

MA 44: Surface Magnetism (Joint Session with O) - Adatoms on surfaces

Time: Thursday 15:00–17:30

Location: H 0110

MA 44.1 Thu 15:00 H 0110

Magnetism of Ho and Er Atoms on Close-Packed Metal Surfaces — ●FABIO DONATI¹, APARAJITA SINGHA¹, SEBASTIAN STEPANOW², CHRISTAN WÄCKERLIN¹, JAN DREISER^{1,3}, PIETRO GAMBARELLA², STEFANO RUSPONI¹, and HARALD BRUNE¹ — ¹Institute of Condensed Matter Physics (ICMP), École Polytechnique Fédérale de Lausanne (EPFL), Switzerland — ²Department of Materials, ETH Zürich, Switzerland — ³Swiss Light Source (SLS), Paul Scherrer Institute (PSI), Switzerland

Single atoms on a surface represent a paradigm for investigating the ultimate size limit of nanomagnets. By combining x-ray magnetic circular dichroism measurements with multiplet calculations, we performed a comparative study of the ground state and magnetic anisotropy of single Ho and Er atoms on Pt(111) and Cu(111). Our results emphasize the different interaction of the 4f orbitals with the substrate electrons, showing that the *s*- or *d*- character of the substrate states plays a major role in determining the hierarchy of the magnetic quantum states [Donati et al., Phys. Rev. Lett., in press]. In particular, Er atoms display a rotation of the magnetization easy axis from out-of-plane on Pt(111) to in-plane on Cu(111), whereas Ho atoms on Pt(111) present a ground state that is incompatible with the long spin relaxation times reported by a recent scanning tunneling microscopy study of the same system [Miyamachi et al., Nature **503**, 242 (2013)].

MA 44.2 Thu 15:15 H 0110

Impact of spin-fluctuations on the magnetic properties of 4d adatoms on metal substrates — ●JULEN IBAÑEZ-AZPIROZ, MANUEL DOS SANTOS DIAS, STEFAN BLÜGEL, and SAMIR LOUNIS — Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

We present a theoretical analysis of the effect of spin-fluctuations on the magnetic properties of 4d adatoms deposited on metallic substrates. These systems have been long predicted to develop a large local magnetic moment by theoretical calculations based on density functional theory (DFT) [1], but experiments have measured negligible magnetic signals so far (see e.g. [2]). Our aim is to clarify the role of the spin-fluctuations, which tend to destabilize the magnetic moment and are not included into the standard DFT. We make use of the fluctuation-dissipation theorem, which relates the magnitude of the spin-fluctuations to the interacting spin-susceptibility as calculated in linear response theory. We access the latter quantity using a fully ab-initio approach based on the Korringa Kohn Rostoker (KKR) Green function formalism within time-dependent DFT [3,4].

We would like to acknowledge support from the Helmholtz Gemeinschaft Deutscher-Young Investigators Group Program No. VH-NG-717 (Functional Nanoscale Structure and Probe Simulation Laboratory).

[1] K.Wildberger et al., Physical Review Letters, **75** 509 (1995)[2] J. Honolka et al., Physical Review B, **76** 144412 (2007)[3] S. Lounis et al., Physical Review B, **83** 035109 (2011)[4] S. Lounis et al., Physical Review Letters, **105** 187205 (2010)

MA 44.3 Thu 15:30 H 0110

Magnetic linear dichroism of 3d metal thin films — ●TORSTEN VELTUM¹, TOBIAS LÖFFLER¹, MATHIAS GEHLMANN², SVEN DÖRING², LUKASZ PLUCINSKI², STEPHAN BOREK³, JAN MINAR³, JÜRGEN BRAUN³, HUBERT EBERT³, and MATHIAS GETZLAFF¹ — ¹Institut für Angewandte Physik, Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf — ²Peter Grünberg Institut PGI-6, Forschungszentrum Jülich, 52428 Jülich — ³Department Chemie, Ludwig-Maximilians-Universität München, 81377 München

Magnetic linear dichroism in the angular distribution of photoelectrons (MLDAD) is a technique that allows the study of both the electronic band structure and the magnetic properties of thin films and single crystals. We are looking for a deeper understanding of the magnetic linear dichroism of 3d metals. We study epitaxially grown Co(0001) and Fe(110) thin films on a W(110) surface.

In this study linearly polarized synchrotron radiation (Beamline 5, DELTA Dortmund) in the VUV regime is used to gain experimental data. Theoretical calculations for these systems are carried out with local spin density approximation (LSDA) and dynamical mean field theory (DMFT).

The electronic structure of the valence band is measured by variation of the photon energy. At excitation energies above 20 eV, dichroism measurements are reconfirmed and extended to angle-resolved spectra in off-normal geometry. The resonance between the 3d core-levels and the valence band of these materials shows an influence on the dichroism.

MA 44.4 Thu 15:45 H 0110

Magnetic properties of Cobalt nanodot arrays on rare-earth-Au₂ surface compounds — ●FREDERIK SCHILLER^{1,2}, LAURA FERNÁNDEZ^{2,3}, MAXIM ILYN¹, ANA MAGAÑA⁴, and ENRIQUE ORTEGA⁴ — ¹Centro de Física de Materiales, San Sebastian, Spain — ²Fachbereich Physik, Phillips Universität Marburg, Germany — ³Donostia International Physics Center, San Sebastian, Spain — ⁴Universidad del País Vasco (UPV/EHU), San Sebastian, Spain

Cobalt deposition on prepatterned rare-earth (RE)Au₂/Au(111) substrates leads to self-organization into very dense hexagonal structures of Co nanodots. Depending on the substrate surface RE material one can achieve different interactions that determine the magnetic properties of the dots. In order to investigate in detail such effects, a combined study involving X-ray Circular Magnetic Dichroism and Scanning Tunneling Microscopy will be presented. Several substrates will be analyzed (SmAu₂, GdAu₂, and YbAu₂) that have the same RE-Au₂ surface structure and lattice but reveal ferromagnetic, anti-ferromagnetic [1], and non-magnetic interaction with the Co nanodot array, respectively. These interactions not only determine the magnetic properties below the Curie temperature T_C of the substrate but also far above T_C and lead to enhancements of the magnetic anisotropy and blocking temperature of the Co nanodot array.

[1] L.Fernandez et al., Nano Letters **14**, 2977 (2014).

MA 44.5 Thu 16:00 H 0110

Magnetism of Fe/Pt surface alloys and Fe/Pt nanostructures embedded in Pt(111) via ab initio calculations — ●SALEEM AYAZ KHAN¹, JÁN MINÁR^{1,2}, and ONDŘEJ ŠÍPR³ — ¹University of West Bohemia, Plzeň, Czech Republic — ²Universität München, Germany — ³Institute of Physics ASCR, Praha, Czech Republic

Embedding Fe atoms in the surface layer of Pt (111) creates low dimensional materials with complex magnetic behavior. To understand the combined effect of coordination and disorder, a systematic theoretical study of spin and orbital magnetic moments and of density of states for a series of embedded Fe/Pt nanostructures was performed within the ab initio density functional theory framework, using the FLAPW method (WIEN2K code) and the KKR-Green's function method (SPRKKR code). Different ways of including relativistic effects were tested. We find that increasing the Pt content in Fe/Pt nanostructures generally results in enhancement of magnetic moments. The effect of hybridization of Fe 3d and Pt 5d electrons in the presence of a surface is discussed in detail.

15 min. break

MA 44.6 Thu 16:30 H 0110

Modifying the magnetic exchange coupling of hybrid organic-ferromagnetic interfaces — ●RICO FRIEDRICH, VASILE CACIUC, NIKOLAY S. KISELEV, NICOLAE ATODIRESEI, and STEFAN BLÜGEL — Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

In molecular spintronics the properties of hybrid organic/ferromagnetic interfaces are of crucial importance [1]. Recently, it has been demonstrated by experimental and theoretical means [2] that an organic layer made of phenalenyl-based molecules on top of a cobalt contact can significantly modify the electronic and magnetic properties of the metal surface.

In this talk we outline a systematic study of this effect by investigating the influence of hetero-atoms within the organic molecules on the magnetic exchange coupling constant J between the surface Fe atoms below the molecule. Our results demonstrate, that a magnetic hardening can be specifically tuned when atoms like boron, carbon or nitrogen influence the magnetic exchange coupling. Moreover, a magnetic softening effect can be realized when either oxygen or a boron-carbon

bond mediate the coupling between surface Fe atoms. Furthermore, we demonstrate that the most important contribution to the modification of the coupling constants is due to the hybridization between the electronic states of the molecule and those of the substrate.

[1] N. Atodiresei et al., *Physical Review Letters* **105**, 066601 (2010).

[2] K. V. Raman et al., *Nature* **493**, 509 (2013).

MA 44.7 Thu 16:45 H 0110

Unexpected antiferromagnetic coupling of Cr-porphyrin to bare cobalt thin film — ●JAN GIROVSKY¹, KARTICK TARAFDER^{2,3}, JAN NOWAKOWSKI¹, CHRISTIAN WÄCKERLIN⁴, MILOŠ BALJOZOVIC¹, DOROTA SIEWERT⁵, ANELIJA WÄCKERLIN⁵, ARMIN KLEIBERT⁶, NIRMALYA BALLAV⁷, THOMAS A. JUNG¹, and PETER M. OPPENEER² — ¹LMN, PSI, Villigen, Switzerland — ²Uppsala University, Uppsala, Sweden — ³BITS, Shameerpet, Andhra Pradesh, India — ⁴LNS, EPFL, Lausanne, Switzerland — ⁵University of Basel, Basel, Switzerland — ⁶SLS, PSI, Villigen, Switzerland — ⁷IISER, Pune, India

Spin bearing square-planar metallo-organic complexes interact magnetically with ferromagnetic (FM) substrates even up to room temperature[1]. So far, exclusively FM ordering has been reported for such molecules adsorbed on bare metallic ferromagnets [2,3]. Here, we present a combined experimental and theoretical study on CrTPP molecules antiferromagnetically (AFM) coupled to bare cobalt substrate. The observed AFM interaction is confirmed by DFT+U calculations and alternatively described within the framework of Goodenough-Kanamori-Anderson (GKA) rules. In the GKA model, the less than half-filled 3d shell of the Chromium ion interacts with the out-of-plane orbitals of the cobalt atoms via indirect 90 degree exchange coupling mediated by the porphyrins' nitrogen atoms[4].

[1] A. Scheybal et al, *Chem Phys Lett* 411, 214 (2005).

[2] N. Ballav et al, *JPCL* 4, 2303 (2013).

[3] A. Lodi Rizzini et al, *Surface Science* 630, 361 (2014).

[4] J. Girovsky et al, *PRB* (R), in press

MA 44.8 Thu 17:00 H 0110

Molecular-driven magnetism on reactive metal surfaces — ●AMILCAR BEDOYA-PINTO¹, STEFAN LACH², CHRISTIANE ZIEGLER², MATS FAHLMAN³, EUGENIO CORONADO⁴, and LUIS HUESO¹ — ¹CIC nanoGUNE, San Sebastián, Spain — ²Department of Physics, University of Kaiserslautern — ³Department of Physics, Chemistry and Biology, Linköping University, Sweden — ⁴ICMOL, Valencia, Spain

The fascinating properties of molecules, due to their wide-ranging chemical functionalities that can be tailored on purpose, are currently

opening new pathways in many fields connected to solid-state physics. As for molecular-based spintronics, the interaction strength between ferromagnetic metals and adsorbed molecules have been found to be determinant to engineer spin-dependent interface properties. Here, with a multi-method study (IR,UPS,XPS,EELS,XMCD,SQUID), we show that the adsorption of high-spin molecules (Tb3q9) on non-magnetic reactive metals induces the formation of room-temperature magnetically active phases, even without the presence of any ferromagnet. This approach relies on a strong chemical reaction at the metal-molecule interface, which dramatically alters the structure and stoichiometry of the molecular species and generates a new phase involving both the high-spin metal atom present in the molecule (Tb) and the metallic surface atoms (Cu). The fact that these purpose-made molecules are able to trigger the creation of a new inorganic phase with robust magnetic properties at a non-magnetic surface underlines the importance and role of interfacial chemistry to crucially modify surface properties and thus design building blocks for spintronic applications.

MA 44.9 Thu 17:15 H 0110

Uncompensated antiferromagnets for artificial magnetic semiconductors — ●MICHALIS CHARILAOU^{1,2,3}, SIMCA BOUMA^{2,3}, CATHERINE BORDEL^{2,3}, and FRANCES HELLMAN^{2,3} — ¹Department of Materials, ETH Zurich, Zurich, Switzerland — ²Department of Physics, University of California Berkeley, Berkeley, California, USA — ³Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California, USA

Like ferromagnets (FM), antiferromagnets (AFM) exhibit spontaneous long-range spin ordering below a transition temperature. The net magnetization of a perfect AFM is zero, however; defects such as vacancies, grain boundaries, or surfaces can create an uncompensated net magnetization. As a specific example we consider AFM CoO, which consists of AFM-coupled FM (111) planes; (111)-oriented epitaxial films with an odd number of planes will exhibit a non-zero net magnetization due to uncompensated surfaces. These uncompensated surfaces have been used to produce an artificially-structured FM semiconductor using epitaxial layers of AFM CoO with a doped semiconductor Al:ZnO (AZO). Both M(T) and the anomalous Hall effect show oscillatory behavior with thickness of either CoO (compensated vs uncompensated) or AZO (RKKY-type oscillations related to the AZO Fermi wavevector due to electron-induced coupling between Co moments at its two CoO surfaces). The experimental results are complemented by theoretical calculations, which show that the thermodynamic behavior of the magnetization in uncompensated AFM is highly versatile, and is dominated by the exchange coupling on the surface.