

# 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 24-26 June 2009. It welcomed 33 participants, 13 tutors and 10 lecturers (the list of participants, tutors 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/workshops/2009/KKRHOC2009/>.

A first introduction to the KKR scheme and its implementation in the SPR-KKR package was given by H. Ebert with some description of the fully relativistic mode. A more detailed introduction to multiple scattering theory was then given by W. Temmermann. E. Engel gave an overview on density functional theory that was dealing primarily with the formal background.

G. Fecher was dealing with practical aspects with density functional theory showing many representative examples. The theory talks were accompanied by a number of contributions from experimental colleagues. J. Honolka gave a talk on the use of XMCD to investigate magnetic properties of supported nanostructures. This was accompanied by a theory talk by O. Sipr on deposited magnetic clusters. The possibilities offered by angle-resolved photo emission was reviewed by J. Fink with an emphasize on many-body properties. The theory talk of P. H. Dederichs dealt with exchange interaction in diluted magnetic semi-conductors. W. Wurth again presented results of experimental XMCD-studies on magnetic clusters. Finally, C. Back gave a talk on the induced magnetism at the (GaMn)As/Fe-interface at room temperature that seems a very promising achievement in the field of spintronics. In addition, many participants presented poster contributions that led to lively discussions during the coffee breaks.

The large number of participants, 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

## Wednesday, 24.6.2009

09:00 - 10:00	H. Ebert	Welcome and Introduction
10:00 - 12:00		Computer session
13:30 - 14.30	W.M. Temmerman	Phase shifts and the KKR-Multiple-Scattering Theory
14:30 - 15:30	E. Engel	Density Functional Theory: An efficient approach to the quantum many-body problem
16:00 - 17:00	G. Fecher	How many functionals do we need? The way to make half-metals half-metallic from $X_{\alpha}$ to $+U$

## Thursday, 25.6.2009

09:00 - 12:00		Computer session
13:30 - 14.30	J. Honolka	Surface supported magnetic nanostructures: insights using XMCD
14:30 - 15:30	O. Sipr	Magnetism and spectroscopy of clusters
16:00 - 17:00	J. Fink	Angular Resolved Photoemission Spectroscopy, a Probe for the Many-Body Properties of Solids

## Friday, 26.6.2009

09:00 - 12:00		Computer session
13:30 - 14:30	P.H. Dederichs	Exchange Interactions in Dilute Magnetic Semiconductors
14:30 - 15:30	W. Wurth	Magnetic Properties of Small Clusters in the Light of X-Ray Magnetic Circular Dichroism
16:00 - 17:00	C. Back	Induced Ferromagnetic Order at Room Temperature in (Ga,Mn)As

## Speakers

H. Ebert	München	The Munich SPR-KKR Package
W.M.Temmerman	Daresbury	Phase shifts and the KKR-Multiple-Scattering Theory
E. Engel	Frankfurt	Density Functional Theory: An efficient approach to the quantum many-body problem
G. Fecher	Mainz	How many functionals do we need? The way to make half-metals half-metallic from $X_{\alpha}$ to $+U$
J. Honolka	Stuttgart	Surface supported magnetic nanostructures: insights using XMCD
O. Šipr	Prague	Magnetism and spectroscopy of clusters
J. Fink	Berlin	Angular Resolved Photoemission Spectroscopy, a Probe for the Many-Body Properties of Solids
W. Wurth	Hamburg	Magnetic Properties of Small Clusters in the Light of X-Ray Magnetic Circular Dichroism
P. Dederichs	Jülich	Exchange Interactions in Dilute Magnetic Semiconductors
C. Back	Regensburg	Induced Ferromagnetic Order at Room Temperature in (Ga,Mn)As

## **Tutors**

Bornemann, Sven – University München  
Chadov, Stanislav – University Mainz  
Ebert, Hubert – University München  
Kardinal, Marianne – University München  
Ködderitzsch, Diemo – University München  
Kuhn, Gerhard – University München  
Lowitzer, Stephan – University München  
Mankovsky, Sergiy – University München  
Minar, Jan – University München  
Polesya, Svitlana – University München  
Šipr, Ondřej – University Prague  
Szotek, Zdzislawa – Daresbury Laboratory  
Temmerman, Walter – Daresbury Laboratory

## **List of participants**

Auge, Alexander – Bielefeld University  
Baev, Ivan – University Hamburg  
Beeck, Torben – University Hamburg  
Borek, Stephan – University Halle-Wittenberg  
Butchers, Matt – University of Warwick  
Chadov, Stanislav – University Mainz  
Chen, Kai, – University Hamburg  
dos Santos Dias, Manuel – University of Warwick  
Edalati Bustan, Saeideh  
Hlil, El Kébir – University Joseph Fourier, Grenoble  
Eugen, Macocian – University of Oradea  
Fiedler, Steffen – University Hamburg  
Fischer, Guntram – University Halle-Wittenberg  
Floare, Calin Gabriel – University Cluj-Napoca  
Gamza, Monika – MPI Dresden  
Glaser, Leif – University Hamburg  
Hammerling, Robert – CMS/WPI Vienna  
Hoda Ahsan, Mohammed Ahsanul – University Halle-Wittenberg  
Hott, Roland – KIT - FZK - IFP Karlsruhe

Kasinathan, Deepa – MPI Dresden  
Khellil, Bouamama – Universite Ferhat Abbas, Setif  
Kronseder, Matthias – University of Regensburg  
Marmodoro, Alberto – University of Warwick  
Meinert, Markus – Bielefeld University  
Miguel, Jorge – Free University of Berlin  
Peace, Jonathan – University of Warwick  
Rohringer, Nina – Lawrence Livermore National Laboratory  
Romanyuk, Oleksandr – Institute of Physics, ASCR  
Rosner, Helge – MPI Dresden  
Sessi, Violetta – MPI Stuttgart  
Sharma, Ghanshyam – Banasthali University  
Sharma, Yamini – Feroze Gandhi College  
Thoene, Jan – IFW Dresden

## Abstracts

– as far as available –

### The Munich SPR-KKR code

H. Ebert

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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 the CPA are described and its implementation within the KKR-method is outlined. Finally, a short outlook on future developments is presented.

### Theory and application of photoelectron diffraction theory in magnetic solids

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It is well known that modulations in the angle-resolved intensity of photoelectrons excited from deep core levels may be considered as a sensor of atomic short-range order in a solid. The modulations in the intensity of photoelectrons are caused by the interference of the directly emitted electron wave with scattered waves at the atoms around the emitting atom (photoelectron diffraction=PD). Therefore, these modulations contain information on the geometric, but in addition on the local magnetic structure [1]. A one-electron non-relativistic multiple-scattering cluster (MSC) model has been applied to calculate spin-resolved PD in magnetic solids. Both spin-orbit interaction and exchange interaction with the spin-polarized valence band are included in the angular and spin part  $|c\rangle$  of the initial core state wave function. In particular spin polarization and magnetism-induced symmetry breaking of the circular dichroism in the angular distribution (CDAD) of photoelectrons are discussed [2-4].

- [1] A.Chassé, J. Phys.: Condens. Matt. 11 (1999) 6475, J. Electr. Spectr. Rel. Phenom. (2004.) 13773.
- [2] T.Okuda, A. Harasawa, T. Kinoshita, K. Nayama, T. Fujikawa, and A. Chasse, Surf. Rev. Lett. 9 (2002) 901.
- [3] A.Chassé, J. Electr. Spectr. Relat. Phenom. 125 (2002) 47; A.Chassé, L. Niebergall, Surf. Sci. 546 (2003) 57.
- [4] A.Chassé, W.Kuch, M.Kotsugi, Xingyu Gao, F. Offi, S. Imada, S. Suga, H. Daimon, and J. Kirschner, Phys. Rev. B71 (2005) 014444

## **Magnetic Compton scattering at Warwick**

M.W. Butchers, J.A. Duffy, J.W. Taylor, S. B. Dugdale, and M.J. Cooper

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The magnetic x-ray scattering group at Warwick uses many techniques to study magnetic materials; XMCD, reflectivity, neutron scattering and most commonly Compton scattering. We use Compton scattering as a probe into



electron momentum distributions of exotic systems. The introduction of circular polarisation allows us to probe the momentum distribution of unpaired electrons, i.e. those electrons which are responsible for the magnetic moment, from the shape of our distributions we can also investigate Fermi surface effects. Our work is mainly done at large scale central facilities (ESRF in Grenoble, SPring-8 in Japan) where we have access to large field, low temperatures and most importantly high energy photons with large flux and variable polarisation. The range of materials we are able to study is very large, we study high Tc superconductors, Invars, frustrated systems, highly spin polarised systems, quantum critical systems to name but a few. Comparison with band structure calculations can reveal the origin of these interesting properties. Recent work includes investigations on  $\text{Co}_{1-x}\text{Fe}_x\text{S}$ , a half metal whose spin polarisation is 'tunable' by doping with iron. Magnetic Compton profiles were taken along different crystallographic directions and band structure models were used to determine the spin polarisation of the system. Another recent investigation was into magnetite ( $\text{Fe}_3\text{O}_4$ ) where we investigated the spin moment of the system across the Verwey transition, a metal/insulator transition in an attempt to settle a dispute over the orbital moment of the system. Future investigations hope to build on work into spin polarisation with a direct link into the field of spintronics.

## **Anisotropic Magnetic Correlations at Finite T in RDLM**

M. dos Santos Dias, J. Staunton and L. Szunyogh

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We present a theory for anisotropic magnetic correlations at finite temperature, in the framework of the Relativistic Disordered Local Moment (RDLM) state. The RDLM is a single site mean field theory of magnetism, formulated in Relativistic Multiple Scattering Theory. It has proven to give a reliable description of magnetic systems in many previous formulations, so our goal is to extend it so as to provide a description of the anisotropic effects that arise

from the coupling between the spins and the lattice, induced by spin-orbit coupling. Starting from the RDLM state, the spin-spin correlation (2),ab function  $SIJ(q)$ , describing interactions between magnetic species a and b of subsystems I and J, respectively, is obtained using linear response theory. This will enable the exploration of anisotropic magnetic interactions in complex systems, such as layered systems, nanoparticles and bulk systems with a large unit cell, as well as the calculation of their magnetic susceptibilities. The exchange bias effect is examined as an example of a possible application of our theory, which we intend to pursue in detail.

## **Magnetic properties of mass selected, deposited alloy clusters and small iron clusters on Nickel**

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Nanoparticles are promising new materials for ultra small magnetic storage devices as their small size allows an increase in storage density [1]. However, for this application in particular a huge magnetic anisotropy is essential to fix the magnetization direction in space [2]. This can potentially be realized by systems with a large orbital magnetic moment and a large spin-orbit coupling. From all ferromagnetic materials the largest “natural” orbital moment is found for Co. An extraordinary huge orbital moment in combination with a large magnetic anisotropy was obtained for Co atoms deposited on a platinum surface by Gambardella et al [3]. In recent work, the electronic and magnetic properties have been studied as a function of the number of atoms per cluster [4-6]. However, by changing also the composition of the clusters a much larger functional space will be available. To tailor their properties a detailed understanding of the basic interaction processes within the nanoparticles and with the supporting surfaces is essential. In order to understand these fundamental interactions, as e.g. the exchange interaction,

and their variation with the particle size, small, mass selected clusters are excellent systems. They are large enough to show complex phenomena and small enough to use sophisticated theoretical methods. Therefore we investigated the influence of different element compositions on the properties of small size selected clusters. We have started experiments on  $\text{Co}_m\text{Pt}_n$  and  $\text{Co}_m\text{Pd}_n$  alloy clusters on different substrates, Pt and Pd representing two candidates with very similar ferromagnetic capabilities [7]. During our last experiment we could amongst others complete the series of measurements performed on small iron clusters [5] by the measurement of single Fe atoms on Nickel. That should of course be a very promising aspirant for theoretical calculations.

All the measurements have been performed using synchrotron radiation at the beamline “UE52-SGM” at Bessy 2 in Berlin. To probe the magnetic properties of the clusters the x- ray magnetic circular dichroism (XMCD) method is applied. In figure 1 the XMCD spectra for  $\text{Co}_n\text{Pd}_1$  cluster deposited on a thin magnetized Ni film are shown. All spectra have been normalized to the same L2 dichroism intensity, so that the L3 dichroism signal reflects roughly the ratio of orbital to spin magnetic moment. By adding a single Pd atom to a Co atom or a  $\text{Co}_2$  cluster respectively the orbital to spin ratio increases drastically. This shows, that tailoring a special property might be possible by choosing the right size and composition of a cluster. This work is performed within the framework of the Sonderforschungsbereich 668.

#### References

- [1] D. Weller and A. Moser, IEEE Trans. Mag. 35, 4423 (1999)
- [2] J. Eisenmenger and I. K. Schuller, Nature Materials 2, 437 (2003)
- [3] P. Gambardella, S. Rusponi, M. Veronese, S. S. Dhesi, C. Grazioli, A. Dallmeyer, I. Cabria, R. Zeller, P. H. Dederichs, K. Kern, C. Carbone and H. Brune, Science 300, 1130 (2003)
- [4] M. Reif, L. Glaser, M. Martins and W. Wurth, Phys. Rev. B 72, 155405 (2005)
- [5] J. T. Lau, A. Föhlisch, R. Nietuby'c, M. Reif, and W. Wurth, Phys. Rev. Lett. 89, 57201 (2002).
- [6] M. Martins, M. Reif, L. Glaser and W. Wurth, Europ. Phys. J. D 45, 539 (2007)
- [7] D. A. Vanleeuwen, J. M. Vanruitenbeek and G. Schmid, L. J. Dejongh, Physica B 194, 263 (1994)

# Calculation of Magnetic Properties in Correlated Systems

G. Fischer, W. Adeagbo, A. Ernst, P. Bruno, M. Däne, M. Lüders, Z. Szotek, W. Temmerman, and W. Hergert

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We present results of calculations of electronic and magnetic properties of different systems. These are the transition metal monoxides (MnO, FeO, CoO and NiO), defect-induced ZnO and the transition metal fluorides (MnF<sub>2</sub>, FeF<sub>2</sub>, CoF<sub>2</sub> and NiF<sub>2</sub>). For the treatment of the localized d-electrons LSIC is applied. CPA is used to simulate the defects in ZnO. Magnetic interactions are mapped onto a Heisenberg Hamiltonian by calculating the exchange parameters  $J_{ij}$  via the Magnetic Force Theorem.

## Electronic structure of CeRhX (X = Sn, In)

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CeRhIn is a non-magnetic Fermi-liquid system with Ce ions in an intermediate valence state [1], whereas the isostructural compound CeRhSn shows the non-Fermi liquid characteristics at low temperatures [2,3] and is supposed to be located on the border between a nonmagnetic and a magnetically ordered ground state, in the vicinity of the antiferromagnetic instability [4]. Numerous experimental data [2] suggest also valence fluctuations of Ce in CeRhSn. To get insight into the interactions responsible for the change in properties between CeRhSn and CeRhIn, we performed a detailed study of electronic structure based on the X-ray photoemission spectroscopy (XPS) experiments at ambient temperature and ab initio band structure calculations.

The Ce core-level XPS spectra revealed an intermediate valence state of Ce ions and the substantial coupling of the Ce 4f and the conduction band states

in both CeRhSn and CeRhIn. The comparative analysis of the theoretical band structures and charge density plots showed distinct changes in chemical bonding and hybridization of the Ce 4f states with the states of the neighbouring Rh atoms introduced by the replacement of In by Sn atoms. The more covalent character of the chemical bonding in the stannide is in line with its smaller thermal expansion. Finally, the temperature dependence of the crystal lattice of CeRhSn shows a distinct anomaly at about 120 K, presumably related to the change in planar Ce-Rh bonds. In contrast, for CeRhIn only a typical thermal expansion was observed.

- [1] D.T. Adroja et al., Phys. Rev. B 39 4831 (1989).
- [2] A. Ślebarski et al., Philos. Mag. B 82, 943 (2002).
- [3] M.S. Kim et al., Phys. Rev. B 68, 054416 (2003).
- [4] H. Tou et al., Phys. Rev. B 70, 100407(R) (2004).

## **XMCD Spectroscopy on Co and Pt Clusters and Nanoparticles**

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Small magnetic clusters and nanoparticles have been of increasing interest in the last years. The miniaturization of magnetic storage technology reduces the magnetic units involved to superparamagnetic cell sizes, but needs to operate at room temperature. While the thermal activation energy at room temperature is constant at 25meV, the magnetic anisotropy energy of an atom on a surface is typically in the range of 1meV, but can reach as much as 8meV [1]. In any case the particles need to be of several hundred to thousand atoms in size (which corresponds to some few nm) in order to provide enough magnetic anisotropy energy to stabilize the imprinted magnetization at room temperature for ten years. High magnetic moment and strong spin orbit coupling are premises for new magnetic storage materials. 3d-5d alloys fulfill those requirements. As a promising candidate the alloys of Cobalt

and Platinum were chosen to investigate. The interaction within a cluster and between cluster and substrate are very complex and need to be fundamentally understood, therefore some experiments were done to investigate the size dependent changes within very small clusters and between identical clusters on different substrates. During those experiments the properties of substrates and clusters were carefully controlled in order to provide reliable experimental data and to compare them with ongoing theoretical calculations to explain the changes. Small mass selected clusters [3] up to 5 atoms per cluster were soft laded in an Ultra High Vacuum (UHV) environment at 40 Kelvin on thin magnetic iron and nickel films and investigated with X-Ray Magnetic Circular Dichroism (XMCD)[5]. The stoichiometry and size of the clusters was varied on both substrates. Figure 2: The orbital to spin magnetic moment ratio depends strongly upon the substrate on which the Cobalt atoms were deposited. For a new material to be applicable to any technological enhancement, a large scale production must be feasible. Wetchemical synthesis methods allow macroscopic output, but have much lower sample quality than physical procedures, as for instance the cluster sputter source used for the above described mass selected clusters. CoPt nanoparticles of a very broad size range but with narrow size distribution can be produced wet-chemically [2]. They were investigated with XAS and XMCD in a UHV experiment providing an external magnetic field of up to 7 Tesla. Primarily the oxidation state, possible aging effects and their magnetic properties [4] were in the focus of these measurements.

[1] Gambardella et al. *Science* (2003), 300,1130

[2] Shevchenko et al *JACS* (2002), 124 ,11480-11485 & *JACS* (2003),125, 9090-9101

[3] Lau et al, *Review of Scientific Instruments*, (2005), 76, 063902-1

[4] Imperia et al, *Phys.Stat.Sol.A*, (2008), 5, 1047

[5] O'Brien et al *PRB* 50,17 (1994) 12672 & Chen et al *PRL* 75,1(1995) 152-155 & B. T. Thole et al., *PRL* 68, (1992) 1943 & P. Carra et al., *PRL* 70, (1993) 694

[6] J. Eisenmenger and I.K. Schuller, *Nature materials* (2003), 437

# Competing interactions in low-dimensional spin 1/2 systems

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Low-dimensional spin systems are one of the actively studied subjects in solid-state physics due to the possibility to observe numerous quantum phenomena and to interpret these phenomena within relatively simple models, e.g., Ising or Heisenberg models. An interesting phenomenon in the spin physics is the formation of a spin liquid a strongly correlated ground-state lacking longrange magnetic order. This ground state is usually related to the electronic mechanism of superconductivity suggested for high-Tc cuprates. Spin liquids originate from quantum fluctuations that are particularly strong in systems with reduced dimensionality and low spin value. The fluctuations can be further enhanced by introducing magnetic frustration which impedes long-range ordering of the system due to a high degree of degeneracy.

On the other hand, many systems tend to avoid degenerate ground states, for instance by lattice distortion, orbital ordering or a combination of both. In our study, we present these phenomena - caused by competing interactions - for selected systems with a square lattice of spin 1/2 transition metals.

## A self-consistent, first-principles method for complex disordered materials

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Realistic materials are always affected by some degree of symmetry-breaking disorder. The Coherent Potential Approximation (CPA)[1] provides a general method to self-consistently determine an effective medium, where translational invariance is restored and first-principle calculations schemes can be deployed to describe averaged properties. Its main limitations emerge from a single site formalism. This has been generalised by the Dynamic Cluster Approximation (DCA)[2] / Non-Local CPA (NLCPA)[3] to account for short range ordering effects (SRO), and by the Multi Sublattice CPA (MSCPA)[4] for materials with complex unit cells. Here we illustrate an unification of

the two developments into a single scheme, which should provide all the flexibility required for describing compounds where both site-specificity and short-range ordering are important. The theory is illustrated through a simple tight-binding model for clarity. A rephrasing within multiple scattering formalism is also offered[5].

#### References

- [1] P. Soven. Coherent-potential model of substitutional disordered alloys. *Physical Review*, 156(3), April 1967.
- [2] M. Jarrell and H. R. Krishnamurthy. Systematic and causal corrections to the coherent potential approximation. *Physical Reviews B*, 63(12):125102, March 2001.
- [3] D. A. Rowlands, J. B. Staunton, and B. L. Gyorffy. Korringa-Kohn-Rostoker nonlocal coherent-potential approximation. *Physical Review B*, 67(11):115109, March 2003.
- [4] A. J. Pindor, W. M. Temmerman, and B. L. Gyorffy. KKR CPA for two atoms per unit cell: application to Pd and PdAg hydrides. *Journal of Physics F*, 13(8):1627?1644, 1983.
- [5] A. Marmodoro and J. B. Staunton. Electrons in systems with several types and degrees of disorder: the Non-Local Coherent Potential Approximation for multi-atom per unit cell materials. Submitted to *Physical Reviews B*, June 2009.

## **Interfacial magnetic domain coupling study in single-crystalline Fe/CoO bilayers using photoelectron emission microscopy**

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X-ray absorption spectroscopy and spectromicroscopy were employed to probe the magnetic and electronic properties of epitaxially grown Fe/CoO bilayers on Ag(001) with elemental selectivity. The use of a photoelectron emission microscope (PEEM) in connection with x-ray magnetic circular and linear dichroisms (XMCD and XMLD) allows layer-selective imaging of ferromagnetic (FM) and antiferromagnetic (AFM) domains. Absorption spectra taken



from bilayers with different Fe thicknesses show only a weak indication for the formation of Fe oxide at the Fe/CoO interface, and a parallel coupling between the Fe magnetization and the spin axis of CoO [1]. XMCD- and XMLD-PEEM images were used to laterally probe both magnetic layers. A magnetic coupling between the layers can be deduced by comparing the magnetic domains in Fe and CoO. In addition to the AFM domains in CoO, which are imaged by XMLD, XMCD images at the Co L3 edge yield a magnetic contrast due to induced magnetic moments. A perfect overlap of the domain walls in the Fe and CoO layers is observed in the thickness range from 5 Fe MLs (monolayers) down to 2 MLs. Furthermore, an enhanced Co XMLD contrast is observed from CoO in contact to thin Fe layers with absent long-range FM order (at 300 K). This effect is explained by the different crystallographic structure of the last CoO monolayers that share oxygen atoms with the adjacent FeO layer, altering the CoO spin axis and affecting the ferromagnetic Co spins at the interface.

References

- [1] R. Abrudan, J. Miguel, M. Bernien, M. Piantek, C. Tieg, J. Kirschner, W. Kuch, *Phys. Rev. B* 77, 014411 (2008)
- [2] J. Miguel, R. Abrudan, M. Bernien, M. Piantek, C. Tieg, J. Kirschner, W. Kuch, *J. Phys.: Condens. Matter* 21, 185004 (2009)

## **Ab-Initio study of one-dimensional disorder on III-V semiconductor surfaces**

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Defects on III-V semiconductor surfaces play crucial role in homo and heteroepitaxial crystal growth by molecular beam epitaxy (MBE). Despite significant efforts are applied to understand surface reconstructions of III-V semiconductors, there are only a limited number of studies related to surface defects. Difficulties arise due to a large system size and, consequently, large

computation resource requirements. Difficulties with large number of atoms are overcome by the Bravais lattice type variation on III-V semiconductor surfaces. Particularly, a rectangular unit cell with oblique translation vectors represents a one-dimensional disorder boundary on a surface. This reduces computational costs significantly. We explain the experimental discrepancy between symmetries resolved by STM and diffraction techniques (RHEED, X-ray) on a number of different surfaces, like the GaSb(001) and GaAs(001) surfaces, by the formation of one-dimensional disorder boundaries. Ab initio calculation within DFT theory are carried out [1, 2] for GaSb(001) (4x3) and GaAs(001)  $\beta 2(2x4)$  and  $c(4x4)$  reconstructions. Specifically, lattice distortion of the (4x3) reconstruction family of GaSb(001) [3] is compared to the GaAs(001)  $\beta 2(2x4)$  and  $c(4x4)$  reconstructions. Very low defect energies are found for specific (4x3) reconstructions with shifts along [-110] direction. A similar behavior is found for the GaAs(001)  $\beta 2(2x4)$  reconstruction. On other reconstructions the calculated defect energies are very high, like for the GaAs(001)  $c(4x4)$ . Low energies would allow for the existence of phase shifted reconstruction regions on short distances which explains, for instance, the thermodynamic stability of the GaSb(001) (4x3) reconstructions, predicted by DFT and observed by STM, and that in diffraction experiments one finds only (1x3) or  $c(2x6)$  diffraction patterns [4].

#### References

- [1] The ABINIT code is used. The ABINIT a common project of the Université Catholique de Louvain, Corning Incorporated, and other contributors ([www.abinit.org](http://www.abinit.org)).
- [2] X. Gonze et al., *Comput. Mater. Sci.* 25, 478 (2002).
- [3] W. Barvosa-Carter, A. S. Bracker, J. C. Culbertson, B. Z. Nosho, B. V. Shanabrook, L. J. Whitman, H. Kim, N. A. Modine, E. Kaxiras, *Phys. Rev. Lett.* 84, 4649 (2000).
- [4] O. Romanyuk, V. M. Kaganer, R. Shayduk, B. P. Tinkham, and W. Braun, *Phys. Rev. B* 77, 235322 (2008).

## **Magnetism of Rh nano-structures on inert Xe buffer layers and in contact with Ag(100) surfaces**

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Previous x-ray magnetic circular dichroism measurements have shown that sub-monolayer coverages of Rh directly deposited on Ag(100) at T=5K are not magnetic [1], in contrast to theoretical predictions [2]. We have investigated this discrepancy and studied the magnetism of Rh nano-structures prepared on inert Xe buffer layers on Ag(100). For Rh nano-structures (monomers, dimers, trimers etc.) situated on the Xe buffer layer we find a cluster size-dependent magnetic moment similar to the one measured on free clusters in the Stern-Gerlach experiment [3]. During desorption of the Xe layer the Rh nano-structures grow in size and make contact with the substrate, which leads to a full quenching of the magnetic moment. The results are discussed modelling the Rh cluster size distribution and magnetic ordering on Xe and Ag(100).

#### References

- [1] J. Honolka et al., Phys. Rev. B 76, 144412 (2007)
- [2] P. Lang, V.S. Stepanyuk, K. Wildberger, R. Zeller, and P.H. Dederichs., Solid State Commun. 92, 755 (1994)
- [3] J.H. Weaver, G.D. Waddill, Science 251, 1444 (1991)
- [4] A.J. Cox, J. G. Louderback, and L.A. Bloomfield, Phys. Rev. Lett. 71, 923 (1993)