O 74: Surface and Interface Magnetism II (O jointly with MA)

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

O 74.1 Thu 10:30 WIL C107

Spin excitations in nanostructures on a Cu(111) surface: Access to the electron self-energy from first-principles — •Benedikt Schweflinghaus, Manuel dos Santos Dias, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Magnetic excitation spectra of nanostructures are nowadays accessible by low-temperature inelastic scanning tunneling spectroscopy, see *e.g.* [1]. We developed a first-principles description of such spectra by combining time-dependent density functional theory and many-body perturbation theory, implemented in a code based on the Korringa-Kohn-Rostoker Green function method [2,3]. The coupling of the electrons to the spin-excitation within the adsorbate is given in terms of the electron self-energy. We analyze this key quantity for a number of clusters with different geometries placed on a Cu(111) substrate. We spin-characterize their excitation spectra and discuss how they change with the number of involved atoms, their kind, and their arrangement on the surface.

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

[1] A. A. Khajetoorians *et al.*, Phys. Rev. Lett. **106**, 037205 (2011).
[2] S. Lounis *et al.*, Phys. Rev. Lett. **105**, 187205 (2010).
[3] S. Lounis *et al.*, Phys. Rev. B **83**, 035109 (2011).

O 74.2 Thu 10:45 WIL C107

Calculation of magnetoelectric coupling at Fe/$BaTiO_3$ and Fe/$SrTiO_3$ interfaces — •Hannes Behrend, Brahim Belhadji, and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, Universität Kiel, 24098 Kiel, Germany

The magnetoelectric coupling effect in composites built out of piezoelectric and ferromagnetic materials has attracted great interest, e.g for sensor applications. The objective of our work is to calculate the magnetoelectric coupling that occurs locally, on an atomic scale, at the Fe/$BaTiO_3$ and Fe/$SrTiO_3$ interfaces by means of spin-density functional calculations. The program VASP by Kresse, Hafner *et al.* from the University Wien is applied. The magnetization density and magnetic moment induced by an external electric field are calculated for electric field strengths chosen sufficiently small so that the system stays in the linear response regime. Currently most of the results refer to frozen-in atomic positions,with additional first results for atomic geometries relaxed under the influence of the electric field. A detailed comparison of the Fe/$BaTiO_3$ and Fe/$SrTiO_3$ interfaces will be given. This will be complemented by a calculation of the magnetoelectric coupling coefficient for Fe/Cu layers, for which we have observed an unexpectedly sensitive dependence of the result on the thickness of the Fe slab. The spacial variation of the induced magnetization density as opposed to the induced electronic charge density will be addressed.

O 74.3 Thu 11:00 WIL C107

Control of ferromagnetism in epitaxial $La_{0.7}Sr_{0.3}MnO_3$ films via $BaTiO_3$ substrate phase transitions investigated by XMCD and XLD — •Arndt Quer[1], Erik Kröger[1], Kerstin Hanff[1], Lars Oloff[1], Rohit Soni[2], Adrian Petraru[2], Matthias Kalläne[1], Herrmann Kohlstedt[2], Lutz Kipp[1], and Kai Rossnagel[1] — [1]Institute of Experimental and Applied Physics, University of Kiel, Germany — [2]Department of Nanoelectronics, University of Kiel, Germany

It is known that $La_{0.7}Sr_{0.3}MnO_3$ thin films grown on $BaTiO_3$ can undergo strain-controlled giant, sharp, and persistent magnetization changes as a result of substrate structural phase transitions. In order to investigate the interplay between lattice strain, magnetism, and electronic structure in this system, we have performed X-ray magnetic circular dichroism (XMCD) and X-ray linear dichroism (XLD) measurements on 20-nm thin, epitaxial $La_{0.7}Sr_{0.3}MnO_3$ films grown by pulsed laser deposition on single-crystalline $BaTiO_3$. Here, we report the obtained results. Experiments were performed at the BACH beamline of the Elettra syncrotron storage ring (Trieste, Italy). This work was supported by the DFG (German Research Foundation) through SFB 855 (Collaborative Research Centre 855) "Magnetoelectric Composites - Future Biomagnetic Interfaces".

O 74.4 Thu 11:15 WIL C107

Spin Excitations in STM Evaluated in Perturbation Theory — •Markus Ternes — Max-Planck Institut für Festkörperphysik, Heisenbergstr. 1, 70569 Stuttgart, Germany

Inelastic spin flip spectroscopy has been very successful to characterize and manipulate the properties of single spins as well as coupled spin structures on surfaces. I will show that a perturbative approach of the interactions between the localized spin system, the probing tip, and the supporting substrate can results in fits to experimental data with unprecedented accuracy. The employed model is based on a transport Hamiltonian which accounts for spin-flip and Coulomb scattering of the tunneling electrons with the magnetic impurity system. Higher order and correlations effects are considered by including spin-spin scattering between the impurity and substrate electrons and by solving the corresponding rate-equations up to 3rd order. Despite its simplicity, the model enables a deeper understanding of the relevant couplings in such systems and provides an easy access to the dynamical properties and correlations in atomic scale spin systems.

O 74.5 Thu 11:30 WIL C107

Interplay between Kondo effect and molecular quenching in magnetic molecules at metal substrates from first principles — •David Jacob[1], Maria Soriano[2], and Juan José Palacios[2] — [1]MPI für Mikrostrukturphysik, Halle, Germany — [2]Universidad Autónoma de Madrid, Madrid, Spain

When a magnetic molecule is deposited on a metallic substrate or attached to metal leads, the Kondo effect can take place, thereby screening its magnetic moment. On the other hand strong coupling of the transition metal center to the organic ligands also leads to quenching of the spin. Using our DFT based ab initio approach for nanoscale devices explicitly taking into account the dynamic correlations originating from strong electronic interactions [1,2], we calculate the electronic structure and STM spectra of high spin complexes on metal surfaces. Our calculations reveal the complex interplay of the Kondo effect and molecular quenching processes in these systems [3]. Furthermore we find that Kondo screening via the organic ligands leads to novel features in the spectral function near the Fermi level different from the usual Kondo peaks. [1] D. Jacob *et al.*, PRL **103**, 016803 (2009); [2] M. Karolak *et al.*, PRL **107**, 146604 (2011); [3] D. Jacob *et al.*, PRB **88**, 134417 (2013).

O 74.6 Thu 11:45 WIL C107

Protection of excited spin states by a superconducting energy gap — •Benjamin W. Heinrich[1], Lukas Braun[1], José I. Pascual[1,2], and Katharina J. Franke[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Germany — [2]CIC nanoGUNE, San Sebastián, and Ikerbasque, Basque Foundation for Science, Bilbao, Spain.

The ability to tune the magnetism of individual atoms or molecules and to control their interaction with the environment is a key requirement for their use in potential spintronic applications. We employ scanning tunneling microscopy and spectroscopy at 1.2 K to characterize the spin state of individual metal-organic complexes, namely Fe(III)-Octaethylporphyrin-Chloride, adsorbed on a superconducting Pb(111) surface. The organic ligand provides an anisotropic environment for the spin of the Fe ion ($S = 5/2$), which leads to a zero field splitting of the spin eigenstates. The superconducting gap in the density of states of the substrate now stabilizes excited spin states of the Fe as it hinders the exchange of energy and angular momentum between the substrate's quasi-particles and the molecular spin. This allows for lifetimes of ≈ 10 ns of the excited spin state [1]. Furthermore we examine the influence of our probe, the STM tip, on the zero field splitting of the Fe ion. Even at a distance of several Angstrom between tip and molecule a sizable change of the magnetic anisotropy is detected.
[1] B. W. Heinrich *et al.* Nature Physics, doi:10.1038/nphys2794.

O 74.7 Thu 12:00 WIL C107

Scanning tunneling microscopy and spectroscopy of transition metal phthalocyanines on noble metal surfaces — •Jens Kügel, Jacob Senkpiel, Pin-Jui Hsu, and Matthias Bode — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Transition metal phthalocyanine (TM-Pc) molecules adsorbed on metal substrate have recently attracted considerable interest, as they offer a versatile platform to study magnetic interaction of the central metal ion with the substrate. Especially the Kondo effect, a collective interaction phenomena with the substrate, arising from unscreened magnetic moments of the metal ion, has been intensively studied [1,2]. In this contribution we present low-temperature ($T = 5\,\mathrm{K}$) scanning tunneling microscopy and spectroscopy data of CuPc and MnPc adsorbed on different noble metal substrates [Ag(001), Cu(001)]. The different molecular spectra will be compared and analyzed in terms of their electronic and magnetic properties. In particular we will focus on the Kondo effect and discuss how superimposed states can lead to misinterpretation of the Kondo temperature.

[1] E. Minamitani *et al.*, Phys. Rev. Lett. **109**, 086602 (2012).
[2] A. Stróżecka *et al.*, Phys. Rev. Lett. **109**, 147202 (2012).

O 74.8 Thu 12:15 WIL C107

Engineering Giant Magnetic Anisotropy and Kondo Resonances in Cobalt Adatoms on the h-BN Nanomesh — •Peter Jacobson[1], Tobias Herden[1], Markus Ternes[1], and Klaus Kern[1,2] — [1]Max-Planck-Institute for Solid State Research, D-70569 Stuttgart, Germany — [2]Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

The magnetic properties of Cobalt adatoms on the h-BN/Rh(111) nanomesh have been investigated by scanning tunneling microscopy at low temperatures (1.5 K) and high magnetic fields (10 T). Isolated Co adatoms show a pronounced Kondo resonance consistent with a spin-1 system with an estimated Kondo temperature well below 1 K possessing negligible magnetic anisotropy. Addition of hydrogen to the Co adatoms results in a remarkable shift in the magnetic properties, the Kondo resonance disappears and inelastic spin flip excitations are observed. The Co-H species remains in a spin-1 state and the spin flip excitations indicate that this species has a substantial magnetic anisotropy of 5 meV. The large magnetic anisotropy is attributed to an unquenched orbital moment. Given the dramatic changes upon hydrogen adsorption, we consider the 'molecular' Co-H system an ideal test system for engineering the magnetic anisotropy in molecular magnets.

O 74.9 Thu 12:30 WIL C107

tuning spin-related transport properties of FePc on Au(111) by single-molecule chemistry — •Jian Shang — BNLMS, college of chemistry and molecular engineering, Peking University, 100871, Beijing, China

Tuning spin-related transport properties at the single molecule level is crucial not only for a fundamental understanding of charge and spin interactions but also represents a prerequisite for development of molecular electronics and spintronics. Here we deposited FePc on Au(111) and then, tuned its spin-related transport properties step by step by single-molecule chemistry. After removing 2H, 4H, 6H and 8H from the molecule, Kondo effect, spin transition, Kondo effect and spin transition were observed in differential conductance spectra, sequentially.

O 74.10 Thu 12:45 WIL C107

Spin state of spin-crossover complexes: from single molecules to ultra-thin films — •Manuel Gruber[1,2], Vincent Davesne[1,2], Martin Bowen[1], Samy Boukari[1], Eric Beaurepaire[1], Wulf Wulfhekel[2], and Toshio Miyamachi[2,3] — [1]IPCMS (UMR 7504 Université de Strasbourg-CNRS), Strasbourg, France — [2]Physikalisches Institut, Karlsruher Institut für Technologie, Germany — [3]Institute for Solid State Physics, University of Tokyo, Chiba, Japan

The spin-state bi-stability of spin-crossover molecules [1] can, in principle, be used as building blocks of memory devices. However, it is not obvious if such complexes deposited on surfaces can sustain their controllable bi-stability. In this work, using a scanning tunneling microscope in ultra-high vacuum at 4K, we investigated Fe(1,10-phenanthroline)2(NCS)2 molecules on Cu(100) and Cu(111) surfaces for coverage going from single molecules to ultra-thin films. For sub-monolayer coverage both spin species coexist at low temperatures [2] while this coexistence seems to be lost for the second-layer molecules. We give insights about the origin of this unexpected spin-state coexistence based on the adsorption geometry. Furthermore, we observe voltage-dependent topographies of the second-layer molecules that we tentatively ascribe to a voltage-dependent steady-state combination of HS and LS in a proportion that reflects the bias- and current-dependent switching rates to/from the HS state [3].

[1] P. Gütlich et al., Chem. Soc. Rev. 29, 419 (2000). [2] T. Miyamachi et al., Nat. Commun. 3, 938 (2012). [3] M. Gruber et al., in preparation.