O 51: Surface and Interface Magnetism I (O jointly with MA)

Time: Wednesday 10:30–13:00 Location: WIL C107

O 51.1 Wed 10:30 WIL C107

Tracing the RKKY-interaction in pairs of adatoms via the peak splitting of a Kondo resonance — Alexander Ako Khajetoorians[1], •Manuel Steinbrecher[1], Mohammed Bouhassoune[2], Samir Lounis[2], Markus Ternes[3], Jens Wiebe[1], and Roland Wiesendanger[1] — [1]Institute of Applied Physics, Universität Hamburg, 20355 Hamburg, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [3]Max-Planck Institut für Festkörperphysik, 70569 Stuttgart, Germany

Ruderman-Kittel-Kasuya-Yoshida (RKKY)-interaction is an indirect exchange interaction between localized magnetic moments in a host mediated by conduction electrons, which oscillates between ferromagnetic and anti-ferromagnetic coupling as a function of distance [L. Zhou *et al.*, Nat. Phys. **6**, 187 (2010)]. We performed scanning tunneling spectroscopy at 300 mK on a Fe-H complex and a clean Fe atom, both adsorbed on Pt(111), for different spacing between the atom and the complex. While the Fe atom shows the well known spin excitation [A. A. Khajetoorians *et al.*, Phys. Rev. Lett. **111**, 157204 (2013)], the hydrogen complex shows a Kondo resonance. As a result of the RKKY-interaction the Kondo resonance reveals a distance dependent peak splitting. Fitting the spectra to model calculations including the coupling to the substrate electrons in third order perturbation enables to determine the distance dependency of the RKKY-interaction, which we compare to our first principles calculations.

O 51.2 Wed 10:45 WIL C107

Controllable Kondo Effect of Fe on Alkali Substrates — •Malte Schüler[1,2], Tim O. Wehling[1,2], Sandra Gardonio[3], and Carlo Carbone[4] — [1]Institut für Theoretische Physik, Universität Bremen, Otto-Hahn-Allee 1, D-28359 Bremen, Germany — [2]Bremen Center for Computational Materials Science, Universität Bremen, Am Fallturm 1a, 28359 Bremen, Germany — [3]Materials Research Laboratory, University of Nova Gorica, Vipavska 13, 5000 Nova Gorica, Slovenia — [4]Istituto di Struttura della Materia, Consiglio Nazionale delle Ricerche, Basovizza, I-34149 Trieste, Italy

The interaction between a magnetic impurity and a non-interacting bath presents a characteristic case of a multiorbital Kondo system. Prototypical realizations are Fe adatoms on alkali-surfaces (in our case Li, Na, K, Cs). The different substrates lead to different hybridization strengths, caused by the decrease of electron density with the increase of the lattice constant.

The electronic configuration and the magnetization of the impurity are measured by XMCD and XAS. Multiplet-broadening and a decrease of magnetic moment with increasing electronic density are observed. The simulation of this behavior leads to understanding how orbital degree of freedom influences the Kondo effect: The orbital resolved hybridization is obtained by fully relaxed DFT calculations and is used as a starting point to model the impurity problem with different complexity. These models are solved by numerical renormalization group, exact diagonalization and quantum Monte Carlo methods and compared to the experimental data.

O 51.3 Wed 11:00 WIL C107

Spin-orbit coupling and spin dynamics of magnetic adatoms — •Manuel dos Santos Dias and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

The control and manipulation of magnetic nanostructures hinges on understanding of their spin dynamics, which have been phenomenologically described for many systems using the Landau-Lifshitz-Gilbert equation (LLGe). Here we investigate the validity and possible extension of this equation down to the single atom limit. The magnetic excitation spectrum is derived from the dynamical magnetic susceptibility of the electronic system, employing Time–Dependent Density Functional Theory, as implemented in the Korringa–Kohn–Rostoker Green function method [1]. We include spin-orbit and Zeeman couplings in our calculations, and explore the key parameters in the LLGe, the precessional frequency and damping, for 3*d* adatoms deposited on the Cu(111) and Pt(111) surfaces. See [2] for an example of a theoretical and experimental investigation of Fe adatoms on Pt(111).

Work supported by the HGF-YIG Programme FunSiLab – Functional Nanoscale Structure Probe and Simulation Laboratory (VH-NG-717).

[1] S. Lounis, A. T. Costa, R. B. Muniz and D. L. Mills, Phys. Rev. Lett. **105**, 187205 (2010), Phys. Rev. B **83**, 035109 (2011)
[2] A. A. Khajetoorians, *et al.*, Phys. Rev. Lett. **111**, 157204 (2013)

O 51.4 Wed 11:15 WIL C107

Exchange coupling and Magnetic anisotropies in 3d atomic chains adsorbed on $Cu_3N - Cu(110)$ molecular network — •Dmitry I. Bazhanov[1,2], Oleg V. Stepanyuk[1,2], and Valeri S. Stepanyuk[2] — [1]Faculty of Physics, Moscow State University, GSP-1, Lenin Hills, 119991 Moscow, Russia — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

Based on first-principles calculations we study the magnetic states and exchange coupling in transition metal Mn, Fe, Co atomic chains deposited on a self-corrugated $Cu_3N - Cu(110)$ molecular network. The various adsorption sites on a bumping area of Cu_3N layer are investigated where the atomic chains grow at the initial stage of nanowires growth [1]. We demonstrate, that the exchange coupling, magnetic order and anisotropies in atomic chains depend sensitively on their chemical composition and adsorption sites on Cu_3N network. We find that the exchange interactions in atomic chains could lead to ferromagnetic or antiferromagnetic coupling depending on the position of the chain on the surface. The dynamics of classical spins is investigated by means of kinetic Monte Carlo method based on transition-state theory. Also using an *ab initio* determined exchange parameters and spin moments we evaluate the Heisenberg-Dirac-Van Vleck quantum spin Hamiltonian for calculations of the magnetic susceptibility, which is used for indicating the existence of quantum entanglement in the antiferromagnetic atomic chains.

This work was supported by the RFBR grant N13-02-01322.

[1] X.-D. Ma *et al.* , Phys. Rev. Lett. 102, 205503 (2009)

O 51.5 Wed 11:30 WIL C107

Complex trend of magnetic order in Fe clusters on Rh(111) and Ru(0001) — •Sören Krotzky[1], Fabian Otte[2], Violetta Sessi[3], Carsten Tieg[3], Paolo Ferriani[2], Stefan Heinze[2], Marta Wasniowska[1], Jan Honolka[1,4], and Klaus Kern[1,5] — [1]Max Planck Institute for Solid State Research, Stuttgart Germany — [2]Institute of Theoretical Physics and Astrophysics, University of Kiel, Kiel Germany — [3]European Synchrotron Radiation Facility, Grenoble France — [4]Institute of Physics of the ASCR, Prague Czech Republic — [5]Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, Switzerland

We investigate the spin configurations in Fe clusters and monolayers on Ru(0001) and Rh(111) by means of X-ray magnetic circular dichroism experiments, first-principles calculations and Monte Carlo simulations. The importance of Fe 3*d* state itinerancy and its hybridization with partly filled 4*d* substrate bands will be studied for monoatomic height Fe clusters of different atomic size N and various geometries. Randomly positioned single Fe atom spins in the dilute regime ($N = 1$) indirectly interact via the Rudermann-Kittel-Kasuya-Yoshida mechanism, which shows inverted character on Ru(0001) and Rh(111). For Fe dimers we prove the antiferromagnetic (Ru) to ferromagnetic (Rh) cross-over of the nearest-neighbour exchange coupling constant J_1. For larger clusters (i.e. $2 \leq N \leq 4$) we show the onset of cluster geometry dependent compensated magnetic structures. Finally, we present experimental evidence for the formation of compensated spin textures both for Ru(0001) and Rh(111) in fully ordered epitaxial Fe islands.

O 51.6 Wed 11:45 WIL C107

Impact of the large substrate polarization on the magnetic anisotropy energy of 3*d* adatoms on Pt(111) — •Mohammed Bouhassoune, Manuel dos Santos Dias, David S. G. Bauer, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

It has been shown recently, from first-principles and experimentally with inelastic tunneling spectroscopy, that the magnetic anisotropy energy (MAE) of single Fe adatoms deposited on Pt(111) surface depends strongly on the adsorption site. Surprisingly the sign of the MAE changes once an Fe adatom is moved from an fcc site to a hcp

site, thus favoring an in-plane orientation of the moment instead of the out-of-plane orientation [1]. We perform ab-initio calcualtions utilizing the full-relativistic full-potential Korringa-Kohn-Rostoker Green function method [2] for Cr, Mn, Fe and Co adatoms, analyse the contribution of the neighboring shells of Pt atoms and demonstrate that the large polarisation cloud of the Pt-substrate impacts strongly on the MAE.

This work is supported by the HGF-YIG Programme
FunSiLab –Functional Nanoscale Structure Probe and Simulation Laboratory (VH-NG-717).

[1] A. A. Khajetoorians, T. Schlenk, B. Schweflinghaus, M. dos Santos Dias, M. Steinbrecher, M. Bouhassoune, S. Lounis, J. Wiebe, R. Wiesendanger, PRL **111**, 157204 (2013)
[2] D. S. G. Bauer, PhD thesis, RWTH-Aachen (2013)

O 51.7 Wed 12:00 WIL C107

Emergent phenomena induced by spin orbit coupling in photoemission from ultrathin ferromagnetic films — •L. Plucinski[1,2], M. Eschbach[1], I. Aguilera[3], G. Bihlmayer[3], S. Blügel[3], and C. M. Schneider[1,2] — [1]PGI-6, FZ Jülich — [2]Fakultät f. Physik, Uni Duisburg-Essen — [3]PGI-1 and IAS-1, FZ Jülich

The existence of easy magnetization axis reduces the crystal symmetry and may manifest itself in lifting the degeneracy of electronic band dispersions along otherwise symmetrical directions in reciprocal space.

In non-magnetic materials spin orbit coupling (SOC) may cause the lifting of the spectral degeneracy of certain surface or bulk bands by means of Rashba or Dresselhaus effects. However, only combining SOC with ferromagnetism offers the possibility of remanent magnetic swapping of the non-degenerate directions which results in discrete switching of the electronic states for certain wave vectors in the Brilloin zone.

We will show the prediction of such phenomena for several monolayers thick films of Fe(001), which have 4-fold in plane easy magnetization axis. The energy scale of the predicted effect (from 20 to 200 meV) is several times larger than the resolution of the state-of-the-art angle-resolved photoemission (ARPES) experiment when performed on cryocooled samples.

Reciprocal space constant energy contours measured by ARPES will be compared with the electronic band structures of Fe calculated using the LDA and GW approximations. Interplay between initial state and photoemission dichroic effects will be discussed.

O 51.8 Wed 12:15 WIL C107

Oscillatory orbital magnetic moment via *d*-band quantum well states in Fe(001) films — •Thiago R. F. Peixoto[1], Maciej Dabrowski[1], Mariusz Pazgan[1], Aimo Winkelmann[1], Takeshi Nakagawa[2], Yasumasa Takagi[2], Toshihiko Yokoyama[2], Uwe Bauer[1], Fikret Yildiz[1], Francesco Bisio[1,3], Marek Przybylski[1,4], and Jürgen Kirschner[1,5] — [1]MPI of Microstructure Physics, Halle, Germany — [2]Institute for Molecular Science, Okazaki, Japan — [3]CNR-SPIN, Genova, Italy — [4]Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, Krakow, Poland — [5]Naturwissenschaftliche Fakultät II, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

Iron films grown on silver surfaces have shown an intriguing thickness-dependent oscillatory magnetic anisotropy [1,2]. We explored the effect of electron confinement on the magnetocrystalline anisotropy of *bcc* Fe films via a combination of spin-resolved photoemission spectroscopy ($h\nu = 6$ eV), x-ray magnetic circular dichroism, and magneto-optical Kerr effect measurements. The thickness-dependent variations in the magnetocrystalline anisotropy are ascribed to periodic changes in the density of states at the Fermi level, induced by confinement of electronic states derived from majority d_{xz}, d_{yz} out-of-plane orbitals. Our results confirm a direct correlation between QWS, the orbital magnetic moment and the magnetocrystalline anisotropy.

[1] U. Bauer and M. Przybylski, Phys. Rev. B 81, 134428 (2010).
[2] J. Li *et al.*, IEEE Trans. on Magn. 47, 1603 (2011).

O 51.9 Wed 12:30 WIL C107

Spin dynamics of a single magnetic adatom coupled to nano-mechanical oscillator operating on the atomic scale — •Michael Schüler[1], Andrey Klavsyuk[2], and Jamal Berakdar[1] — [1]Martin-Luther University Halle-Wittenberg, Institute for Physics, Karl-Heinrich-von-Fritsch-Straße 3, 06120 Halle, Germany — [2]M. V. Lomonosov Moscow State University, Faculty of Physics, Vorob'evy gory, 119899 Moskow, Russia

Great advances have been achieved recently in fabricating, manipulating, and imaging in a controlled way the properties of small magnetic systems. One of the most versatile approaches is the scanning tunnelling microscopy (STM) or spectroscopy (STS) setup, allowing to access the dynamics of single magnetic adatoms on the surface. Within a simple model system, we demonstrate how the transport properties and the relaxation spin dynamics are related to the anisotropic environment. As a second step, we have computed the magnetic anisotropy parameters for the typical Fe@Cu(001) systems by ab initio methods which allows to compare the calculations including the STM tip with the result in absence of the tip. As it turns out, the presence of the tip has a considerable influence on the anisotropy energy. Therefore, depositing the tip apex on a nano-scaled cantilever yields a nanomechanical oscillator coupled to a single spin - a kind of hybrid systems that are subject of recent experimental investigations. We analyse the resulting spin dynamics and point out how the magnetic moment of the Fe atom can be controlled coherently.

O 51.10 Wed 12:45 WIL C107

Surface electronic properties of Ni(111) investigated by low-temperature scanning tunneling spectroscopy — •Andreas Krönlein, Jeannette Kemmer, Pin-Jui Hsu, and Matthias Bode — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Although the general electronic properties of Ni(111) have been intensively investigated theoretically and experimentally, the exact position of the majority and minority surface state bands is still under debate [1,2,3,4]. We have performed scanning tunneling spectroscopy measurements at $T = 5.5$ K to investigate the electronic properties of Ni(111) above and below the Fermi level with high energy resolution. Our data allow for the precise determination of band onsets and effective masses of the *sp*-derived surface states and thereby enable us to quantify their magnetic exchange splitting.

[1] M. Donath *et al.*, Phys. Rev. Lett. **70**, 2802 (1993).
[2] J. Braun *et al.*, J. Phys.: Condens. Matter **16**, S2539 (2004).
[3] T. Ohwaki *et al.*, Phys. Rev. B **73**, 235424 (2006).
[4] J. Lobo-Checa *et al.*, Phys. Rev. B **77**, 075415 (2008).