

## O 60: [MA] Joint Session "Surface Magnetism II" (jointly with O)

Time: Thursday 9:30–13:00

Location: EB 301

O 60.1 Thu 9:30 EB 301

**Magnetism of Cobalt Nanoclusters on Graphene on Ir(111)** — ●STEFAN SCHUMACHER<sup>1</sup>, CHI VO-VAN<sup>2</sup>, JOHANN CORAUX<sup>2</sup>, VIOLETTA SESSI<sup>3</sup>, OLIVIER FRUCHART<sup>2</sup>, NICK B. BROOKES<sup>3</sup>, PHILIPPE OHRESSER<sup>4</sup>, and THOMAS MICHELY<sup>1</sup> — <sup>1</sup>II. Physikalisches Institut, Universität zu Köln, D-50937 Köln — <sup>2</sup>Institut Néel, CNRS et Université Joseph Fourier, F-38042 Grenoble — <sup>3</sup>European Synchrotron Radiation Facility, F-38043 Grenoble — <sup>4</sup>Synchrotron SOLEIL, F-91192 Gif-sur-Yvette

On the moiré pattern of graphene on Ir(111) a variety of highly perfect cluster superlattices with narrow size distribution can be grown. The magnetic properties of Co clusters comprising from 26 to 2700 atoms, densely self-organized on the graphene/Ir(111) moiré as well as in more sparse arrangements, were studied *in situ* by means of scanning tunneling microscopy (STM) and X-ray magnetic circular dichroism (XMCD). Surprisingly the small clusters show almost no magnetic anisotropy. We find indication for a magnetic coupling between the clusters. Experiments have to be performed carefully as the clusters get readily damaged by soft X-rays.

O 60.2 Thu 9:45 EB 301

**The role of the chemical and van der Waals interactions in defining the spin-polarization at the hybrid graphene-metal interfaces** — ●NICOLAE ATODIRESEI<sup>1</sup>, VASILE CACIUC<sup>1</sup>, PREDRAG LAZIĆ<sup>2</sup>, MARTIN CALLSEN<sup>1</sup>, and STEFAN BLÜGEL<sup>1</sup> — <sup>1</sup>Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — <sup>2</sup>Massachusetts Institute of Technology, Cambridge, 02139 Massachusetts, USA

By performing density functional theory calculations we reveal the bonding mechanism and the adsorption geometry of graphene on Ir(111) and Co/Ir(111) surfaces. Our simulations included the van der Waals interactions by employing a semi-empirical [1] and an *ab initio* [2] approach, as implemented in the JuNoLo code [3]. The binding of the graphene to the metal is dominated by van der Waals interactions although, locally, a polar covalent-like chemical interaction takes place. In turn, this leads to strong variation of the local spin-polarization at the hybrid graphene-Co/Ir(111) interface. [1] S. Grimme, J. Comput. Chem. **27** 1787 (2006); [2] M. Dion *et al.*, Phys. Rev. Lett. **92**, 246401 (2004); [3] P. Lazić *et al.*, Comp. Phys. Commun. **181**, 371 (2010).

O 60.3 Thu 10:00 EB 301

**Magnetic coupling in metal organic networks on surfaces** — ●TOBIAS R. UMBACH, CHRISTIAN FELIX HERMANN, MATTHIAS BERNIEN, ALEX KRÜGER, ISABEL FERÁNDEZ-TORRENTE, PAUL STOLL, KATHARINA J. FRANKE, JOSE I. PASCUAL, and WOLFGANG KUCH — Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Metal organic networks offer the possibility to alter the electronic and magnetic functionality of surfaces on a nanometer scale. Here we report on the bilayer metal organic network of Fe atoms and 2,4,6-Tris(4-pyridyl)-1,3,5-triazine (T4PT) on a Au(111) surface. The network is investigated in terms of scanning tunneling microscopy (STM) and X-ray circular dichroism (XMCD). Fe atoms and T4PT molecules form a mixed ordered phase consisting of two distinct layers. The first layer has a triangular structure and every Fe atom is surrounded by three pyridyl groups of three different T4PT molecules. The second layer is exclusively built of T4PT molecules, centered with the triazine ring on top of the Fe atoms of the first layer. XMCD measurements reveal sizable magnetic moments of the Fe sites and an out of plane magnetic anisotropy. The field dependence of the XMCD signal reveals a finite ferromagnetic coupling of the Fe atoms in the Fe-T4PT network.

O 60.4 Thu 10:15 EB 301

**Electronic and magnetic properties of free and supported transition metal phthalocyanines** — ●ROBERTO ROBLES, RICHARD KORYTAR, and NICOLÁS LORENTE — Centre d'Investigacions en Nanociència i Nanotecnologia, CIN2 (CSIC-ICN), Barcelona, Spain

By performing density functional theory calculations we have studied the electronic and magnetic properties of transition metal phthalocyanines (MPc, with M=Fe,Co,Ni,Cu), both in the gas phase and sup-

ported on Ag (100) surfaces. First we investigate the properties of the gas-phase MPC's as we change the transition metal and ionize the system. Then we deposit the molecules on the Ag (100) surface, showing how charge transfer and spin moment change by the hybridization with the surface states. We discuss the utility of the anion as a model of the supported situation. We also explore the effect of different exchange-correlation potentials, as well as the influence of van-der-Waals interactions and electronic correlation beyond DFT (GGA+U). Finally, we analyse our results in view of recent STM experiments on the same systems, specially regarding the Kondo effect observed in some of the systems.

- Mugarza, A. et al. Spin coupling and relaxation inside molecule-metal contacts. Nat. Commun. **2**:490 doi: 10.1038/ncomms1497 (2011).

O 60.5 Thu 10:30 EB 301

**Spin resolved measurements of magnetic molecules on surfaces** — ●JENS BREDE<sup>1</sup>, RÉGIS DECKER<sup>1</sup>, JÖRG SCHWÖBEL<sup>1</sup>, SVETLANA KLYATSKAYA<sup>2</sup>, MARIO RUBEN<sup>2,3</sup>, and ROLAND WIESENDANGER<sup>1</sup> — <sup>1</sup>Institute of Applied Physics, University of Hamburg, 20355 Hamburg, Germany — <sup>2</sup>Institute of Nanotechnology, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany — <sup>3</sup>IPCMS, Université de Strasbourg, 67034 Strasbourg, France

The use of magnetic molecules opens a gateway to a flexible design of novel spintronic devices to store, manipulate, and read spin information at nanoscale. Crucial is the precise knowledge of molecular properties at the interface towards an electrode. Progress in this field relies on resolving and understanding the physics at the relevant interfaces. In particular the role of individual molecular constituents and the impact of the atomic environment on molecular properties, determine device relevant parameters, such as conductance and spin polarization. Here, we applied spin-polarized scanning tunneling microscopy to resolve the physics of the molecule-ferromagnet interface. The analysis focuses on different phthalocyanine molecules. The phthalocyanine constitutes of an organic macrocyclic ligand and can be functionalized with various metal ions in order to modify, e.g. the molecular spin state. We will discuss the spin-dependent transport from magnetic surfaces through such molecules.

O 60.6 Thu 10:45 EB 301

**Controlling the spin and the magnetic coupling of adsorbed molecules by on-surface coordination chemistry** — ●CHRISTIAN WÄCKERLIN<sup>1</sup>, KARTICK TARAFDAR<sup>3</sup>, DOROTA CHYLARECKA<sup>1</sup>, JAN GIROVSKY<sup>1</sup>, TATJANA HÄHLEN<sup>1</sup>, CRISTIAN IACOVITA<sup>4</sup>, ARMIN KLEIBERT<sup>2</sup>, FRITHJOF NOLTING<sup>2</sup>, THOMAS A. JUNG<sup>1</sup>, PETER M. OPPENEER<sup>3</sup>, and NIRMALYA BALLAV<sup>5</sup> — <sup>1</sup>Laboratory for Micro- and Nanotechnology and — <sup>2</sup>Swiss Light Source, Paul Scherrer Institute, Switzerland — <sup>3</sup>Department of Physics and Astronomy, Uppsala University, Sweden — <sup>4</sup>Department of Physics, University of Basel, Switzerland — <sup>5</sup>Department of Chemistry, Indian Institute of Science Education and Research, India

The chemical and magneto-electronic interaction of metalloporphyrins with axial ligands has been investigated for the specific case where the paramagnetic molecules [1] are supported on ferromagnetic substrates. Specifically, nitric oxide (NO) can coordinate to the porphyrin center and compete with the surface ligand in its influence of the structural and electronic integrity of the porphyrin [2]. The coordination of NO (S=1/2) with Co(II) (S=1/2) [3], Fe(II) (S=1) and Mn(II) (S=5/2) tetraphenyl porphyrins on ferromagnetic Ni or Co thin film substrates is analyzed by combining X-ray magnetic circular dichroism (XMCD), scanning tunneling microscopy (STM) and density functional theory + additional Hubbard U interaction (DFT+U) calculations.

[1] A. Scheybal et al, Chem Phys Lett **411**, 214 (2005). [2] W. Heringer et al, J Am Chem Soc **133**, 6206 (2011). [3] C. Wäckerlin et al, Nat Comms **1**:61 (2010).

O 60.7 Thu 11:00 EB 301

**Probing individual spin states of Fe-Porphyrins on a superconductor** — ●BENJAMIN W. HEINRICH, LUKAS Z. BRAUN, JOSÉ I. PASCUAL, and KATHARINA J. FRANKE — Institut für Experimentalphysik, Freie Universität Berlin, Germany

Scanning Tunneling Microscopy/Spectroscopy (STM/STS) allows for

studying the competition between magnetism and superconductivity at a single-impurity level. Commonly, the adsorption of a magnetic atom [1,2], or molecule [3], on a superconductor locally breaks the time-reversal symmetry and gives rise to bound states in the superconducting (SC) gap [4], and/or Kondo quasi-particle states [3]. However, here we can show that decoupling the impurity spin from the SC substrate preserves both the local spin and the SC state.

We use inelastic electron tunneling spectroscopy (IETS) to probe the spin state of single Fe(III)-Octaethylporphyrin-Chloride (FeOEP-Cl) molecules adsorbed on Pb(111). Due to the bulky ligand, the interaction between the central Fe ion, holding the molecular spin, and the substrate is strongly reduced. At 4.5 K, we can observe spin flips on the molecule, while the SC quasi-particle resonances remain unchanged. Reducing the tip-sample distance allows for altering the local anisotropy, while desorbing the chlorine ligand via controlled voltage pulses results in a change of the spin state as revealed by energy shifts of the IETS signal.

[1] A. Yazdani et al., Science 275, 1767 (1997) [2] S.-H. Ji et al., Phys. Rev. Lett. 100, 226801 (2008) [3] K.J. Franke et al., Science 332, 940 (2011) [4] H. Shiba, Prog. Theor. Phys. 40, 435 (1968)

## 15 min. break

O 60.8 Thu 11:30 EB 301

**Spatially modulated tunnel magnetoresistance on the nanoscale** — ●HIROFUMI OKA, KUN TAO, SEBASTIAN WEDEKIND, GUILLEMIN RODARY, VALERI STEPANYUK, DIRK SANDER, and JÜRGEN KIRSCHNER — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

We investigate the tunnel magnetoresistance (TMR) effect within a single Co nano-island by low-temperature spin-polarized scanning tunneling microscopy in magnetic fields. We measure the tunnel current as a function of the bias voltage and extract the TMR. We find a TMR of 290 MΩ for the anti-parallel and 190 MΩ for the parallel state at  $-0.27$  V at the center of a Co island. This gives a TMR ratio of  $\sim 50\%$ . The TMR ratio depends on energy and position within the nano-island. We observe a clear spatial modulation of the TMR ratio with an amplitude of  $\sim 20\%$  and a spacing of  $\sim 1.3$  nm between maxima and minima around the Fermi level. This result can be ascribed to a spatially modulated spin-polarization within the Co island due to spin-dependent quantum interference [1]. Our combined experimental and theoretical study reveals that spin-dependent electron confinement affects all transport properties such as differential conductance, conductance and TMR. We demonstrate that the TMR within a nanostructured magnetic tunnel junction can be controlled on a length scale of 1 nm through spin-dependent quantum interference [2].

[1] H. Oka et al., Science 327, 843 (2010).

[2] H. Oka et al., PRL 107, 187201 (2011).

O 60.9 Thu 11:45 EB 301

**First-principles investigation of g-shifts and damping of dynamical magnetic excitations in adatoms on surfaces** —

●SAMIR LOUNIS<sup>1</sup>, ANTONIO T. COSTA<sup>2</sup>, BRUNO CHILIAN<sup>3</sup>, ALEXANDER A. KHAJETOORIANS<sup>3</sup>, JENS WIEBE<sup>3</sup>, ROLAND WIESENDANGER<sup>3</sup>, and DOUGLAS L. MILLS<sup>4</sup> — <sup>1</sup>Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — <sup>2</sup>Instituto de Física, Universidade Federal Fluminense, 24210-340 Niterói, Rio de Janeiro, Brazil — <sup>3</sup>Institute of Applied Physics, Hamburg University, Jungiusstrasse 11, D-20355 Hamburg, Germany — <sup>4</sup>Department of Physics and Astronomy, University of California Irvine, California, 92697 USA

Recently, spin excitations in Fe adatoms on Cu(111) and Ag(111) surfaces are probed with magnetic field dependent inelastic scanning tunneling spectroscopy[1]. The calculation of the transverse dynamical magnetic susceptibility allows to analyse the electronic signature of these excitations[2]. We show that an Fe adatom on Ag(111) surface, contrary to other atoms embedded in various lattice configurations, has a surprisingly large g-value of 3 instead of the regular value of 2.

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

[1] A. A. Khajetoorians et al., Phys. Rev. Lett. 106, 037205 (2011); B. Chilian et al., Arxiv:1108.2443

[2] S. Lounis et al., Phys. Rev. Lett. 105, 187205 (2010); S. Lounis et al., Phys. Rev. B 83, 035109 (2011)

O 60.10 Thu 12:00 EB 301

**Anomalous large g-factor of single atoms adsorbed on a metal substrate** — ●JENS WIEBE<sup>1</sup>, ALEXANDER A. KHAJETOORIANS<sup>1</sup>, SAMIR LOUNIS<sup>2</sup>, ANTONIO T. COSTA<sup>3</sup>, BRUNO CHILIAN<sup>1</sup>, DOUGLAS L. MILLS<sup>4</sup>, and ROLAND WIESENDANGER<sup>1</sup> —

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We performed magnetic field dependent inelastic scanning tunneling spectroscopy (ISTS) on individual Fe atoms adsorbed on different metal surfaces. ISTS reveals a spin excitation which is shifting linearly to higher energies in the magnetic field. The magnetic anisotropies and the g-factors of the Fe atoms, as well as the lifetimes of the excitations, are extracted. We find lifetimes of hundreds of fs limited by coupling to electron-hole pairs in the substrate and decreasing linearly in the magnetic field. As expected, the magnetic anisotropy strongly depends on the substrate. Astoundingly, the g-factor is  $g \approx 3.1$  for Ag(111) [1] instead of the regular value of 2 which is observed for the Cu(111) substrate [2]. This very large g-shift can be understood when considering the complete electronic structure of both the Ag(111) surface state and the Fe atom, as shown by *ab initio* calculations of the magnetic susceptibility.

[1] B. Chilian et al., Phys. Rev. B, accepted (2011).

[2] A. A. Khajetoorians et al., Phys. Rev. Lett. 106, 037205 (2011).

O 60.11 Thu 12:15 EB 301

**Detecting spin excitation of rare-earth atoms and clusters on metallic surfaces** — ●TOSHIO MIYAMACHI<sup>1</sup>, TOBIAS SCHUH<sup>1</sup>, STEFAN GERSTL<sup>1</sup>, ARTHUR ERNST<sup>2</sup>, and WULF WULFHEKEL<sup>1</sup> —

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At the heart of the stability of magnetic bits in information storage is a magnetic anisotropy energy (MAE) and magnetization dynamics. Recent inelastic tunneling spectroscopy (ITS) studies have revealed that the spin states of 3d transition metal atoms and clusters on metallic substrates have extremely short lifetimes of the order of femtosecond due to strong hybridization of 3d states and substrates [1]. To reduce the influence of substrates from atoms and clusters, 4f rare-earth Gd atoms and clusters on Pt(111) and Cu(111) were studied with ITS. Since the 4f states are inner orbitals, the hybridization with substrates could be decreased. In addition, as the relativistic spin orbit interaction plays a crucial role for the MAE, 4f atoms with larger spin and orbital momenta could show larger MAEs than 3d atoms [2]. Obtained results show that the spin excitation of 4f states can be accessed with ITS, and that giant magnetic anisotropies and lifetimes of the excited states of Gd are nearly independent of supporting substrate or size of the cluster, reflecting the strongly localized character of 4f electrons in Gd atoms and clusters.

[1] T. Balashov et al., Phys. Rev. Lett. 102, 257203 (2009)

[2] T. Schuh et al., Phys. Rev. B. 84, 104401 (2011)

O 60.12 Thu 12:30 EB 301

**Spin-transfer torque switching efficiency in SP-STM experiments** — ●ANDREAS SONNTAG, STEFAN KRAUSE, GABRIELA HERZOG,

ANIKA SCHLENHOFF, and ROLAND WIESENDANGER — Institute of Applied Physics, University of Hamburg, Germany

The tunnel current generated in spin-polarized scanning tunneling microscopy (SP-STM) experiments can be used to manipulate the switching behavior of superparamagnets [1] or even to reverse the quasistable magnetization of nano-islands [2]. Two main contributions involved in magnetization switching could be identified: Joule heating and the spin-transfer torque.

In our study we investigate the influence of a spin-polarized tunneling current on the switching behavior of superparamagnetic Fe nano-islands on the W(110) surface. Analyzing the lifetimes of the two magnetic states in dependence of the current, Joule heating and spin-torque effects are separated and quantified [3]. While the Joule heating decreases both lifetimes equally, the spin-torque lifts their degeneracy. Both effects are found to scale linearly with the tunneling current. By introducing the so-called spin-transfer torque viscosity and normalizing the torque with respect to the magnetic moment of the free layer, we compare our findings to experiments performed on lithographically fabricated magneto-tunnel junctions. The results show a comparatively high spin-transfer torque efficiency in our experiments.

[1] S. Krause et al., Science 317, 1537 (2007).

[2] G. Herzog et al., Appl. Phys. Lett. 96, 102505 (2010).

[3] S. Krause *et al.*, Phys. Rev. Lett. **107**, 186601 (2011).

O 60.13 Thu 12:45 EB 301

**Spin transfer torque and Joule heating of field-emitted electrons** — ● ANIKA SCHLENHOFF, ANDREAS SONNTAG, STEFAN KRAUSE, and ROLAND WIESENDANGER — Institute of Applied Physics, University of Hamburg

Since the detection of the spin polarization of field-emitted electrons in the 1970's [1], it is an open question which type of effects a high spin-polarized current of field-emitted electrons has onto a magnetic sample. Though spin-polarized two-photon photoemission has gained first insight into the interaction of hot electrons with an underlying spin system [2], the microscopic details still remain to be discovered.

In our studies, we utilize spin-polarized scanning tunneling microscopy (SP-STM) in the field emission mode [3] for the direct observation of the influence of field-emitted electrons onto atomic-scale superparamagnets [4]. The experiments reveal that the injection of high spin-polarized currents via the first field emission resonance (FER) significantly changes the superparamagnet's switching behavior. Telegraphic noise experiments allow for a detailed current-dependent lifetime analysis, thereby quantifying the spin-transfer torque and Joule heating of the field-emitted electrons. The results are compared to low energy electrons tunneling directly into the nanoisland.

[1] N. Müller *et al.*, Phys. Rev. Lett. **29**, 1651 (1972).

[2] A. B. Schmidt *et al.*, Phys. Rev. Lett **105**, 197401(2010).

[3] A. Kubetzka *et al.*, Appl. Phys: Lett. **91**, 012508 (2007).

[4] S. Krause *et al.*, Phys. Rev. Lett. **103**, 127202 (2009).