MA 26 Electron Theory

Time: Thursday 10:15–13:15 Room: HSZ 401

MA 26.1 Thu 10:15 HSZ 401

Spin-polarised systems treated with a relativistic optimised potential method. — •D. Ködderitzsch and H. Ebert — Ludwig-Maximilians-Universität München, Department Chemie, Physikalische Chemie, Germany

The optimised effective potential (OEP) method (OPM) opens a way to explore orbital dependent exchange-correlation (xc) functionals (E_{xc}) within density-functional theory (DFT) in order to tailor new functionals for, e. g. an improved description of spin-orbit induced orbital magnetism.
Here we present the first implementation of a spin-polarised fully relativistic OPM-method (ROPM) for open-shell systems. We have reformulated the ROPM in terms of Green's functions and sketch our subsequent implementation within the framework of the KKR-scattering theory for spin-polarised solids. We adopted and extended different approaches for solving the ROEP-equation [1,2,3] and present first applications to open-shell systems (free atoms) using exact exchange in our approximation for E_{xc}. Further we outline our route towards an implementation for magnetic solids including the random-phase approximation for the correlation functional and make contact to current-DFT.

[1] J.D. Talman and W.F. Shadwick, Phys. Rev. A **14**, 36 (1976).
[2] T.Kreibich *et al.*, Phys. Rev A **57**, 138 (1998).
[3] S.Kümmel and J.P.Perdew, Phys. Rev Lett. **90**, 43004 (2003).

MA 26.2 Thu 10:30 HSZ 401

Orbital magnetism of Co impurities in Au — •Mahdi Sargolzaei, Ingo Opahle, Manuel Richter, Klaus Koepernik, Ulrike Nitzsche, and Helmut Eschrig — IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

The electronic structure of cobalt impurities inside gold has been calculated in the framework of local spin density approximation including two dufferent variants of orbital polarization corrections [1,2]. Orbital and spin magnetic moments have been evaluated using the relativistic version of the full-potential local-orbital minimum-basis code. In agreement with recent experimental and theoretical findings, the orbital moment is considerably enhanced in comparison with Co metal. It is demonstrated that lattice relaxation around the impurities reduces the orbital moment by about 15%. Co in Au is also an example for systems with high anisotropy energy and large orbital moment which compared to hcp Co are one order of magnitude larger.

1- O. Eriksson, B. Johansson, M. S. S. Brooks, J. Phys. Cond. Mat. 1, 4005 (1989).
2- H. Eschrig, M. Sargolzaei, K. Koepernik, M. Richter, Europhys. Lett. 72, 611 (2005).

MA 26.3 Thu 10:45 HSZ 401

Fully relativistic one-step theory of ultraviolet (inverse) photoemission for correlated systems: Application to ferromagnetic Ni and Fe. — •Jürgen Braun, Jan Minar, and Hubert Ebert — Department Chemie/Phys. Chemie, Ludwig-Maximilians-Universität München, Butenandt Str. 11, 81377 München

An improved formulation of the one-step model of photoemission from crystal surfaces is proposed which overcomes different limitations of the original theory. Considering the electronic one-particle potential and the many-body self-energy as given quantities, we derive an explicit expression for the spin-polarized photocurrent. The theory is formulated within a fully relativistic framework for a general nonlocal and space-filling, complex and energy-dependent self-energy which is based on a self-consistent DFT-DMFT calculation. Using the relativistic version of the layer-dependent Korringa-Kohn-Rostocker (KKR) multiple scattering formalism, the theory applies to semi-infinite lattices with perfect lateral translational invariance and arbitrary number of atoms per unit cell. Here, we present a quantitative analysis of experimental photoemission data from ferromagnetic Ni and Fe.

MA 26.4 Thu 11:00 HSZ 401

Spontaneous magnetostriction in elemental ferromagnets investigated with a DLM approach — •Ulrike Nitzsche, Manuel Richter, Klaus Koepernik, and Helmut Eschrig — IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

The large change of lattice parameters caused by magnetic order of elemental hcp Gd was been a subject of intensive studies in the past. In several ab-initio calculations the value of the spontaneous volume magnetostriction of Gd was overestimated by a factor of 2 to 4. An important point is the modelling of the paramagnetic state of Gd above T_C characterized by the non-vanishing fluctuating f-moments. Besides the usually used method to model this state by a supercell with ordered antiferromagnetic spin configurations one can simulate the magnetic disorder in the paramagnetic state by disordered local moments (DLM) within the coherent potential approximation (CPA).
Up to now no comparison of both models has been published using the same numerical method. Aim of this talk is to investigate the influence of the different models for the paramagnetic state on the value of the spontaneous magnetostriction for the elemental ferromagnets Gd, Fe and Ni. Additional contributions to the spontaneous magnetostriction are discussed.

MA 26.5 Thu 11:15 HSZ 401

Giant magneto-crystalline anisotropies in transition-metal monowires — •Yuriy Mokrousov[1,2], Gustav Bihlmayer[2], Stefan Heinze[1], and Stefan Blügel[2] — [1]Institute for Applied Physics, University of Hamburg, 20355 Hamburg, Germany — [2]Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany

We report on first-principles calculations of the magnetic properties of freestanding 3d, 4d and 5d transition-metal (TM) monoatomic chains. Our calculations were performed with the one-dimensional (1D) version of the full-potential linearized augmented plane-wave (FLAPW) method, as implemented in the FLEUR code [1]. The new 1D-FLAPW scheme is extremely fast and allows a natural treatment of structures with 1D geometry. We investigate the origin of magnetism in TM monoatomic wires, paying special attention to the influence of spin-orbit interaction on the magnetic properties. We present equilibrium interatomic distances, spin- and orbital moments and the values of the magneto-crystalline anisotropy energy (MAE). Across the series the easy axis of magnetization oscillates between two possible directions: perpendicular and along the wire axis. The largest values of the MAE occur at the end of the series. Giant values of 30-100 meV/atom can be obtained upon stretching of 4d- and 5d-TM wires. Certain chains change the magnetization direction upon wire stretching, opening new perspectives in controlling the spin-dependent ballistic conductance in these structures.

[1] Y. Mokrousov, G. Bihlmayer and S. Blügel, Phys. Rev. B, 72, 045402 (2005)

MA 26.6 Thu 11:30 HSZ 401

Pressure induced magnetic collapse in $ZrFe_2$ predicted by theoritical calculation — •Wenxu Zhang, Klaus Koepernik, Ulrike Nitzsche, and Manuel Richter — IFW Dresden, P.O. Box 270016, D-01171 Dresden,Germany

Electronic structure and magnetic properties of $ZrFe_2$ with the cubic Laves phase are investigated by scalar and full-relativistic full-potential local-orbital minimum basis band structure calculations. The total magnetic moment of $3.06\mu_B$ is obtained at experimental lattice constant ($7.06\AA$), which is a little larger than the one at equilibrium lattice constant($2.6\mu_B$ at $6.85\AA$). The scenario of a localized $3d$ magnetic moment in negative diffusive sp background moment is in accordance with previous results by P. Mohn. We predict a two steps magnetic collapse: one is from $3.06\mu_B$ to $1.26\mu_B$ at about 3.6GPa, and the other is from $1\mu_B$ to paramagnetic state at about 20 GPa. The magnetic moment(m) decreases under the pressure at the vinicity of the experimental lattice constant with $d\ln m/dp = -0.038GPa^{-1}$. The spantanous magnetostriction is 0.015. The Invar effect in this alloy is suggested to relate to the magnetic transition.

MA 26.7 Thu 11:45 HSZ 401

Exchange coupling and finite temperature magnetism in chromium-chalcogenide compounds — •Sergey Mankovsky[1], Svetlana Polesya[1], Hubert Ebert[1], Wolfgang Bensch[2], and Zhong-Le Huang[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

Using the Korringa-Kohn-Rostoker (KKR) band structure method, a detailed theoretical investigation of the electronic and magnetic properties of $Cr_{1+x}Q_2$ (Q=(Te-Se), $x = 0.25 \div 1$) alloys having a trigonal crystal structure have been performed. The disorder in the system has been accounted for by means of the Coherent Potential Approximation (CPA). The influence of Cr content on structural and magnetic properties was studied within the whole region of Te and Se concentrations. The stability of magnetic structures in these alloys have been studied both for $T = 0K$ and $T \neq 0K$. The temperature dependent magnetic properties have been performed using the Monte Carlo simulations based on the Heisenberg model. The required exchange coupling parameters were obtained from ab-initio electronic structure calculations. The detailed analysis of our theoretical results have been done in comparison with the experimental data.

MA 26.8 Thu 12:00 HSZ 401

Organic Antiferromagnets, Diluted Magnetic Semiconductors, and Iron — Novel Features in the Magnetism in Correlated Electrons — •Avinash Singh — Department of Physics, Indian Institute of Technology Kanpur — Institute for Physics, Humboldt University at Berlin

There has been renewed interest in correlated electron systems on triangular lattices, as evidenced by recent studies of antiferromagnetism, superconductivity and metal-insulator transition in the organic systems $\kappa - (BEDT - TTF)_2X$, the discovery of "water superconductors" $Na_xCoO_2.yH_2O$, the observation of low-temperature insulating phases in some $\sqrt{3}$-adlayer structures such as K on Si[111], and quasi two-dimensional 120° spin ordering and spin-wave excitations in $RbFe(MoO_4)_2$ and the multiferroic material $HoMnO_3$. The discovery of ferromagnetism in Mn-doped III-V semiconductors such as $Ga_{1-x}Mn_xAs$, has led to considerable interest in these diluted magnetic semiconductors (DMS) in view of their potential applications such as optical isolators, magnetic sensors, non-volatile memories seamlessly integrated into semiconductor circuits etc. and the possibility of studying new magnetic cooperative phenomena such as spin-dependent tunneling, magnetoresistance, spin-dependent light emission etc. in semiconductor heterostructures arising from the new (spin) degrees of freedom. I will describe some novel features in the magnetism of these materials of current interest, and also discuss recent progress in our understanding of the classic strong-coupling problem of a band ferromagnet such as iron.

MA 26.9 Thu 12:15 HSZ 401

Electronic structure of *RE*AuMg and *RE*AgMg (*RE* = Eu, Gd, Yb) — •Jan Gegner[1], T.C. Koethe[1], Hua Wu[1], H. Hartmann[1], T. Lorenz[1], T. Fickenscher[2], R. Pöttgen[2], and L.H. Tjeng[1] — [1]II. Physikalisches Institut der Universität zu Köln, Germany — [2]Institut für Anorganische und Analytische Chemie,Westfälische Wilhelms-Universität Münster, Germany

We have investigated the electronic structure of the equiatomic EuAuMg, GdAuMg, YbAuMg and GdAgMg intermetallics using x-ray photoelectron spectroscopy. The spectra revealed that the Yb and Eu are divalent while the Gd is trivalent. The spectral weight in the vicinity of the Fermi level is in all cases dominated by the mix of Mg *s*, Au/Ag *sp* and *RE spd* bands, and not by the *RE* $4f$. We also found that the Au and Ag *d* bands are extraordinarily narrow, as if the noble metal atoms were impurities submerged in a low density *sp* metal host. The experimental results were compared with band structure calculations, and we found good agreement provided that the spin-orbit interaction in the Au an Ag *d* bands is included and correlation effects in the open $4f$ shells are accounted for using the LDA+U scheme. Nevertheless, limitations of such mean-field scheme to explain excitation spectra are also evident.

MA 26.10 Thu 12:30 HSZ 401

Calculated de Haas-van Alphen frequencies of $NpCoGa_5$ — •Ingo Opahle[1], Saad Elgazzar[1], Vito D.P. Servedio[2], Manuel Richter[1], and Peter M. Oppeneer[3] — [1]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]Dip. di Fisica, Univ. di Roma "La Sapienza", 00185 Roma, Italy — [3]Department of Physics, Uppsala University, Box 530, S-751 21 Uppsala, Sweden

The electronic structure and magnetic properties of $NpCoGa_5$ are investigated in the framework of relativistic density functional theory in the local spin density approximation (LSDA) with and without orbital polarization (OP) corrections. A detailed analysis of the Fermi surface is presented. Comparison of the calculated angular dependence of the de Haas-van Alphen frequencies with recent experimental data shows that LSDA reproduces the main features of the Fermi surface topology, while the spin and orbital moments of $NpCoGa_5$ are less well described. The inclusion of OP corrections leads to a very good agreement between calculated and measured de Haas-van Alphen frequencies, but does not yield a significant improvement of the calculated magnetic properties. We predict that $NpCoGa_5$ shows an intrinsic GMR effect at moderate magnetic field.

MA 26.11 Thu 12:45 HSZ 401

Accounting for correlation effects in the calculation of the spin-orbit induced properties of magnetic transition metals — •Stanislav Chadov[1], Jan Minár[1], Hubert Ebert[1], Leonid Pourovskii[2], Michael Katsnelson[2], and Alexander Lichtenstein[3] — [1]Department Chemie und Biochemie, Physikalische Chemie, Universität München, Butenandtstr. 5-13, D-81377 München, Germany — [2]Institute for Molecules and Materials, Radboud University of Nijmegen, NL-6525 ED Nijmegen, The Netherlands — [3]Institut für Theoretische Physik, Universität Hamburg, 20355 Hamburg, Germany

Recently we proposed a charge- and self-energy- self-consistent computational scheme on the basis of the Korringa-Kohn-Rostoker (KKR) multiple scattering theory including many-body effects described by the dynamical mean field theory (DMFT). It was successfully applied to moderately correlated systems, showing the importance to account for the electronic correlations in the calculation of a wide range of their spectroscopic properties (Fano effect, spin-resolved VB-XPS, magneto-optical spectra).

Here we present an extention of the scheme allowing one to consider the influence of electronic correlations on the spin-orbit induced properties by taking into account spin polarization as well as spin-orbit coupling in the many-body solver. The latter is important for systems pocessing both localized and itinerant features as the interplay of relativistic effects and electron-electron correlations makes the calculation of the corresponding electronic properties quite complicated. First results of investigations on 3d transition metals will be presented.

MA 26.12 Thu 13:00 HSZ 401

Electronic structure and Fermi Surfaces of Transuranium* Copmounds UMGa$_5$ ($M=$Pd and Pt)* compounds — •Saad Elgazzar, Ingo Opahle, and Manuel Richter — IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

We report a critical analysis of the electronic structures and de Haas-van Alphen (dHvA) quantities of the heavy-fermion UPdGa$_5$ and UPtGa$_5 $. The electronic structures are investigated {\it ab initio} on the basis of full-potential band-structure calculations, adopting the fully relativistic formulations in the framework of the local spin-density approximation (LSDA) with and without orbital polarization (OP) corrections. The calculated calculated dHvA quantities are in good agreement with experimental data for both compounds recently published \cite{Ikeda}

\bibitem{Ikeda} S. Ikeda, {\em et al.}, JPSJ, {\bf 74} (2005) pp.2277-2281.