Report on Hands-on Course
”KKR Bandstructure and Spectroscopy Calculations”

A hands-on course on the KKR method entitled ”KKR Bandstructure and Spectroscopy Calculations” took place in München 9-11 June 2005. It welcomed 28 participants and 20 lecturers (the list of participants and lecturers is given below).

The aim of the workshop was to introduce new users from theory as well as experiment into the Munich SPR-KKR (spin polarized relativistic Korringa-Kohn-Rostoker) program package (see http://olymp.cup.uni-muenchen.de/ak/ebert/SPRKKR/). The highly automated program package not only allows to study the electronic structure of solids by calculating bands, densities of states, total energies etc, but also gives access to the calculations of many spectroscopic properties as probed for example by XANES, EXAFS, magneto-optics, angle integrated photoemission, Auger electron spectroscopy or Compton scattering. The codes can be run in a non-relativistic and relativistic manner and contain several tools to analyse the effect of the spin-orbit interaction. Moreover, the package can treat ordered and disordered alloys and magnetic multilayers. In addition, the package supplies many tools to analyse the electronic structure such as wave function, phase shift or matrix element plots. All of this was embedded into an easy to use multi purpose Graphical User Interface (GUI) called XBAND (see http://olymp.cup.uni-muenchen.de/ak/ebert/xband.html), that can easily be adopted to support other bandstructure packages. Set exercises for three afternoons were prepared to give the participants the opportunity to acquaint themselves with all features of performing electronic structure and spectroscopy calculations. In addition, the participants were also given the opportunity to investigate systems of their own interest together with their spectroscopic properties.

A series of lectures accompanied the practical hands-on sessions. Nearly all lecture notes can be found under:
http://olymp.cup.uni-muenchen.de/ak/ebert/Handson_2005/. The fundamentals of the KKR method were taught by W. Temmerman and Z. Szotek. The relativistic version of the KKR and its implementation in the Munich SPR-KKR package were introduced by H. Ebert. The calculation of spectroscopic properties using the program package was demonstrated by J. Minar. As recent applications results on the high-field susceptibility of ferromagnetic

metals, ferromagnetic clusters at finite temperature and free transition metal clusters were presented by S. Mankovskyy, S. Polesya and O. Sipr, respectively. In addition, there were invited theoretical talks: P. H. Dederichs dealt with diluted magnetic semiconductors and A. Soldatov reported on his work on XAFS of small nanoclusters. These presentations were complemented by invited talks given by experimentalists: H. Wende dealt with XAS of light 3d elements as a benchmark for ab initio calculations, K. Baberschke also addressed the relationship of experiment and theory concerning the magnetism of 3d monolayers grown with oxygen surfactant, J. Schmalhorst demonstrated the power of soft X-ray spectroscopy to investigate the interface structure and magnetism of magnetic tunnel junctions with Heusler alloy electrodes and W. Warth reported on investigations of the magnetic properties of deposited transition metal clusters by using X-ray spectroscopy.

In addition, many participants presented poster contributions that led to lively discussions during the coffee breaks.

The large number of participants (not all applications could be accepted because the limited number of tutors and available computers), in particular with an experimental background, reflects the need for hands on courses introducing also non-experts to the field. The course in Munich surely succeeded in teaching the participants the basics of the rather complex KKR formalism as well as the use of the very user-friendly Munich SPR-KKR package.

Program:

	Thursday	Friday	Saturday	
9	Ebert	Mankovsky Polesya	Schmalhorst	
10	Minar	Soldatov	Sipr	
	▨	▨	▨	Coffee
11	Wende	Baberschke	Wurth	
12	Dederichs	Temmerman	Szotek	
13	▨	▨	▨	Lunch
14 15	xband SCF	E(k) DOS	spectroscopies	
16	▨	▨	▨	Coffee
17	SCF CPA	ground state properties	spectroscopies	
18				
19 20		Dinner Weißes Bräuhaus		

Speakers:

H. Ebert	München	The Munich SPRKKR package
J. Minar	München	Calculating spectroscopic properties with the Munich SPRKKR package
H. Wende	Berlin	XAS of light 3d elements: a benchmark for ab initio calculations
P. H. Dederichs	Jülich	Diluted magnetic semiconductors
S. Mankovsky	München	High-field magnetic susceptibility of ferromagnetic metals
S. Polesya	München	Ferromagnetic clusters at finite temperatures
A. Soldatov	Rostov State University	XAFS of small nanoclusters
K. Baberschke	Berlin	New magnetism of 3d monolayers grown with oxygen surfactant: Experiment vs. ab initio calculations
W. M. Temmerman	Daresbury	KKR-basics I
J. Schmalhorst	Bielefeld	Magnetic tunnel junctions with Heusler alloy electrode: Interface structure and magnetism explored by soft X-rays
O. Sipr	Prague	Free clusters
W. Wurth	Hamburg	Magnetic properties of deposited transition metal clusters from x-ray spectroscopy
D. Szotek	Daresbury	KKR-basics II

Invited speakers and tutors

Baberschke, Klaus – Institut für Experimentalphysik, FU Berlin, Germany
Benea, Diana – Ludwig-Maximilians-Universität München, Germany
Bornemann, Sven – Ludwig-Maximilians-Universität München, Germany
Chadov, Stanislav – Ludwig-Maximilians-Universität München, Germany
Dederichs, P.H. – Forschungszentrum Jülich GmbH, Jülich, Germany
Ebert, Hubert – Ludwig-Maximilians-Universität München, Germany
Kardinal, Marianne – Ludwig-Maximilians-Universität München, Germany
Ködderitzsch, Diemo – Ludwig-Maximilians-Universität München, Germany
Kosuth, Michal – Ludwig-Maximilians-Universität München, Germany
Mankovsky, Sergey – Ludwig-Maximilians-Universität München, Germany

Minar, Jan – Ludwig-Maximilians-Universität München, Germany
Polesya, Svetlana – Ludwig-Maximilians-Universität München, Germany
Popescu, Voicu – Ludwig-Maximilians-Universität München, Germany
Schmalhorst, Jan Michael – University of Bielefeld, Bielefeld, Germany
Sipr, Ondrej – Institute of Physics AS CR, Praha, Czech Republic
Soldatov, Alexander – Rostov State University, Faculty of Physics, Rostov-Don, Russia
Szotek, Zdzislawa – Daresbury Laboratory Daresbury
Temmerman, Walter – Daresbury Laboratory Daresbury
Wende, Heiko – Insitut für Experimentalphysik, Freie Universität Berlin, Germany
Wurth, Wilfried – Institut für Experimentalphysik, Hamburg, Germany

List of participants

Antoniak, Carolin – Universität Duisburg-Essen, Germany
Aziz,Bekhit, Emad Flear – BESSY GmbH, Berlin, Germany
Batt, Gary – Bristol University, UK
Bauer, Matthias – Inst. f. Physik. Chemie, Univ. Stuttgart, Germany
Belhadji, Brahim – Forschungszentrum Jülich GmbH Jülich
Däne, Markus – Martin Luther University, Halle, Germany
Emtsev, Konstantin – Institute of Technical Physics, University Erlangen-Nuremberg, Germany
Fecher, Gerhard H. – Johannes Gutenberg - Universität, Mainz, Germany
Flege, Jan Ingo – University of Bremen, Bremen, Germany
Go, Anna – Institute of Experimental Physics, University of Bialystok, Poland
Goraus, Jerzy – University of Silesia, Katowice, Poland
Johal, Tarnjit – CCLRC Daresbury Laboratory, Daresbury, UK
Kandpal, Hem – University Mainz, Mainz, Germany
Laverock, Jude – University of Bristol, UK
Lueders, Martin – Daresbury Laboratory, UK
Mouketo, Landry – The Abdus Salam ICTP, Trieste, Italy
Müller, Martina – FZ Jülich, Jülich, Germany
M'Passi-Mabiala, Bernard – The Abdus Salam ICTP, Trieste, Italy
Olimov, Khusniddin – Physikalisches Institut, Bonn, Germany
Rowlands, Derwyn – University of Bristol, Bristol, UK

Saha, Kamal – Max Planck Institute of Microstructure Physics Theory Department, Halle (Saale), Germany
Sahnoun, Mohammed – Department of Chemistry, University of Fribourg, Switzerland
Tallarida, Massimo – BTU Cottbus, Germany
Umeno, Yoshitaka – Institut fuer Zuverlaessigkeit von Bauteilen und Systemen (IZBS), Uni Karlsruhe, Germany
Welter, Edmund – HASYLAB at DESY, Hamburg, Germany
Winkelmann, Aimo – MPI für Mikrostrukturphysik, Halle, Germany
Zenia, Hand – Daresbury Laboratory, UK
Zhang, LingFei – University of Salford, Institute for Materials Research, UK

Abstracts

Molecular Structure of NaCl Electrolytes of Varing Concentration

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New magnetism of 3d monolayers grown with oxygen surfactant: Experiment vs. ab initio calculations

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Surfactant assisted growth of nanoscale structures on surfaces is a well established technique. Moreover, it is known that for ultrathin films of Fe, Co, and Ni the magnetic properties are highly sensitive to minimal structural changes: If the nearest neighbour distance varies by 0.03-0.05 $\AA$, only, the magnetic anisotropy energy (MAE) may change by 102-103. So the question arises: Can the growth of ultrathin 3d ferromagnets on single crystal substrates be manipulated using oxygen as a surfactant, or will an antiferromagnetic metal oxide be formed? The answer is threefold: i) We could indeed show by MEED and XAS that the growth is improved up to ¿20 ML and that finally the O atoms "float" on top of the ferromagnetic film (Surf. Sci. **566-568**, 100, *ibid* **565**, 197 (2004)). ii) Recent measurements demonstrate that the magnetic anisotropy energy is significantly enhanced using surfactants. Theory reveals that this is mainly due to the decrease in the magnitude of the surface anisotropy (PRL **92**, 147202 (2004)). iii) Preliminary experiments show that the chemisorbed oxygen atoms on the surface of the ferromagnetic film carry an induced magnetic moment.
The experiments will be discussed in context with ab initio calculations from the groups at Uppsala, Vienna, LMU and UCI.

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Comparative studies of methods for calculating the Fermi Surface of random metallic alloys

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We report on a comprehensive study of the similarities and differences between Molecular CPA [1] and the recently developed Non Local CPA [2] methods for calculating the electronic structure of random metallic alloys (solid solution). In particular we investigate their predictions for the Bloch spectral functions and effective Fermi surface. Furthermore we study the solution of the Fermi surface with bond filling and short ranged chemical order. Our results will be illustrated by explicit calculation based on a one band two dimensional tight-binding model.

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A. Gonis, Greens Functions for Ordered and Disordered Systems, in the series Studies in Mathematical Physics, edited by E. van Groesen and E. M. de Jager (North Holland, Amsterdam, 1992).

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EXAFS/XANES Investigations into the Fe(III)-catalyzed Michael addition Reaction

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The Michael reaction of 1,3-dicarbonyl compounds with α,β-unsaturated carbonyls like methyl vinyl ketone is catalysed by Iron(III) salts under mild conditions with remarkable efficiency. Using $FeCl_3$ $6H_2O$ and $Fe(ClO_4)_3$ $9H_2O$ the disadvantages of traditional catalysts like Brönsted bases such as side and subsequent reactions can be avoided. In addition the environmentally friendly and cheap catalysts do not require special reaction conditions and no solvent is needed. The mechanism for this reaction has been proposed.

In this contribution we focus on the first step of the reaction cycle. The nature of complex 1 formed by dissolving $FeCl_3$ $6H_2O$ or $Fe(ClO4)_3$ $9H_2O$

in the β-keto ester Ethyl 2-oxocyclopentanecarboxylate (EOP) is so far unknown. Experimentally $FeCl_3$ $6H_2O$ shows a reduced catalytic activity compared to $Fe(ClO_4)_3$ $9H_2O$. Additionally the catalytic activity of $Fe(ClO_4)_3$ $9H_2O$ is reduced when Cl^- ions are added to the reaction mixture. Calculations in the gas phase predict binding of the chloride ions to the iron centre resulting in a reduced ability of the iron to coordinate ester molecules. To provide experimental proof, EXAFS and XANES-spectra of 2 mol% solutions of $FeCl_3$ $6H_2O$ and $Fe(ClO_4)_3$ $9H_2O$ in EOP were recorded together with several references and were analyzed with special focus on the coordination geometry of the iron centre by pre-peak evaluation.

The Munich SPR-KKR code

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The talk gives a short introduction to the functionality and formal background of the Munich spin-polarised relativistic (SPR-KKR) program package (see http://olymp.phys.chemie.uni-muenchen.de/ak/ebert/SPRKKR/). First, in short the various available calculation modes, the electron structure information that can be obtained and the various kinds of electronic spectroscopy that can be studied are surveyed. Presenting the formal background of the SPR-KKR package emphasise is laid on the fully relativistic mode for magnetic solids. Technical details connected with that as for example the coupled radial Dirac equations, the single site t-matrix, symmetry considerations are discussed in some detail. Two ways to determine the so-called scattering path operator are explained: The real space cluster mode is used for high energies (EXAFS) and to deal with surfaces at the moment. The Brillouin zone integration technique, on the other hand, is used as the standard method for most other purposes. Using this technique exploiting symmetry is indispensable. The simultaneous presence of spin-orbit coupling and spin magnetisation, however, has rather important consequences for this as it is demonstrated. An important feature of the program package is the ability to deal with disordered systems by using the CPA (Coherent Potential Approximation). The basic ideas of he CPA are described and its implementation within the KKR-method is outlined. Finally, a short outlook on future developments is presented.

Electronic properties of clean unreconstructed 6H-SiC(0001) surfaces studied by angle resolved photoelectron spectroscopy

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The properties of the clean and unreconstructed SiC(0001) and SiC(000-1) surfaces were investigated by means of angle-resolved ultraviolet photoelectron spectroscopy. The measurements were conducted at the synchrotron light source BESSYII using a newly designed spectrometer of toroidal geometry (TEA) allowing us to collect all emission angles in one azimuthal plane simultaneously.

The clean, unreconstructed surfaces were prepared by exposing hydrogen terminated surfaces to a high flux of synchrotron radiation. Earlier findings on Si-rich $(\sqrt{3} \times \sqrt{3})R30^o$ and (3x3) reconstructed surfaces of SiC show an interesting behavior in that the dangling bond surface bands undergo a Mott-Hubbard metal-insulator transition. The question addressed in this report is whether 11 unreconstructed SiC(0001) surfaces are still in the Mott-Hubbard regime or whether they exhibit the metallic surface suggested by theoretical calculations that don't take correlation effects into account.

First of all, valence band spectra show no states at the Fermi level before and after irradiation, that is, clean surfaces are semiconducting. Second, for Si and C terminated surfaces irradiation results in the appearance of the dangling bond states ≈0.8eV above, and close to the valence band maximum, respectively. These states lie in the gap of the projected bulk band structure. The bandwidth amounts to 0.2 and 0.6 eV for Si and C dangling bonds, respectively. Hydrogen desorption is accompanied by the disappearance of H-induced states in the valence band. Except for the location of the dangling bond band the electronic structure of the clean unreconstructed surfaces agrees with the existing band structure calculations. Therefore, clean unreconstructed Si- and C-truncated surfaces of 6H-SiC surfaces represent further examples of a Mott-Hubbard insulating surface despite a separation of the dangling bonds that is markedly reduced in comparison with the reconstructed surfaces.

Photon-stimulated Desorption and X-ray Standing Waves

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X-ray standing waves (XSW) using electrons and fluorescence photons as secondary signals have become a standard technique to determine adsorbate structures. However, when a sample is irradiated by intense light, desorption of ions is also a frequently observed phenomenon that is known as photon-stimulated desorption (PSD). But this signal is of a fundamentally different physical nature. The identification of this process has been a persistent topic in surface science throughout the last decades. By virtue of the inherent periodic time structure of synchrotron radiation, an efficient detection of positive ions emitted from the surface is feasible using time-of-flight spectroscopy. In this review, we will survey the relevant desorption mechanisms which initiate the prevailing processes. We will show that the combination of X-ray standing waves with X-ray PSD (XPSD) is a unique tool to identify the underlying desorption processes in a site-specific manner. In the contribution we will deal with the systems Si(111)-(7 x 7), H/Si(111)- (1 x 1), Ge/Si(111)-(1 x 1):H, and Cl/Si(111). This choice serves to illustrate the peculiarities of the different kinds of desorption processes and to demonstrate the general approach to the interpretation of XSW-XPSD data.

Site preference of manganese in $Fe_{3-x}Mn_xAl$ alloys

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A lot of attention has recently been paid to understand the fascinating structural and physical properties of iron aluminides that arise when some Fe atoms are substituted by other transition-metal atoms. Intermetallic compound Fe_3Al is a ferromagnet with DO_3-type crystal structure. The crystal lattice can be described as four interpenetrated face-centred cubic Bravais lattices originated at (0,0,0), (1/4,1/4,1/4), (1/2,1/2,1/2) and (3/4,3/4,3/4), and abbreviated as A, B, C and D, respectively. In the perfectly ordered structure there are two non- equivalent iron sites with different chemical neighbourhood - (A,C) and B sublattices. As a consequence different electronic and magnetic properties connected with these positions are observed as well as different site preferences depending on the element substituting for iron take place. According to Mössbauer and electron spectroscopy the doping manganese atoms have been found to occupy B sublattice [1]. However, nonempirical studies indicate that for x=0.2 manganese atoms preferentially occupy (A,C) sublattice and does not show any site preference for the lower of the considered concentrations [2]. The aim of our research is to investigate the site preference of atoms in compound $Fe_{3-x}Mn_xAl$ where iron is substituted by manganese. Results of the calculations carried out with the SPRKKR method [3] with the experimental values of the lattice parameter [4] are presented.

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Electronic structure of Ce2Rh3Al9

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Ce2Rh3Al9 is an interesting compound, known to possess mixed valence properties and unusual temperature dependence of resistivity. We have measured specific heat, electrical resistivity, magnetical susceptibility and XPS spectra of that compound. Moreover we calculated DOS by means of FP-LAPW and TB-LMTO-ASA method. Both methods predict pseudogap located on Fermi level. FP-LAPW result in half-metalic and LMTO in non-magnetic character of this compound. In low temperature resistivity, however, we do not see activated part, our explanation is that due to atomic disorder the gap is destroyed. Magnetical measurements don't show any ordering down to 2K, therefore the LMTO calculations seems to depict better the properties of that compound. Agreement between measured valence band spectra and calculated one is also quite good.

Calculated electronic structure of X_2YZ Heusler compounds

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Half metallicity has long been predicted using band structure method in the half Heulser NiMnSb and some other materials. More recently, certain full Heusler alloys have been predicted to show half metallicity. In this work, we present calculations on a series of X_2YZ full Heusler compounds which show the phenomenon of half metallic ferromagnetism. The crystal structures have been obtained for some of the compounds through structural relaxation in the first principles framework determining the minimum total energy as function of the lattice parameter. We find that mostly Co based Heusler compounds are exhibiting half metallic behaviour. We also analyze the influence of the lattice parameter on the minority band gap. We find that smaller lattice parameter result in larger minority band gaps. The width of the gap is seemingly a linear function of the lattice constant. X=Co based Heusler compounds exhibit high Curie temperature with a linear dependence on the number of valence electrons. Our results show that Co based Hesuler compounds obey the Slater-Pauling rule, while most of the others do not. There are slight changes in the magnetic moment of the Co atoms, while the magnetic moment of Y increases with the number of valence electrons. The pecularities of the electronic structure suggest that the Co based Heusler compounds are the best candidates for various spintronics applications.

Fermi surface nesting and charge-density-wave order in rare earth tri-tellurides

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The Fermi surface of rare-earth tri-tellurides ($R\mathrm{Te}_3$) is investigated in terms of the nesting driven charge-density wave formation using positron annihilation and first-principles LMTO calculations. Fermi surface nesting is revealed as a strong candidate for driving charge-density wave formation in these compounds. The nesting vector obtained from positron annihilation experiments on GdTe_3 is determined to be $\mathbf{q} = (0.28 \pm 0.02, 0, 0)\ \mathbf{a}^*$, $(\mathbf{a}^* = 2\pi/\mathbf{a})$, in excellent agreement with previous experimental and theoretical studies.

Self-interaction correction (SIC) in multiple-scattering theory

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We present applications of the Layer-KKR method, including the coherent potential approximation (CPA) to the calculation of the electronic structure and the photocurrents of magnetic multilayers. We discuss how the photoemission calculations can help to analyse experimental spectra. We present photo-emission spectra of quantum well systems. Furthermore we report on calculations of the magnetic moments of ultrathin films of Ni and V.

Self-interaction correction (SIC) in multiple-scattering theory

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We propose a simplified version of self-interaction corrected local spin-density (SIC-LSD) approximation, based on multiple scattering theory, which implements self-interaction correction locally, within the KKR method. The multiple scattering aspect of this new SIC-LSD method allows for the description of crystal potentials which vary from site to site in a random fashion and the calculation of physical quantities averaged over ensembles of such potentials using the coherent potential approximation (CPA). This facilitates applications of the SIC to alloys and pseudoalloys which could describe disordered local moment systems, as well as intermediate valences. As a demonstration of the method, we study the well-known α-γ phase transition in Ce, where we also explain how SIC operates in terms of multiple scattering theory.

Influence of atomic relaxation on the magnetic properties of Mn/Ni(001) system

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The Mn bulk ground state being essentially of non-ferromagnetic type, a spin flop towards ferromagnetism can be induced by strong 3d ferromagnets (Fe, Co, Ni) [1, 2]. We discuss the geometric optimization and the onset of ferromagnetism in Mn/Ni(001) system. Spin-polarized (with collinear magnetism) calculations within the density functional approach of *Kohn and Sham* and beyond local density approximation are performed by the pseudopotential code PWscf. This calculations are supported by the recent experimental works [3, 4, 5]. The results obtained showing evidence of NiMn surface alloy formation, a contraction of the Ni atomic positions in the overlayer after relaxation in the cases of Ni(001) clean surface and NiMn alloy on Ni(001) and, an outwards buckling of Mn atoms in the cases of Mn metallic and NiMn alloy on Ni(001).

References

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Determination of lattice site occupation and oxidation state of Fe and Mn ions in doped $LiNbO_3$ and investigation of structural changes of $Ni_{50}Mn_{30}Ga_{20}$

freestanding films in dependence on the temperature of RTA (Rapid Thermal Annealing) by means of XAS (X-ray Absorption Spectroscopy)

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In the present work experimental XANES (X-ray Absorption Near Edge Structure) spectra of both Mn and Fe (EQ70 and EQ729 sample) in doped $LiNbO_3$, at Mn and Fe K-edge respectively, are analyzed and compared to the calculated using FEFF8 code[1] spectra. In FEFF8 code calculations the FMS (Full Multiple Scattering) approach within the cluster of atoms (within the R=6.35 $\AA$ around absorbing atom) constructed according to the crystal structure data of $LiNbO_3$ (where Mn (Fe) is assumed to be either on Li or Nb site in $LiNbO_3$ matrix) is applied. From analysis of comparison between experimental and calculated with the use of FEFF8 code XANES and PDOS (P Density of states) spectra, the conclusion about lattice site occupation of both Mn and Fe in $LiNbO_3$ matrix is made. The oxidation states of Fe and Mn ions in doped $LiNbO_3$ are determined comparing their corresponding main absorption edge positions at their Fe and Mn K-edge experimental XANES spectra to the appropriate reference spectra.

XANES qualitative analysis results along with FEFF8 calculations and first coordination shell EXAFS (Extended X-ray Absorption Fine Structure) fit at Mn K-edge are also presented in this work for $Ni_{50}Mn_{30}Ga_{20}$ films, as-deposited and annealed at t=200 ^{o}C, 400 ^{o}C, 600 ^{o}C, and 650 ^{o}C. From analysis of experimental XANES and calculated FEFF8 spectra and Modified FT of freestanding $Ni_{50}Mn_{30}Ga_{20}$ films, the dependence of structural disorder of the samples on annealing temperature and existence of different phases of films are obtained. The dependence of structural disorder on annealing temperature is confirmed by first coordination shell Mn-Ni EXAFS fit results.

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Electronic Structure Calculations with Short Range Order

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For many years the Korringa-Kohn-Rostoker coherent-potential approximation (KKR-CPA) has been widely used to describe the electronic structure of disordered systems based upon a first-principles description of the crystal potential. However, as a single-site theory the KKR-CPA is unable to account for important environmental effects such as short-range order (SRO) in alloys and spin fluctuations in magnets, amongst others. Using the recently devised KKR-NLCPA (where NL stands for nonlocal), we show how to remedy this by presenting explicit calculations for the effects of SRO on the electronic structure of the bcc $Cu_{50}Zn_{50}$ solid solution.

Computing conductances of tunnel junctions by the Korringa-Kokn-Rostoker method : Formulation and test of a Green function approach.

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An approach to computing conductances of tunnel junctions within the framework of the Landauer-Büttiker theory for the electronic transport is introduced and formulated for the Korringa-Kohn-Rostoker (KKR) method for electronic-structure calculations. After a general introduction to the idea behind the approach, tests and comparisons with other methods, namely a 'transmission of Bloch-waves' approach and an approach based on the Kubo-Greenwood formula for the conductivity tensor, reveal a high accuracy and robustness of the proposed method, thus proving its suitability for state-of-the-art computations of spin-dependent ballistic transport. Based on Green functions, it is flexible and can easily be implemented in present KKR computer codes.

Magnetic tunnel junctions with Heusler alloy electrode: Interface structure and magnetism explored by soft X-rays

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The implementation of half-metallic materials like full Heusler alloys for spintronic applications, e.g., as electrode in magnetic tunnel junctions, is of highest technological relevance. The major challenge is the preparation of preferably defect free interfaces.

We fabricate Co_2MnSi / AlO_x / Co-Fe MTJs with more than 100% tunneling magnetoresistance (TMR) at low temperature and low bias voltage. However, the TMR bias voltage and temperature dependence is considerably stronger than usually found for optimized MTJs with 3d-alloy electrodes. For explaining this conclusively, knowledge of the structural and magnetic properties of the Co_2MnSi / AlO_x interface is of vital importance. In this talk investigations of the Co_2MnSi / AlO_x interface and the Co_2MnSi bulk material by X-ray absorption spectroscopy will be presented and discussed with respect to the temperature dependent transport properties of the junctions.

The authors gratefully acknowledge the opportunity to perform soft X-ray absorption spectroscopy at the Advanced Light Source, Berkeley, USA and at the BESSY mbH, Berlin, Germany.

Free clusters

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Clusters comprising few tens or hundreds of atoms form an interesting class of materials, because they form a bridge between atoms and molecules on the one hand and solids on the other hand and yet their properties cannot be described by a simple interpolation between the two extremes. Magnetic properties of transition metal clusters, in particular, attracted a lot of attention recently - both due to fundamental reasons and due to potential applications in magnetic recording technology. As clusters contain a large portion of surface atoms, it is interesting to study the relation between the electronic and magnetic properties of atoms which are close to a cluster surface and of atoms which are close to a planar surface of a crystal. A frequently used tool for studying magnetism in complex systems is x-ray magnetic circular dichroism (XMCD), defined as the difference between the absorption rate for left- and right-circularly polarized x-rays in magnetic targets.

The talk will thus focus on theoretical investigations of electronic, magnetic and spectroscopic properties of free Fe clusters of 9 to 89 atoms with bcc geometry and bulk interatomic distances and on comparing their properties with properties of bulk Fe and of bcc-Fe crystal surfaces. The theoretical framework is based on an ab-initio fully-relativistic spin-polarized real-space multiple-scattering technique, as implemented in the SPRKKR code.

X-ray absorption spectroscopy analysis of small nanoclusters

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Free and supported clusters of atoms are the novel physical objects which probably can make a bridge from atomic to solid state physics. Therefore the study of their structure and electronic subsystem in a function of cluster size is of great importance. The status of modern research shows XANES spectroscopy to be a useful tool for the investigation of both local structure and electronic subsystem of free clusters. X-ray absorption spectra of clusters with different type of chemical bonding covering the whole size range from several atoms to the solid are reported. The clusters have been generated using 'pick-up' method and their XANES spectra have been measured by both TEY and Auger YIELD techniques at BW3 beamline of HASYLAB at DESY. The x-ray absorption fine structure is shown to be sensitive to the size of cluster. For theoretical analysis of the experimental spectra a modern, self consistent full multiple-scattering method has been applied. In the framework of this approach dependence of the XANES vs. the cluster size has been analysed. In order to study the sensitivity of XANES on cluster symmetry, theoretical simulations have been performed for different structural models.

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X-ray absorption spectroscopy of SiC

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We have measured X-ray absorption spectra (XAS) of 3C- and 4H- SiC at the Si-$L_{2,3}$ and C-K edges. For the two polytypes the near edge spectra are very different in shape. We have compared our spectra with total and partial density of states calculations, addressing the various XAS features to Si- and C-derived states. By considering the different crystal structure symmetry of the two polytypes, we can put in evidence the influence of electronic band symmetry in the absorption cross sections of both edges.

Multiple Scattering Theory: KKR and KKR-CPA
I. Ordered Systems
II. Disordered Systems

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In these talks we briefly overview the multiple scattering theory and elaborate on the KKR and KKR-CPA methods that are based on this theory. In the first part we derive the single scatterer and multiple scattering quantities, leading to the single particle Green's function from which a number of observables can be calculated. Screened structure constants and impurity Green's functions are introduced and applications to surfaces and interfaces are also briefly discused. In the second part we concentrate on disordered systems and discuss the KKR-CPA band structure method in some detail. We introduce the configurationally averaged Green's function, density of states, integrated density of states, and spectral functions. The power of the method

is demonstrated by showing that one can not only study real substitutional alloys, composed of different elements, but can utilize the alloy analogy to describe properties of pseudo alloys, comprising different phases of a system, as for example localized (γ) and delocalized (α) phases of Ce. The calculated finite temperature phase diagram of Ce α to γ phase transition is discussed to illustrate the great potential of this methodology.

Ab initio simulation of deformation of nanostructure and its relation to electronic properties

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Nanostructures have been attracting attention because of their prominent properties, and their applications for novel devices with advanced functions have been attempted. Since such nanostructured materials are subject to high strain conditions it is important to clarify the mechanical properties and its relation to electronic structure. We have conducted ab initio simulations to elucidate the mechanical and electronic properties of materials placing our focus on the behavior of materials under high strain condition. Single crystal such as silicon and silicon carbide under ideal shear is investigated to find the relation between deformation and electronic structure. Tensile simulation of silicon thin film is performed to manifest the effect of surface structure on the mechanical properties and the electronic structure. The mechanical and electronic properties of carbon nanotubes under large deformation are also introduced. Investigation of structure and properties of perovskite thin films and ferromagnetic materials will be our future project.

A new X-ray Spectrometer with large Focusing Crystal Analyzer

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A new focusing spectrometer in Johann geometry that was build and permanently installed at the wiggler beamlime W1 at the Hamburger Synchrotron Strahlungslabor (HASYLAB) am Deutschen Elektronen Synchrotron (DESY) is described. It is now available for user operation. The usable energy range of the spectrometer which is installed inside a vacuum tank is 2.1 keV - 25 keV. Currently it is however limited by the source to 4.5 keV - 10.5 keV. The design of the spectrometer is optimised for the usage of a large source spot size at the DORIS storage ring as well as for simple operation and robustness under the conditions of user operation. Nevertheless, in the future, an undulator at a PETRA III beamline would be the ideal source to enlarge the number of possible applications. The spectrometer uses spherically and cylindrically bent crystals with typical bending radii of 100 cm (spherical) and 70 cm (cylindrical). The performance of the spectrometer is demonstrated by three bench mark experiments, Resonant Inelastic X-ray Scattering (RIXS), X-ray Absorption Fluorescence Spectroscopy (XAFS) in samples with complicated matrices and the determination of the chemical shift of Kβ emission lines of Cr in different valence states.

XAS of light 3d elements: a benchmark for *ab initio* calculations

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The element- and shell-specific XMCD technique provides a unique tool for the investigation of the magnetism of ultrathin films and nanostructures. Detailed fine structures in the L-edge XMCD are resolved at the new generation synchrotron sources. They allow for the study of the induced magnetism of light 3d elements like Ti, V and Cr at the interface to ferromagnetic layers [1-3]. However, it turns out that for these elements the strong electron-hole interaction leads to a shift of the spectral weights from the L3 to the L2 edge and thereby to the breakdown of the standard analysis (sum rules). Therefore, *ab initio* calculations were performed with the Munich SPR-KKR package to determine the magnetic ground state properties of these systems and the corresponding X-ray absorption spectra. Furthermore, a double-pole approximation within the time-dependent DFT will be presented, which allows for an experimental assessment of the exchange-correlation kernel. The experimentally determined correlation energies can be used to test advanced exchange kernels in the future. This work is supported by BMBF (05 KS4 KEB/5).

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Interface effects observed by magneto-optical Kerr effect of ultrathin transition metal films on palladium substrates

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We have measured the magneto-optical Kerr effect (MOKE) of ultrathin iron and cobalt films epitaxially grown on palladium substrates of different crystallographic orientations. Anomalous changes in the Kerr rotation observed at low thicknesses of the films are attributed to the influence of the interface between the ultrathin film and the substrate. In particular, sign reversals of the Kerr signal are observed. Due to the complexity of the magneto-optical response, no direct conclusions can be drawn about the magnetic moments at the interface. However, it could be possible to attribute the measured effects to influences from the electronic and spin structure of the interface. Theoretical calculations of MOKE for different compositions and magnetic configurations of the Co/Pd and Fe/Pd interfaces would be helpful in this case.

Electronic and magnetic properties of the surfaces and interfaces of hole doped manganites from model and first principles calculations

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The electronic and magnetic properties of hole-doped manganite surfaces are investigated in a model and a Self-Interaction Corrected (SIC-LSDA) calculations. The model incorporates the kinetic energy of the e_g electrons, their coupling through Hund's rule to the core-like t_{2g} spin and the superexchange interaction between the latter. A shift is added to the onsite energy at the surface in order to mimic the effects of the changes with respect to the cubic symmertry in the bulk. We looked at negative values of the shift added to one orbital or both with respect to the bulk levels. We found that the most favourable scenario is when a small shift is added to the $3z^2$-r^2. The stability of the ferromagnetic (FM) coupling between surface and bulk is enhanced as a result. But a larger shift would deplete the other orbital and thus would disfavour in-plane FM coupling at the surface which would be detrimental to the tunnelling magnetoresistance (TMR) of manganite-based junctions. In the SIC-LSDA calculation we found that the subsurface Mn ion localises an extra e_g electron whereas when at the surface only the t_{2g} orbits are localised. We have also studied $La_{0.7}Sr_{0.3}MnO_3/SrTiO_3$ within SIC-LSDA to look at the interfaces. Important changes are found to occur at the interface but given that we used only one unit cell for $SrTiO_3$ this becomes metallic. We are looking at bigger cells and also different interfaces, ie La-Ti and Mn-Sr.

SIC-LSD Description of Spintronics Materials

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We discuss an application of the self-interaction corrected local spin density approximation (SIC-LSD) to half-metallic transition metal oxides, and among them double perovskites and magnetite (Fe_3O_4), and diluted magnetic semiconductors such as Mn-doped Ga-group V compounds and ZnO. In addition we explore also spinel ferromagnetic insulators for exploiting in spin filtering heterostructures. Also, Eu chalcogenides and pnictides, as well as rare earth sulphides, are scrutinised for possible technological applications. We concentrate on the electronic and magnetic properties of all the compounds and in magnetite, in addition, issues of charge order are also thoroughly investigated.