of magnetic materials. We focus on the Andreev reflection at the interface between a magnetic and a superconducting material, the two particle process which governs the low energy transport properties. We use high sensitivity of Andreev reflection to the degree of spin-polarization and the interfacial scattering to propose studies of spin-polarized transport in semiconductor/superconductor junctions. We give results for charge and spin conductance as a function of spin subband splitting, and potential and spin-flip scattering strengths. Our findings can serve to investigate the nature of magnetically active interface formed between ferromagnetic semiconductor and metal. Such an interface could change the degree of spin polarization as compared to the bulk of the magnetic material and have important implications on the spin-injection experiments. We also consider spin-polarized transport in unconventional superconductors which in the last several years were successfully grown as heterostructures with manganite perovskites. We reveal several novel effects arising from the anisotropic superconducting order parameter combined with the difference between electronic densities of superconductor and ferromagnet.

H. Ohno, *Science* **281**, 951 (1998).

R. J. Soulen Jr. *et al.*, *Science* **282**, 85 (1998).

I. Žutić and S. Das Sarma, *Phys. Rev. B* **60**, R16322 (1999).

I. Žutić and O.T. Valls, *Phys. Rev. B* **60**, 6320 (1999).

I. Žutić and O.T. Valls, *Phys. Rev. B* **61**, 1555 (2000).

Thursday, July 27

Oral Sessions

Reiss Science Building
Room 103

- | | |
|-------|--|
| 08:30 | Session 5: Ohno, Schulthess, MacDonald |
| 10:35 | Session 6: van Schilfgaarde, Hellberg, Cohen |
| 13:15 | Session 7: Lichtenstein, Jarrell, Savrasov, Kioussis |
| 15:30 | Session 8: Pederson, Yee, Epstein, Khanna,
Blugel, Momi |

Conference Lecture (Following Banquet)

ICC Galleria

- | | |
|-------|--------------------------------|
| 20:00 | Conference Lecture: G.A. Prinz |
|-------|--------------------------------|

Ferromagnetism and Heterostructures of Magnetic III-V Semiconductors

Hideo Ohno

Laboratory for Electronic Intelligent Systems
Research Institute of Electrical Communication, Tohoku University
Katahira 2-1-1, Aoba-ku, Sendai 980-8577, Japan
Phone/Fax: +81-22-217-5553, E-mail: ohno@riec.tohoku.ac.jp

Modern information technology is based on charge and spin degrees of freedom of electrons; transistors utilize charge of carriers in semiconductors, whereas magnetic storage takes advantage of spin of electrons in magnetic materials. An emerging new field in semiconductor physics and technology, semiconductor spintronics, involves the use of both charge and spin degrees of freedom to create new functionality and to enhance the performance of the existing devices. In order to utilize the spin degree of freedom in semiconductors, we need to be able to create, sustain, control, and detect the spin of carriers.

Here, I review our recent study on magnetic semiconductors based on III-V's and spin-dependent phenomena related to them. Introduction of magnetic ion, Mn, in III-V compounds such as GaAs leads to hole-induced ferromagnetism, where transition temperature can be as high as 110 K for 5% Mn concentration [1]. The origin of ferromagnetism is explained in terms of a mean-field theory, which predicts transition temperatures over room temperature for GaN and ZnO based magnetic semiconductors [2]. Due to the exchange interaction between spins of carriers and localized magnetic electrons, spin-splitting of the semiconductor bands takes place when ferromagnetism sets in, and carriers become partially spin polarized. Electrical spin injection across a ferromagnetic/nonmagnetic semiconductor heterojunction and into an InGaAs quantum well (QW) has been demonstrated using ferromagnetic (Ga,Mn)As as a source of spin polarized carriers [3]. Magnetic/nonmagnetic trilayer structures based on III-V's have been shown to exhibit spin-dependent scattering as well as interlayer coupling [4]. We have also studied spin relaxation in nonmagnetic GaAs QW's and found that QW's grown on (110) substrates exhibit prolonged spin relaxation time [5], which can be over 10 ns from *room temperature* down to 5 K when modulation doped.

[1] H. Ohno, *Science*, **281**, 951 (1998), *J. Mag. Mag. Materials*, **200**, 110 (1999).

[2] T. Dietl, H. Ohno, F. Matsukura, J. Cibert, and D. Ferrand, *Science*, **287**, 1019 (2000).

[3] Y. Ohno, D. K. Young, B. Beschoten, F. Matsukura, H. Ohno, and D. D. Awschalom, *Nature*, **402**, 790 (1999).

[4] N. Akiba, D. Chiba, K. Nakata, F. Matsukura, Y. Ohno, and H. Ohno, to appear in *J. Appl. Phys.*

[5] Y. Ohno, R. Terauchi, T. Adachi, F. Matsukura, and H. Ohno, *Phys. Rev. Lett.*, **83**, 4196 (1999).

On the ferromagnetic interactions in Mn doped III-V semiconductors

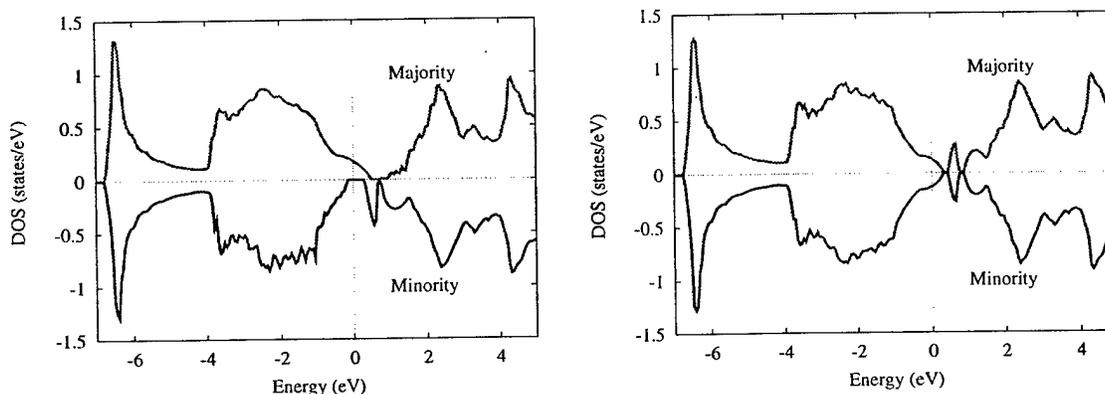
T. C. Schulthess

Computer Science and Mathematics Division
Oak Ridge National Laboratory, Oak Ridge TN 37631-6114

W. H. Butler

Metals and Ceramics Division
Oak Ridge National Laboratory, Oak Ridge TN 37631-6114

Ferromagnetism has been observed in several III-V-based semiconductors with Mn concentrations of the order of several atomic %. For (Ga,Mn)-As the Curie temperature can be as high as 110 Kelvin (H. Ohno, Science 281, 951). In order to understand the origin of the ferromagnetic coupling we have performed a study of (Ga,Mn)-As, (In,Mn)-As, and (Ga,Mn)-Sb using the layer-KKR multiple scattering approach in conjunction with the single site CPA. The strength of the magnetic coupling is determined by comparing the energies of the ferromagnetically (FM) ordered state with the disordered local moment (DLM) state. In all cases we find that both, the DLM and the FM ordered state exist, with the FM ordered state being favored energetically. The density of states (DOS) for (Ga,Mn)-As shows the majority Mn *d*-states to be strongly hybridized with the As *p*-band. It is therefore more appropriate to view the electronic structure of Mn in terms of bands than in terms of atomic states. Comparing the DOS of the FM and DLM states (see Figure) reveals that in the FM ordered state the minority bands are shifted so that the Fermi level falls in the minority gap. This not only stabilizes the FM state but also renders the system halfmetallic. It also implies that when the Mn moments are aligned, a small anti-parallel polarization is induced on the As *p*-band. This is in accordance with a recent experiment of Beschoten et. al. (Phys. Rev. Lett. 83, 3073), in which a negative magnetic circular dichroism signal was observed below the FM ordering temperature.



DOS for (Ga_{0.95}Mn_{0.05})-As in the FM (left) and the DLM (right) states.

Theory of $\text{III}_{1-x}\text{Mn}_x\text{V}$ Semiconductor Ferromagnetism

A.H. MacDonald, R. Abolfath, T. Jungwirth, J. König, B.H. Lee and J. Schliemann
Indiana University
Bloomington IN, 47405

It has recently been discovered that III-V semiconductors like GaAs and InAs become ferromagnetic when Mn is substituted on a small fraction of the group III element sites. I will discuss a theory of the magnetic, transport, and optical properties of these materials. The theory is semi-phenomenological and based on envelope function descriptions of semiconductor valence bands holes exchange coupled to Mn local moments. This basic model has been solidly established in studies of closely related paramagnetic II-VI semiconductor systems. Within this framework, I will discuss insights which can be obtained at different levels of approximation from mean-field theory, to perturbative treatments of magnetic fluctuations, to numerically exact results based on hybrid quantum Monte Carlo simulations in which the local moment orientations are treated as classical degrees of freedom. The utility of first principles calculations in estimating the parameters of this phenomenology will also be discussed.

Exchange Interactions in Mn-doped GaN and GaAs

Mark van Schilfgaarde
Sandia National Laboratories
MS 9161, Livermore, CA 94551-0969

Using the local spin-density approximation, the coupling between effects of magnetic elements Mn, Fe and Cr substituting for the cation in the III-V semiconductors GaN, AlN, and GaAs, is investigated for concentrations between 1 and 10%. The short-ranged magnetic interactions are large, inducing a tendency to form magnetic nanoclusters of a few (3 to 4) magnetic atoms.

The magnetic d states are strongly spin polarized and form deep levels ranging throughout the host bandgap; and they are responsible for magnetic exchange interactions that are found to be anomalous in several respects. Fe substitutes isoelectronically with Ga, and behaves approximately as does Mn in the usual dilute magnetic semiconductors, e.g. Mn:ZnTe. Mn dopes the host; thus the t_{2g} defect level is partially filled. The deeper e_g levels are entirely filled and thus are stabilized in an antiferromagnetic alignment (superexchange), while the t_{2g} level is stabilized in the ferromagnetic alignment (Zener double exchange) and predominates. Nevertheless, the total energy of a Mn "dimer" as a function of canting angle θ does not show the hallmark of the Zener double exchange, namely $E = \cos(\theta/2)$. In GaAs, the t_{2g} level of an isolated Mn lies about 0.1 eV above the valence band maximum and forms a resonance with it. The resonance is partially delocalized, but the strong scattering from the magnetic dopant causes states at the fermi level to differ qualitatively from the usual itinerant, effective-mass like character in a p -doped semiconductor. Thus, prospects for spin-polarized hole transport in these materials are poor.

We also show that the exchange interactions, while falling off algebraically in GaAs owing to the quasi-itinerant character of the resonance, are not RKKY-like. The coupling strength decreases with increasing Mn concentration, and they are not decomposable into a sum of pairwise interactions. A tight-binding model appears to be a more appropriate description of the magnetic electronic structure in these complex materials.

Correlation Induced Magnetism in the Sn/Ge Surface

C. Stephen Hellberg, Naval Research Laboratory

Electrons at the Sn/Ge(111) surface form a narrow band. Experimentally, the surface distorts at low temperatures, but LDA fails to find the distortion. We describe the surface electrons with a Hubbard model, the parameters of which are derived from LDA calculations. Solving the Hubbard model exactly, we find the surface distorts in agreement with experiments, and the distortion is driven by a magnetic transition.

Metal-insulator transitions and energetics of FeO and CoO at high pressures within LDA+U

R.E. Cohen and S.A. Gramsch
Carnegie Institution of Washington
5251 Broad Branch Rd., N.W., Washington, D.C. 20015

S.Y. Savrasov
Rutgers University
Piscataway, N.J. 08854

We have studied the predictions of GGA and LDA+U for the high pressure behavior of FeO and CoO, and the effects of lattice strain. Studying the predictions of high pressure behavior will help test the viability of a model for the transition metal oxides, as many methods might produce an insulating state at zero pressure, but might not accurately predict high pressure behavior. The experimental situation is also uncertain. A high-spin low-spin transition was detected by Mössbauer at 90 GPa (Pasternak et al., PRL 79, 5046, 1997) but was not seen by x-ray spectroscopy to 140 GPa (Badro et al., PRL 83, 4101, 1999). GGA shows discontinuous high-spin low-spin transitions in FeO and CoO with cubic lattices. In FeO, the optimal rhombohedral strain causes the transition to be spread out continuously, ending with a low-spin configuration at about 250 GPa. LDA+U totally changes the predicted behavior. With $U=4.6$ eV (Pickett et al., PRB 58, 1201, 1998), LDA+U predicts insulating behavior at low pressures, with a metal insulator transition at 75 GPa in FeO with optimal rhombohedral strain, but the high-spin low-spin transition is pushed up to very high pressures (310 GPa). We find two different insulating solutions for FeO, one with rhombohedral symmetry, and one with monoclinic symmetry. The latter, lower symmetry solution, is lower in energy for both the cubic and rhombohedrally strained lattices. A similar picture is found for CoO, where GGA gives a high-spin low-spin transition at about 30 GPa, but drives this transition up to extreme pressures. Thus a strong test of the reasonableness of LDA+U is whether high-spin low-spin transitions are found experimentally at high pressures in the transition metal oxides, or if instead metal-insulator transitions are found.

For both FeO and CoO we find that LDA+U gives accurate equations of state, and gives reasonable energetics for lattice distortions. For FeO with optimal rhombohedral strain, GGA gives $V_0=265$ au, $K_0=158$ GPa, and $K'_0=3.05$, LDA+U ($U=4.6$ eV) gives 289 au, 183 GPa, and 3.64, respectively, compared with 274 au, 142-180 GPa, and 4.9 from experiments. For CoO we find the LDA+U equation of state to be more accurate than GGA. GGA gives $V_0=225$ au, $K_0=305$ GPa, compared with 261 au and 181 GPa from experiment. $U=4$ eV gives $V_0=274$ au, $K_0=201$ GPa, a significant improvement.

**Electronic structure and magnetism of correlated systems:
beyond the LDA.**

A.I. Lichtenstein
University of Nijmegen
6525 ED Nijmegen, The Netherlands

Local spin density approximation (LSDA) have been highly successful for electronic structure and zero temperature magnetic properties of non-correlated systems. We discuss some failures of the LDA-scheme for the charge, spin and orbital ordering in transition metal compounds. Starting from a general formulation of the LDA+U approach with local Coulomb correlations for d- or f- ions, the different ways to go beyond the mean-field approximation and include an effect of the spin- and charge-fluctuations have been analyzed. Dynamical mean field theory (DMFT) which takes into account a frequency dependence of the self energy was implemented on the basis of first-principle LMTO-TB scheme and the QMC-solution of an effective multi-orbital spin-polarized quantum-impurity problem. The calculated quasiparticle spectrum of ferromagnetic iron and antiferromagnetic manganese shows an important correlation effects. Finally we address some problems of the finite-temperature transition-metal magnetism.

The Dynamical Cluster Approximation

M. Jarrell, C. Huscroft and S. Moukouri
University of Cincinnati
Cincinnati Ohio

H.R. Krishnamurthy
Indian Institute of Science
Bangalore, India

Th. Maier and Th. Pruschke
University of Regensburg
Regensburg, Germany

The Dynamical Cluster Approximation (DCA) includes short-ranged corrections to local approximations such as the Dynamical Mean Field or the Coherent Potential by mapping the thermodynamic lattice problem onto a self-consistently embedded periodic cluster of size N_c . It is a fully causal and systematic approximation to the full lattice problem, with corrections $\mathcal{O}(1/N_c)$. The effective cluster problem can be solved with a variety of methods including Quantum Monte Carlo, the Non-Crossing Approximation, Exact Diagonalization, etc. The DCA formalism and an adaptively parallel QMC algorithm will be discussed, and results for the one-particle and two-particle properties of the Hubbard model will be shown. At half filling a pseudogap is found in the charge but not the spin response. Away from half filling the pseudogap is accompanied by a d-wave pairing instability.

Electronic Structure Calculations with DMFT

S. Savrasov

Department of Physics and Astronomy, Rutgers University
136 Frelinghysen Rd., Piscataway NJ 08854

A novel electronic structure method for dealing with realistic systems which gives both ground state properties and excitations spectra will be reviewed. The method is based on dynamical mean field theory of strongly correlated electronic systems which treats many-body effects locally via self-consistent solutions of the Anderson impurity-like models. Applications of the method to several long standing problems known in LDA will be discussed.

DEVELOPMENT OF MAGNETISM IN STRONGLY CORRELATED ELECTRON SYSTEMS: NON-KONDO MECHANISM FOR MOMENT COLLAPSE

Nicholas Kioussis,* Eric Collins,* Say Peng Lim,* and Bernard R. Cooper**

**Department of Physics, California State University Northridge, Northridge, CA 91330*

***Department of Physics, West Virginia University, Morgantown, WV 26506*

We present an *ab initio* based method which gives clear insight into the interplay between the band-f hybridization, the band-f coulomb exchange, and the crystal-field interactions, as the degree of 4f localization is varied across a series of strongly correlated electron systems. The predictions for the ordered moments, magnetic structure, and ordering temperatures are in excellent agreement with experiment, including the occurrence of a *moment collapse* of non-Kondo origin. In contrast, spin and orbitally polarized *ab initio* density functional calculations fail to predict, even qualitatively, the trend of the unusual magnetic properties.

Anisotropy Barriers and Spin-Tunneling Fields of Nanoscale Magnets

M. R. Pederson¹, J. Kortus¹, S. N. Khanna²

¹Naval Research Laboratory

Washington DC 20375-5345

²Virginia Commonwealth University

Richmond VA

Recent work aimed at the density-functional-based understanding and optimization of nanoscale magnets is discussed. In addition to electronic structures and spin ordering in these systems, we discuss a new method for incorporating the spin-orbit interaction that has been developed for the calculation of anisotropy hamiltonians and for determining the fields at which resonant tunneling of magnetization occurs. Some mechanisms, amenable to study within density-functional theory, for determination of spin-tunneling *mechanisms* and higher-order anisotropy will also be presented. Systems that will be discussed include the $\text{Mn}_{12}\text{O}_{12}(\text{RCOO})_{16}(\text{H}_2\text{O})_4$ molecule and the $\text{Fe}_8\text{O}_2(\text{OH})_{12}(\text{C}_6\text{N}_3\text{H}_{15})_6\text{Br}_8$ molecule which both have large spins and reasonably large anisotropy barriers as well as the $\text{V}_{15}\text{As}_6\text{O}_{42}(\text{H}_2\text{O})$ molecule which behaves as a half integer low-spin molecular magnet with smaller anisotropic effects. Other examples include transition-metal-oxide nanotowers and pure transition-metal nanostructures. By way of example we show that the optimization of anisotropy barriers and net moments are separate issues which may be competing. For example we find that many high-spin pure transition metal structures also have high symmetry leading to a vanishing of the second-order anisotropy barriers. Also, upon proper variation of the transition-metal atoms in the intrinsically uniaxial molecular magnets we show that the net moments are indeed enhanced but only at the expense of significantly smaller anisotropy barriers.

Molecule-Based Ferromagnets, Ferrimagnets, Metamagnets and Spin-Glasses

G. T. Yee, B. B. Kaul, M. A. Taylor, M. W. Whitton, J. P. Fitzgerald

University of Colorado, Boulder, CO 80309

Our continuing investigation into decamethylmetallocene-based charge-transfer (CT) salt magnets (where M = Cr, Fe or Mn) has yielded a number of well-characterized solids exhibiting a variety of phenomena. The palette of acceptors we have examined includes examples culled from the extensive conductive CT salt literature, such as 2,3-dicyano-1,4-naphthoquinone. We have also found viable building blocks in the similarly extensive organic polymer precursor and Diels-Alder reaction literature such as dimethyl dicyanofumarate. Single crystal X-ray diffraction analysis of the CT compounds shows that they adopt similar mixed-stack pseudo-1D structures common to others in this class. Magnetic characterization utilizing ac and dc SQUID susceptometry reveals a variety of behaviors ranging from ferromagnetism to glassy ferromagnetism to metamagnetism. A particular strength of the CT salt strategy is that we can prepare families of structurally related materials in which the number of unpaired electrons is systematically varied. Another strength is that cyclic voltammetry can be a valuable guide to reactivity.

We have extended these ideas to the synthesis of a radical-anion-bridged, three-dimensional coordination polymer network that exhibits order below 210 K. Although this compound is not yet structurally characterized, it clearly demonstrates the importance of dimensionality and represents the apparent first high T_c magnetic compound related to the remarkable V[TCNE]₂ where TCNE=tetracyanoethylene, the first room temperature molecule-based magnet.

Organic Magnets - Chemistry and Physics

Joel S. Miller^a and Arthur J. Epstein^b

^a Department of Chemistry, 315 S. 1400 E. RM 2124, Salt Lake City, UT 84112-0850

^b Department of Physics and Department of Chemistry, The Ohio State University, 174 West 18th Street, Columbus, OH 43210-1106

Organic-based materials exhibiting the technologically important property of bulk magnetism have been sought and studied.¹ These magnets are prepared via conventional organic chemistry methodologies and unlike conventional inorganic-based magnets do not require metallurgical processing. Furthermore, these magnets are frequently soluble in conventional solvents (*e. g.*, toluene, dichloromethane, and acetonitrile, THF) and examples have saturation magnetizations more than twice that of iron metal on a mole basis. Also magnets with critical temperatures exceeding room temperature and magnets with coercive field exceeding that of Co₅Sm have been prepared.

In addition to an overview of magnetic behavior, a plethora of examples of magnets made from molecules as well as their physics will be reviewed. These will include [M(III)(C₅Me₅)₂][A], [Mn(III)(porphyrin)][A] (A = cyanocarbon etc. electron acceptors) as well as a V-based room-temperature magnet etc.

We acknowledge the support from the U. S. Department of Energy (Grant Nos. DE FG 02-86BR45271 and DE FG 03-93ER45504) as well as the U. S. National Science Foundation (Grant No. CHE-9730948)

¹ J. S. Miller, A. J. Epstein, *Angew. Chem.* 106, 399-432; *Angew. Chem. internat. edit.* 33, 385-415 (1994). J. S. Miller, A. J. Epstein, *Chem. Eng. News*, 73(#40), 30-41 (1995).

Measuring Cluster Magnetic Moments Without Magnetic Experiments

G. L. Gutsev, M. Beltran, S. N. Khanna, and P. Jena
Physics Department,
Virginia Commonwealth University
Richmond, Va. 23284-2000.

It is proposed that the magnetic moment of clusters can be determined by combining the results of ab-initio calculations on the anionic and neutral clusters with experiments involving negative ion photoelectron spectroscopy. The method is particularly applicable at small sizes where the Stern-Gerlach determination of the moment is difficult. More importantly, the method avoids ambiguities in the derived moments associated with the uncertainties in the cluster temperature. The method is applied to pure Fe_n and Ni_n clusters containing up to 5 atoms. In the case of Fe_3 cluster, which is marked by nearly degenerate isomers, this new approach is shown to be able to uniquely identify the ground state multiplicity. In the case of Ni_5 where the existing calculations and experiments have wide disagreement, the approach yields the ground state to have a moment of $1.2 \mu_B$ per atom. A critical comparison of the present results with previous calculations and experiments will be presented.

Magnetism of two-dimensional itinerant antiferromagnets on a triangular lattice

Ph. Kurz, G. Bihlmayer, and S. Blügel
Institut für Festkörperforschung, Forschungszentrum Jülich
D-52425 Jülich, Germany

K. Hirai
Department of Physics, Nara Medical University
Kashihara, Nara 634-8521, Japan

Based on vector spin-density first-principles total-energy calculations of Cr and Mn transition-metal monolayers on a triangular lattice provided by (111) oriented Cu or Ag substrates we conclude that the magnetism of Cr is well described by the n.n. Heisenberg model and the coplanar non-collinear periodic Néel state is the magnetic ground state. For Mn the physics is much richer: (i) Exchange interactions beyond nearest neighbors and (ii) due to more than two spins (such as the four-spin interaction) play an important role. The consequences of (i) and (ii) for the magnetic ground state will be discussed. The search for the magnetic minimum-energy configurations included surface unit-cells with one, two, three, and four atoms. Non-collinear magnetic configurations changing along continuous paths in real space connecting high symmetry states and spin-spiral states along high-symmetry lines in the surface Brillouin-zone of the momentum vector have been investigated. Selfconsistently determined external magnetic constraint fields guarantee, that the average magnetic moment around each atom points in the prescribed direction. The results are obtained employing the full-potential linearized augmented plane-wave (FLAPW) method in film geometry, extended by the vector spin-density description for the interstitial and vacuum region in order to deal with non-collinear structures.

Magnetization Plateaus of Two-Dimensional Frustrated Antiferromagnets

Tsutomu Momoi*, Lyman Laboratory of Physics, Harvard University
Cambridge, MA 02138

Keisuke Totsuka, Department of Physics, Kyushu University
Hakozaki, Higashi-ku, Fukuoka-shi, 812-8581 Japan

We studied the magnetization process of two-dimensional frustrated antiferromagnets, and found that plateau structures can appear in a few systems. All of these plateaus can be understood as superfluid-insulator transitions of magnetic excitations. As an example, we discussed the Heisenberg antiferromagnet on Shastry-Sutherland lattice, which is a possible model for $\text{SrCu}_2(\text{BO}_3)_2$, and found plateaus at $m/m_{\text{sat}} = 1/3$ and $1/2$. Treating magnetic excitations as bosonic particles and using strong coupling expansion, we derived effective Hamiltonian for the magnetic particles. This effective Hamiltonian contains repulsive interactions and correlated hopping terms. These repulsive interactions induce Mott insulators of the magnetic excitations at $m/m_{\text{sat}} = 1/2$ and $1/3$, and thereby create magnetization plateaus. In the plateaus, the magnetic excitations are crystallized and form a checkerboard structure at $m/m_{\text{sat}} = 1/2$ and a stripe structure at $m/m_{\text{sat}} = 1/3$. The correlated hopping terms have remarkable consequences on the dynamics of excitations. At zero and very low magnetization, bound states of triplet excitations are formed by the correlated hopping. This explains the peculiar results of inelastic neutron scattering.

[*] On leave of absence from Inst. of Physics, Univ. of Tsukuba, Ibaraki 305-8571, Japan.

[1] T. Momoi and K. Totsuka, Phys. Rev. B **61**, 3231 (2000).

Friday, July 28

Oral Sessions

Reiss Science Building
Room 103

08:30	Session 9: Pickett, Mazin, Butler
10:35	Session 10: Szunyogh, Nadgorny, Cottenier, Qiu
13:20	Session 11: Dobrovitski, Sabiryanov, Ayuela
14:50	Session 12: Andersen, Hobbs, Heinonen, Mryasov
16:35	Conference Closing

**Coexisting Superconductivity and Magnetism:
The Novel Case of $\text{RuSr}_2\text{GdCu}_2\text{O}_8$**

Warren E. Pickett and Alexander B. Shick
Department of Physics, University of California
Davis CA 95616

Ruben Weht
Departamento de Física, CNEA
Avda. General Paz 1499 y Constituyentes, 1650 San Martin, Argentina

Superconductivity and magnetism are both macroscopic manifestations of quantum mechanical effects, and generally they compete for the attention of electrons, hence they rarely coexist except in tiny temperature ranges near one (or both) of the transition temperatures. The hybrid ruthenocuprate $\text{RuSr}_2\text{GdCu}_2\text{O}_8$ presents a completely new aspect of this competition – it seems agreed that it orders magnetically near 135 K and then superconducts at 45 K without disturbing the magnetism. There is conflicting data about the magnetism, originally thought to be ferromagnetism but new data suggesting that a strongly canted antiferromagnetic phase accounts for the data better. In either case superconductivity arises within a phase that has a net magnetic moment.

The structure of this compound itself is worthy of notice. It can be regarded as a $\text{YBa}_2\text{Cu}_3\text{O}_7$ -like structure, with the CuO chain replaced by a RuO_2 layer with the same structure as the CuO_2 layers (and $\text{Y} \rightarrow \text{Gd}$). Thus it has the common CuO_2 bilayer structure that occurs in several high temperature superconductors (YBCO, BSCCO, ...). Remarkably, the remaining part of the cell is a Sr_2RuO_4 substructure exactly like the layered ruthenate that superconducts at 1.5 K, and is believed to be a triplet superconductor. The superconductivity in $\text{RuSr}_2\text{GdCu}_2\text{O}_8$ (often now called Ru1212), at 45 K, is naturally expected to be singlet as in other cuprate superconductors.

We will review the current understanding of this compound, and lay out the results of electronic structure studies that indicate (1) the Ru ion definitely favors magnetism. (2) the antiferromagnetically ordered phase is preferred energetically over the ferromagnetic phase, and (3) the RuO_2 layer distorts in a $\sqrt{2} \times \sqrt{2}$ fashion but the antiferromagnetic phase is still favored. One important feature of this compound is that the magnetism resides in the t_{2g} orbitals in Ru, and these orbitals are coupled only very weakly to the primary superconducting orbital, which is the Cu $d_{x^2-y^2}$ orbital. This weak coupling is what ultimately allows coexistence of superconductivity with magnetism. We will also comment on the possibility of canting of spins in this magnetic phase.

Work supported by the Office of Naval Research.

Fermiology and Spin-polarized Tunneling

I.I. Mazin

Code 6391, Naval Research Laboratory, Washington, DC 20375, USA

I will discuss the role of Fermiology in such experiments as (1) Ballistic no-barrier tunneling (2) Diffusive no-barrier tunneling (3) Ballistic tunneling through a rectangular (vacuum) barrier (4) Ballistic tunneling through a semiconductor (5) Ballistic Andreev tunneling (6) Diffusive Andreev tunneling. All these experiments will be discussed both in non-magnetic and in spin-polarized cases. Particular attention will be paid to defining the experimentally measurable spin polarization in all these cases, when a ferromagnet is involved. It will be demonstrated that for complex Fermi surfaces all experiments above probe different, sometimes extremely different, properties. Some first principle, as well as some model calculations will be presented to illustrate this point.

Spin Dependent Tunneling Conductance of Fe|MgO|Fe Sandwiches

W. H. Butler and X.-G. Zhang
Oak Ridge National Laboratory
Oak Ridge, TN 37831-6114

J. M. MacLaren
Tulane University
New Orleans, LA, 70018

We present first-principles based calculations of the tunneling conductance and magnetoconductance of Fe|MgO|Fe sandwiches. The calculations assume an epitaxial relationship between the Fe and MgO (100) layers similar to that achieved in recent experimental measurements of tunneling conductance. We describe the physical, magnetic, and electronic structure of a system consisting of an MgO layer embedded between two semi-infinite Fe layers as calculated self-consistently using the layer Korringa-Kohn-Rostoker technique. The tunneling conductance was calculated from first-principles without adjustable parameters by summing the tunneling transmission probability over Bloch states in the Fe electrodes. Our calculations indicate that quite different tunneling mechanisms dominate the conductance in the two spin channels. In the majority channel, the conductance is primarily via Bloch electrons with zero transverse momentum. One particular state with Δ_1 symmetry is able to effectively couple from the Fe into the MgO. In the minority channel, the conductance is primarily through interface resonance states, especially for thinner layers. We predict a large magnetoresistance that increases with thickness.

**Theoretical investigation of magnetotransport of
Co and $\text{Ni}_x\text{Fe}_{1-x}$ related spin valves**

L. Szunyogh, Department of Theoretical Physics, Technical University of Budapest,
Budafoki, út 8, H-1111, Budapest, Hungary

C. Blaas, Center of Computational Materials Science, Technical University of Vienna,
Gumpendorferstr. 1.a, A-1060, Vienna, Austria

P. Weinberger, Center of Computational Materials Science, Technical University of Vienna,
Gumpendorferstr. 1.a, A-1060, Vienna, Austria

P.M. Levy, Department of Physics, New York University,
4 Washington Place, New York, NY 10003, USA

C.B. Sommers, Laboratoire de Physique des Solides, Université de Paris-Sud,
91405 Orsay, France

We present results of ab-initio calculations of the electric conductivity of magnetic multilayers. Our approach builds on the Kubo-Greenwood formalism as evaluated by using the spin-polarized relativistic Screened Korringa-Kohn-Rostoker method and the coherent-potential approximation. The ultimate goal of our study is to explore quantitative predictions to the GMR properties of commonly used spin valve systems comprising ferromagnetic Co or $\text{Ni}_x\text{Fe}_{1-x}$ slabs and nonmagnetic Cu spacer. After analyzing the role of different boundary conditions as well as an imaginary part for the energy used inherently in the method we are able to provide both resistivities and GMR ratios that are in quite good agreement with experiments. Particular attention is paid to effects of interdiffusion across the Co/Cu interface and alloying in the non-magnetic Cu spacer. We demonstrate that these effects dramatically change the calculated value of GMR. An attempt is also made to attribute these changes to different (intrinsic and defect) scattering mechanism present in the system.

Spin Dependent Transport in Real Systems

Boris E. Nadgorny*
Naval Research Laboratory
Washington, DC 20375, U.S.A.

Spin-dependent transport is playing an increasingly important role due to the rapid advance of a new area of electronics dubbed *spintronics*, which is based on electron spin imbalance in ferromagnets or semiconductors. Not surprisingly, the spin degree of freedom makes the treatment of spin-polarized systems significantly more complicated compared to conventional transport systems. We will discuss experimental and theoretical issues that have important implications for spin dependent transport and tunneling, as well as for Andreev reflection in magnetic materials. As an example, we will demonstrate that a material (Sr-doped LaMnO_3) may have a high degree of current spin polarization without being half-metallic.

* in collaboration with I. Mazin, A. Golubov, M. Osofsky, V. Harris and R. J. Soulen, Jr.

Hyperfine fields and local relaxations for impurities in bcc Fe: an FLAPW study

Stefaan Cottenier

Instituut voor Kern- en Stralingsfysica
Celestijnenlaan 200 D, B-3001 Leuven, Belgium

Heinz Haas
Hahn-Meitner-Institut Berlin
D-14109 Berlin, Germany

The experimental and theoretical study of magnetic hyperfine fields¹ situates at the border of materials and nuclear physics. Known hyperfine fields (a materials property) can be used to study unknown nuclear magnetic moments (=nuclear physics). Known nuclear magnetic moments (a nuclear property) can be used to measure unknown hyperfine fields (=materials science). The present work shows how an accurate theoretical approach can shed new light on existing experiments.

Magnetic hyperfine fields are hard to calculate. In contrast to many other properties they depend not only on the Density Of States (DOS) at the Fermi energy (E_F), but on the integral of the (s-)DOS up to E_F . One should therefore use an electronic structure method which accurately reproduces the DOS over this entire energy range. Moreover, it is not the crystalline DOS itself, but rather the DOS limited to the small region where the nucleus sits, which is important. This puts even higher requirements on the calculational method.

Since a decade or so, the FLAPW-code WIEN has proven to be a reliable tool to calculate magnetic hyperfine fields. Both hyperfine fields on nuclei in pure materials and on nuclei as impurities in materials – the experimentally most important case – can be calculated almost routinely. Current computer resources make it even possible to calculate a large group of impurity/material combinations at once. The study of such systematics can give much more insight in the physics of the problem.

In the present work, hyperfine fields on a number of medium-Z impurities in bcc Fe are studied (Rb → Xe and a few others). These hyperfine fields never have been satisfactorily calculated before, despite several attempts since as early as 1975. We confront our results with the wealth of existing experimental data, and show how the calculations can help to interpret the experiments in a more reliable way. It will be pointed out that (and why) a few particular cases (Cs, Fr, ...) are extremely sensitive to external perturbations, such as e.g. application of pressure. Although these cases have been measured, their exceptional status was never realized.

The relaxation of the Fe-neighbors due to the presence of the impurity is studied as well.

¹A magnetic hyperfine field is defined as the magnetic field felt by a nucleus and generated by the surrounding electron cloud.

Magnetic Phases of Mn and Fe and the Epitaxial Bain Path

S. L. Qiu †, P. M. Marcus ‡ and Hong Ma †

† Alloy Research Center, Department of Physics,
Florida Atlantic University, Boca Raton, FL 33431-0991
‡ IBM Research Division, T. J. Watson Research Center,
Yorktown Heights, NY 10598

The appropriate theoretical procedure for comparison of theory with experiment for crystalline phases of a material, both stable and metastable, in equilibrium or under strain, is to find the epitaxial Bain path (EBP) of the material. For magnetic materials several EBPs may be needed including non-magnetic (NM), ferromagnetic (FM) and antiferromagnetic (AF); there may be several AF phases. The simplest EBPs are for the tetragonal structures produced by isotropic epitaxy on (001) surfaces that are considered here, but other crystal faces and structures may be epitaxially strained to give an EBP. The effects of epitaxial strain for tetragonal structure are graphically represented by two plots – the energy along the EBP as a function of c/a or a and the volume per atom as a function of c/a or a . Minima of the energy locate the equilibrium states, including the ground state; strained epitaxial states are located on the volume plot. First-principles calculations on EBP's of tetragonal Mn and Fe were made using the all-electron full-potential linearized-augmented-plane-wave (FLAPW) method with two different potentials: (1) the local-spin-density-approximation without relativistic corrections (LSDA-NREL) and (2) the Perdew-Burke-Ernzerhof exchange-correlation potential in a generalized-gradient-approximation with relativistic corrections (GGA-REL). Study of tetragonal EBPs for all c/a leads to the useful concept of an “extended ground state”, which means the state of lowest energy at each c/a . Such states are, except for ranges of c/a in which they are unstable, experimentally accessible. However, they may require strains imposed by external constraints to stabilize them. The extended ground state of Mn is then shown to be almost entirely the AF EBP, but the extended ground state of Fe is the FM EBP for low c/a but for a range of high c/a uses the AF EBP. The AF EBP of Mn shows that the c/a of γ -Mn (which is not fcc) agrees very closely with experiment, but that Mn films on V(001) are strained δ -Mn (which is not bcc). The AF EBP of Fe shows that Fe epitaxial on Cu(001) is strained γ -Fe (which is not fcc).

Statistical coarse-graining as an approach to multiscale problems in magnetism

V. V. Dobrovitski, M. I. Katsnelson, and B. N. Harmon

Ames Laboratory

Iowa State University, Dept. of Physics and Astronomy, Ames, Iowa, 50011

Multiscale phenomena which include several coupled processes occurring at different length scales, are widespread in magnetism. For example, the magnetization reversal in a magnet often starts from a domain of opposite polarity nucleated near some defect. Here, the different length scales involved can be clearly identified. First, the microscopic scale (several interatomic distances) in the vicinity of the defect. Next, there is a “micromagnetic” length scale (several thousands of angstroms) where the formation of the general structure of the domain nucleus takes place. And, finally, the macroscopic length scale responsible for propagation of the magnons created in the course of the reversal; these magnons play an important role in energy transfer. A similar picture of several interacting length scales appears in many situations, such as the breakthrough of a domain wall pinned by a defect [1], exchange coupling in spin-valve systems [2] etc.

A correct description of such problems is of importance both for fundamental science and for applications. At present, there are many tools used to work at different length scales. E.g., micromagnetic modeling provides a description of the length scales of order of the domain wall width (and larger), and atomistic simulations can be used for smaller scale. However, for the description of real systems all the length scales should be coupled, i.e. modeled simultaneously and seamlessly, with the possibility of energy transfer between them. Simple schemes, where the region of micromagnetic simulations is just attached to the region of atomic spin simulations, do not give a satisfactory description of the energy transfer between the lengthscales. Some impedance matching region between the micromagnetic and atomic regions is necessary, which would allow for gradual exclusion of short-wavelength modes until they die out.

In the present paper, we apply the ideas of coarse grained molecular dynamics (recently developed by Rudd and Broughton [3]) to magnetic materials modeling. We propose a computational scheme which employs basic concepts of nonequilibrium statistical mechanics to couple micromagnetism and the dynamical modeling of classical spins [4]. We identify the key problems arising in the course of implementation of this scheme and their possible solutions. In particular, we have analyzed the optimal choice of the weighting function used in coarse graining. Simple one-dimensional tests indicate that this approach may be suitable for realistic modeling of magnetic systems.

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Magnetic Properties of Co clusters embedded in Cu matrix

R.F. Sabyrivanov and S.S. Jaswal

116 Brace, University of Nebraska, Lincoln 68588-0111

First-principle methods are used to study the magnetic properties of Co clusters in a Cu matrix. The local magnetic moments (LMM) are calculated for different cluster sizes. As expected, the LMM of the inner-shell Co atoms are close to the bulk value. The LMM of the outer shell Co atoms (\sim three outer shells) are smaller than the bulk value. The LMM of the outer-shell Co atoms are quite sensitive to the relaxation at the Co-Cu interface. For example, the LMM of a single Co atom in Cu matrix is $\sim 0.9\mu_B$ without any relaxation but $0.0\mu_B$ (non-magnetic) with 1% and 0.5% relaxations of the first and second shells respectively. The small induced moments on the Cu shells near the interface oscillate with the size of the cluster. The cluster-cluster exchange interactions are studied as a functions of the separation distance by calculating the energy of the system as a function of the angle between the magnetic moments of two clusters of 141 atoms. The exchange interactions have oscillatory behavior with large amplitude at low distances (less than 2.5 nm). The oscillatory nature of interactions is the origin of the peak in zero field cooled magnetization curve obtained in experiment. This research is supported by NSF, DARPA, AFOSR and DOE.

Electronic properties in Magnetic Heusler alloys: Ni_2MnGa

A. Ayuela , J . Enkovaara, and R. M. Nieminen

Laboratory of Physics, Helsinki University of Technology, 02015 Espoo, Finland

K. Ullakko

Materials Physics Laboratory, Helsinki University of Technology, 02015 Espoo, Finland.

Some alloys which are plastically deformed at low temperatures and revert to their original shape upon heating (Shape Memory Effect - SME), are already being used as actuators. Also the magnetically driven actuators- such as the ternary and intermetallic Heusler alloys with composition X_2YM - are being developed. The application of magnetic fields on nearly stequiometric compounds around the Ni_2MnGa Heusler alloy gives strains up to 2 % as the recent experimental results showed [1,2].

The Heusler alloys with composition X_2YM , are studied within the density-functional theory (DFT) with the generalized gradient approximation (GGA) for the electronic exchange and correlation [3]. The geometrical and electronic structures for the magnetic $L2_1$ structure are calculated. The structures and magnetic moments at equilibrium are in good agreement with the experimental values. The structural trends with varying X and Y are explained by a d -occupation model , while a rigid band model can account for the trends with changing M.

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3rd Generation Muffin-Tin Orbitals of Arbitrary Order

O.K. Andersen

Max-Planck-Institut für Festkörperforschung
Stuttgart, Germany

Abstract not available.

Fully unconstrained noncollinear magnetism within the projector augmented wave method

D. Hobbs, G. Kresse, and J. Hafner

Institute for Material Physics and Center for Computational Material Science
Sensengasse 8, A-1090, Vienna, Austria

Spin-polarized calculations in solids have generally been confined to a global quantization axis to simplify both the theoretical model and its implementation in self-consistent codes. This approximation is justified as many materials exhibit a collinear magnetic order. However, in recent years much interest has been directed towards noncollinear magnetism in which the magnetization density is a continuous vector variable of position. In this paper we develop the all-electron projector augmented wave (PAW) method for noncollinear magnetic structures, based on a generalized local-spin-density theory. The method allows both the atomic and magnetic structures to relax simultaneously and self-consistently. The algorithms have been implemented within a powerful package called VASP (Vienna *ab-initio* simulation package), which has been used successfully for a large variety of different systems such as crystalline and amorphous semiconductors, simple liquids and transition metals. The approach has been used to study small clusters of Fe and Cr, some of these clusters show noncollinear magnetic arrangements.

A fully parallelized pseudopotential code for noncollinear magnetic systems

Olle Heinonen

Seagate Technology

7801 Computer Ave. S., Bloomington, MN 55435

Magnetic recording sensors based on Giant Magnetoresistance consist of multilayers of non-magnetic and magnetic metallic layers of the order of 10 Å thin. In order to optimize designs, it becomes imperative to understand the electronic and magnetic structure of such multilayered structures. This poses a formidable problem for electronic structure calculations, which have to be able to take into account both relaxation of the atomic and electronic structure and spontaneous breaking, or absence, of point group symmetries of the single-particle density matrix. In other words, calculations cannot be restricted to k -points in the irreducible wedge of the Brillouin zone since this one generally may not be known *a priori*. For example, spin structures near interfaces may be non-collinear. Furthermore, the use of heavy transition metals necessitates the inclusion of spin-orbit interactions, which further complicates the calculations. I have constructed a plane-wave pseudopotential code designed to be able to deal with these kinds of systems. The pseudopotentials are those of Hartwigsen, Goedecker and Hutter, which explicitly include both spin-orbit interactions as well as semi-core electrons in the calculations in order to accurately capture exchange-split states in transition metals. The minimization of the LSDA energy functional does not employ standard sub-space diagonalizations at distinct k -points, but uses a direct conjugate gradient minimization of an extended energy functional which includes all states, occupied and un-occupied, at once. This way, the code can be used for arbitrarily large real-space unit cells and no assumptions about the symmetry of the single-particle density matrix have been made. The code has been fully adapted for parallelization using MPI.

Magnetic interactions in the vicinity of extended lattice defects: examples of calculations for para, soft and hard magnets.

Oleg N. Mryasov, UC Berkeley
Mark van Schilfgaarde, Sandia Natl. Labs
Renat F. Sabiryanov, Nebraska University
Yuri N. Gornostyrev, Metals Physics Institute, Russia

It is commonly accepted extended lattice defects strongly influence magnetic properties of materials. However, the role of specific lattice defects is very poorly understood due to the fundamental difficulties of the modeling extended lattice (dislocations, grain boundaries) and magnetic defects (domain walls) interaction. These principal difficulties originate in that extended lattice defects properties are predetermined by complex balance of (i) atomistic (non-linear) and continuum (linear elastic) static lattice response. Resulting equilibrium lattice distortions, local variation of the symmetry and atomic coordination produce non-trivial variations of the exchange interactions and local magnetic anisotropies which can probably be reliably described only on the basis of electronic structure calculations. In contrast with interatomic interactions, degree of magnetic interactions variation and contribution non-linearities of magnetic response in the vicinity of extended defects remain open questions.

We summarize here our recent experience in addressing these questions using modeling schemes starting from the first-principles electronic structure calculations. Since answers on above general questions are likely to be dependent on the type of magnetic material, we consider examples of : (i) paramagnetic under ambient conditions material (CoTi), (ii) soft magnet (FeCo) and (iii) hard magnet (FePt). In particular, we employ tractable hybrid continuum/atomistic Peierls-Nabarro model with ab-initio parameterization¹ to determine dislocation structure for para (CoTi), soft (FeCo) and hard (FePt) materials. Distribution of the magnetic exchange interactions and magnetic anisotropies determined using real space TB-LMTO and Green Function methods. Characteristic variations of magnetic interaction parameters in the vicinity of lattice defects are related with changes in coordination number, lowering of the symmetry and distribution of distortion fields. Implication of the difference in the length scale of lattice (few tenth of angstroms for dislocation cores) and magnetic defects (hundreds of angstroms for domain walls) for estimates of their interactions using calculated parameters of magnetic interactions is discussed.

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