MA 4: Electron Theory of Magnetism

Time: Monday 10:15–13:15 Location: H23

MA 4.1 Mon 10:15 H23
Magnetic EXAFS on Fe/Ag(100): Experiment and Theory —
●J. Kurde[1], N. Ponpandian[1], J. Luo[1], C. Sorg[1], K. Baberschke[1], and H. Wende[1,2] — [1]Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin-Dahlem, Germany — [2]Angewandte Physik, Fachbereich Physik, Universität Duisburg-Essen, Lotharstr. 1, D-47048 Duisburg, Germany

The $L_{2,3}$ edges of a bcc iron film (13 ML) on Ag(100) have been investigated with magnetic EXAFS (MEXAFS). The absorption spectra were recorded in a k range up to 12 Å^{-1}. The normal or spin-averaged EXAFS confirms clearly a bcc structure. The well known differences [1] of the spin-averaged and magnetic spectra are observed. Beyond this significant intensities for distances larger than 6 Å in the Fourier transform of the magnetic signal are seen and analysed. To achieve a more fundamental understanding of the spin-selective scattering phenomena that determine the MEXAFS, we applied two theoretical models: 1) *ab initio* calculations and 2) the rigid band model [2]. From 1) we can identify each contributing scattering path. Method 2) works surprisingly good, since we can clearly reproduce the observed structures. Hence, one can describe the magnetic scattering by a spin-dependend shift of the scattering potential due to exchange coupling, which can be modeled by the energy-shifted EXAFS spectra. Supported by BMBF (05 KS4 KEB 5).
[1] H. Wende *et al.*, J. Synch. Rad. 6, 696 – 698 (1999)
[2] H. Wende, Rep. Prog. Phys. 67, 2105-2181 (2004)

MA 4.2 Mon 10:30 H23
Relativistic formulation of the Korringa-Kohn-Rostoker nonlocal coherent-potential approximation — ●Diemo D. Ködderitzsch[1], Hubert Ebert[1], and Derwyn Rowlands[2] — [1]Ludwig-Maximilians-Universität München, Department Chemie und Biochemie, Physikalische Chemie — [2]H. H. Wills Physics Laboratory, University of Bristol, Bristol BS8 1TL, United Kingdom

For years the Korringa-Kohn-Rostoker (KKR) coherent-potential approximation (CPA) has been widely and successfully used to describe the electronic structure of disordered systems like alloys. As a single-site mean field theory the CPA is not able to describe short-range order (e.g. clustering) effects. The recently introduced [1] KKR nonlocal coherent-potential approximation (KKR-NLCPA) provides a sound basis for systematically including important environmental effects within an *ab initio* description of disordered systems.

Here we propose a fully relativistic formulation of the KKR-NLCPA which is designed for the treatment of magnetically-ordered alloys. Crucial to its implementation is a reformulation of the basic algorithm and a symmetrisation of the fundamental coarse-graining procedure, which we describe in detail. As a first application of the approach we study the electronic and magnetic properties of the ferromagnetic FePt system.

[1] D.A. Rowlands, J. Phys.: Condensed Matter **16**, 3179, (2006) and references therein; D.A. Rowlands, J.B. Staunton, and B.L.Györffy. Phys. Rev. **B67**, 115109 (2003).

MA 4.3 Mon 10:45 H23
Recent developments in the theory of angle-resolved photoemission (UPS and XPS) — Jan Minar[1], ●Juergen Braun[2], and Hubert Ebert[1] — [1]Dep. Chemie und Biochemie, Physikalische Chemie, Universität München, Butenandtstr. 5-13, D-81377 München, Germany — [2]Inst. f. Mathematik, Universität Hildesheim, Germany

Recent developments and improvements in the resolution of angle-resolved photoemission experiments in the UPS as well as in the XPS regime require an improved (or revised) theoretical description of the photoemission process based on the one-step model. In particular, in several earlies studies the measured spectra were described either within a single particle approach based on DFT(LSDA) including matrix elements effects or by sophisticated many-body approaches neglecting these effects. In our analysis [1], we combined for the first time electronic correlations with matrix elements effects to achieve an improved interpretation of photoemission data from Ni and Fe. This has been done by means of a combined fully-relativistic self-consistent LSDA+DMFT approach [2].

In the second part we present the results for angle-resolved photoe-

mission of Ag in the soft X-ray range. In particular k$_∥$ and photon momentum transfer effects, which are often neglected in the high energy photoemission, are discussed in detail.[3]
1. J. Braun et al., Phys. Rev. Lett 97, 227601 (2006)
2. J. Minár et al., Phys. Rev. B 72, 45125 (2005)
3. F. Venturini, J. Phys.: Cond. Matt., submitted (2006)

MA 4.4 Mon 11:00 H23
Residual resistance calculations of $Ga_{1-x}Mn_xAs$ using the Kubo-Greenwood formalism — ●Stephan Lowitzer[1], Stanislav Chadov[1], Voicu Popescu[2,1], and Hubert Ebert[1] — [1]Department Chemie/Physikalische Chemie, LMU München, Butenandstraße 5-13, 81377 München — [2]Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart

The residual resistance (at T = 0K) of the diluted magnetic semiconductor system (DMS) $Ga_{1-x}Mn_xAs$ has been calculated. For these calculations the Kubo-Greenwood formalism has been employed. The electronic structure calculations is based on the Korringa-Kohn-Rostoker (KKR) band structure method in connection with the coherent potential approximation (CPA) alloy theory. The results show in accordance with other authors a fast decrease of the resistivity with increasing Mn-concentration. This behavior is due to an increase of the density of states at the Fermi edge. Additional calculations show, that the occupation of interstitial positions or the occupation of antisites lead to a clear increase of the resistivity due to disorder. These calculations are in good agreement with experimental data for untreated and tempered samples. Further calculations indicate a small influence of the spin-orbit-coupling on the isotropic residual resistance.

MA 4.5 Mon 11:15 H23
Temperature dependent magnetic properties of low-dimensional systems — ●Svetlana Polesya[1], Sergey Mankovsky[1], Voicu Popescu[2], and Hubert Ebert[1] — [1]Dept. Chemie und Biochemie, Universität München, Butenandtstr. 5-13, D-81377 München, Germany — [2]Max-Planck-Institut für Metallforschung Abt. Schütz, Heisenbergstr. 3, D-70569 Stuttgart, Germany

Temperature dependent magnetic properties of metallic clusters and ultra-thin magnetic films deposited on metallic substrate have been studied on the basis of Heisenberg model using the Monte Carlo simulations as well as Green's function random-phase approximation. The exchange coupling parameters were obtained on the basis of calculations of electronic structure performed within the KKR Green's functions method.

We studied the dependence of the Curie temperature of ultra-thin magnetic films of 3d transition metals on the thickness of these films. The influence of magnetic anisotropy and inter-diffusion at the interface on the temperature dependent magnetic properties of films were studied as well. The effect of covering layers of non-magnetic metals having different thickness on the anisotropy in magnetic films as well as on the Curie temperature have been investigated.

MA 4.6 Mon 11:30 H23
Influence of correlation effects on spin-orbit induced magnetic properties of disordered systems — ●Stanislav Chadov[1], Jan Minár[1], Diemo Ködderitzsch[1], Hubert Ebert[1], and Leonid Pourovskii[2] — [1]Universität München, Dept. Chemie und Biochemie, Physikalische Chemie, Butenandtstr. 5-13, 81377 München — [2]Institute for Molecules and Materials, Radboud University of Nijmegen, NL-6525 ED Nijmegen, The Netherlands

We present results for orbital magnetic moments of the ferromagnets Fe, Co and Ni as well as for disorderd Fe_xCo_{1-x} alloys calculated within the relativistic full potential Korringa-Kohn-Rostoker (KKR) method using the Coherent Potential Approximation (CPA). Particular attention is paid to the influence of local correlation effects which have a noticable effect on the spin-orbit induced properties of 3d transition metal compounds. Local correlations are taken into account within the framework of the Dynamical Mean Field Theory (DMFT) combined with the KKR in a fully self-consistent scheme. The relativistic version of the DMFT solver used in the present work allows to take into account explicitly the interplay of the spin-orbit coupling and local correlations. Therefore, a more accurate treatment of the orbital magnetic moments is obtained. A corresponding comparison

with experimental data is presented.

MA 4.7   Mon 11:45   H23

Magnetic properties of Cr teluride-selenide alloys — •Sergey Mankovsky[1], Svetlana Polesya[1], Hubert Ebert[1], Zhong-Le Huang[2], and Wolfgang Bensch[2] — [1]Dept. Chemie und Biochemie, Universität München, Butenandtstr. 5-13, D-81377 München, Germany — [2]Institute for Anorganic Chemistry, Olshausenstr. 40, D-24098, Kiel, Germany

Results of a theoretical study of the magnetic properties of Cr teluride-selenide alloys having trigonal crystal structure are presented in comparison with experimental results. Both ground state and temperature-dependent magnetic properties of $Cr_{1-\delta}Te$ and $Cr_x(Te_\alpha Se_\beta)_2$ (with ratio $\alpha : \beta = 7 : 1, 6 : 2, 5 : 3$) have been investigated in a wide region of chromium content. For the alloys $Cr_x(Te_\alpha Se_\beta)_2$ a transition to the state with antiferromagnetic order in a fully occupied sub-lattice and with no order in a partially occupied sub-lattice was obtained. For the alloys $Li_x Cr_{0.5} Ti_{0.75} Se_2$, a non-monotonic dependence of structural and magnetic properties have been found upon increase of Li concentration x, that is in agreement with experimental results.

The ground state properties have been studied on the basis of electronic structure calculations using the Korringa-Kohn-Rostoker (KKR) band structure method combined with the CPA alloy theory. Using Monte Carlo simulations we obtained the magnetic configuration at $T = 0K$ and studied the magnetic properties at $T > 0K$ as well. The required exchange coupling parameters were obtained from our ab-initio electronic structure calculations.

MA 4.8   Mon 12:00   H23

Magneto-kristalline Anisotropie von FePt in Abhängigkeit von der Unordnung — •Gerhard Kuhn, Michal Kosuth, Diemo Koedderitzsch und Hubert Ebert — Department Chemie und Biochemie / Physikalische Chemie, Universität München, Butenandtstr. 5-13, D-81377 München, Germany

Die magnetischen Eigenschaften von FePt in der CuAu-Struktur wurden mittels des KKR (Korringa-Kohn-Rostoker)-Bandstrukturverfahrens untersucht. Die Verwendung der Coherent Potential Approximation erlaubte dabei den Einfluß einer Interdiffusion der beiden Teilgitter zu untersuchen. Die Verwendung der relativistischen Version ermöglichte die Berechnung von Spin-Bahn-induzierten Größen wie orbitales Moment und die magneto-kristalline Anisotropie. Für tetragonales geordnetes FePt wurde, im Einklang mit dem Experiment, die leichte Achse senkrecht zu den Fe- bzw. Pt-Atomlagen gefunden. Eine Interdiffusion zwischen den Fe- und Pt-Atomlagen führt zu einem raschen Abbau der Anisotropie. Im Grenzfall einer tetragonalen Legierung verbleibt eine kleine Anisotropie mit der leichten Richtung längs der c-Achse. Die Annahme einer kubischen Einheitszelle verändert die Ergebnisse nur geringfügig, wobei im Falle der Legierung die drei kubischen Achsen äquivalent sind.

MA 4.9   Mon 12:15   H23

Magnetic behaviors under pressure of some cubic Laves phase compounds — •Wenxu Zhang, Manuel Richter, and Helmut Eschrig — Leibniz Institute for Solid State and Materials Research Dresden,Dresden,Germany

The electronic structures of four *Laves* phase iron compounds(e.g. YFe_2,$ZrFe_2$,$LuFe_2$,and $HfFe_2$) have been calculated by the state-of-the-art LSDA code FPLO. The magnetic moments collapse under hydrostatic pressure. This feature is found to be universal in these materials. Its electronic origin is provided by the sharp peaks in the density of states near the Fermi level. The bonding characteristics are discussed to elucidate the equilibrium lattice constant variation. Possible occurrence of superconductivity under pressure, e.g. close to the quantum critical points, is proposed.

MA 4.10   Mon 12:30   H23

Representation of the adiabatic magnetic energy on the atomic level by the spin-cluster expansion technique — •Reinhard Singer, Frank Dietermann, and Manfred Fähnle — Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart

The adiabatic magnetic energy on an atomic level may be represented in principle exactly within the spin-cluster expansion (SCE) [1] by contributions arising from all possible spin clusters. The basis functions for this representation thereby are constructed from a complete set of one-spin basis functions (like, e.g. spherical harmonics $Y_{lm}(\mathbf{e}_i)$) of the unit vector $\mathbf{e}_i$ describing the orientation of the atomic magnetic moment at site i. The complete set of cluster basis functions is then obtained by reducing each corresponding direct product of one-spin functions according to the symmetry restrictions of the magnetic system under consideration, i.e., time-reversal and rotational invariance in the case of isotropic magnets.[2] The expansion coefficients corresponding to the cluster basis functions can be practically obtained by carefully fitting to reference configurations calculated with the ab-initio electron theory. The so constructed SCE of the magnetic energy comprises ab-initio accuracy and thus lends itself to quickly find the true magnetic ground state in complicated systems, to thermo-statistical methods like Monte-Carlo simulations, or to large scale spin dynamics simulations. First results for the SCE of fcc Fe and fcc Ni are presented.

[1] R. Drautz and M. Fähnle, Phys. Rev. B 69, 104404 (2004).
[2] R. Singer and M. Fähnle, J. Math. Phys. 47, 113503 (2006).

MA 4.11   Mon 12:45   H23

On the theory of x-ray absorption spectroscopy in solids: Mixing of the core states by the aspherical effective potential — •Christos Kostoglou[1], Matej Komelj[2], and Manfred Fähnle[1] — [1]Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart — [2]Jožef Stefan Institute, Jamova 39, SI 1000 Ljubljana, Slovenia

For the early transition metals the spin-orbit splitting of the $2p_{1/2}$ and the $2p_{3/2}$ core states is rather small. As a consequence, the $2p_{1/2}$ and $2p_{3/2}$ excitations by x-ray absorption at the L edges exhibit a quantum mechanical mixing which has an influence on the x-ray absorption spectrum. The main source for this mixing is a many-electron effect, i.e., the Coulomb interaction between the core hole (created by the absorption) and the valence electron. We discuss another possible source which so far has never been quantified and which is a one-electron contribution, i.e., the mixing of the two core states by the aspherical part of the static effective potential. We calculate the influence of this mixing on the x-ray magnetic dichroism spectrum of CrO_2 within the framework of the perutbation theory for nearly-degenerate states and within the ab-initio density functional electron theory in the LDA+U version. It turns out that the effect of this type of mixing on the spectrum is rather small.

MA 4.12   Mon 13:00   H23

Orbital magnetism in UN and UT$_2$Si$_2$ compounds — •Carsten Neise, Mahdi Sargolzaei, Klaus Koepernik, Ingo Opahle, Manuel Richter, and Helmut Eschrig — IFW Dresden, P.O.B. 270016,D-01171 Dresden Germany

Usually orbital moments are underestimated in spin polarized relativistic density functional calculations. To get rid of this problem, so-called orbital polarisation (OP) corrections were introduced first in [1] and later derived in a slightly different form in [2].
In this work OP corrections have been applied for UN compound and UT_2Si_2 compounds, where T is (Co,Cu,Cr,Fe,Mn,Ni,Os,Pd,Rh,Ru), with a focus on the orbital moment. The results of the individual atomic moments in these compounds will be compared with available experimental data and calculations in literature.

[1] O. Eriksson, M.S.S. Brooks and B. Johansson, Phys. Rev. B 41 (1990), 7311-7314
[2] H. Eschrig, M. Sargolzaei, K. Koepernik and M. Richter, Europhys. Lett. 72 (2005), 611-617