

O 110: Surface Magnetism I (joint session O/MA)

Time: Thursday 15:00–18:00

Location: WIL A317

O 110.1 Thu 15:00 WIL A317

Magnetic properties of multilayer vanadyl phthalocyanine on Pb(111) — ●PIOTR KOT, MAXIMILLIAN UHL, ROBERT DROST, and CHRISTIAN R. AST — Max Planck Institute for Solid State Research

Single-molecule magnets have been of great interest to the condensed matter community due to their potential applications in memory storage and quantum computing [1], and their inherent usefulness in studying fundamental quantum mechanics [2]. Here we present a study of vanadyl phthalocyanine (VOPc) molecules which, when deposited in the correct conditions, form multilayer nano-crystals on the surface of Pb(111) with two possible molecular orientations at each layer. Only one of the VOPc orientations on the first layer shows a spin excitation with energy splitting consistent with a spin half system, which agrees with recent findings [3]. The magnetic properties found on the second layer of molecules is also only observed in one of the molecular orientations, and shows strong zero-field splitting. This suggests that the way the first and second layer molecules interact with their environments varies significantly.

1. Leuenberger, Michael N., and Daniel Loss. "Quantum computing in molecular magnets." *Nature* 410.6830 (2001): 789.
2. Gatteschi, Dante, and Roberta Sessoli. "Quantum tunneling of magnetization and related phenomena in molecular materials." *Angewandte Chemie International Edition* 42.3 (2003): 268-297.
3. Malavolti, Luigi, et al. "Tunable Spin*Superconductor Coupling of Spin 1/2 Vanadyl Phthalocyanine Molecules." *Nano letters* 18.12 (2018): 7955-7961.

O 110.2 Thu 15:15 WIL A317

Influence of the Molecular Arrangement on the Magnetic Properties of FePc and FePcF₁₆ thin films — ●KATHARINA GREULICH¹, AXEL BELSER¹, SVEN BÖLKE¹, REIMER KARSTENS¹, PETER NAGEL², STEFAN SCHUPPLER², MICHAEL MERZ², THOMAS CHASSÉ¹, and HEIKO PEISERT¹ — ¹Institute of Physical and Theoretical Chemistry, University of Tübingen — ²Institute for Solid-State Physics, Karlsruhe Institute of Technology

The electronic configuration and thus the magnetic properties of the central metal atom of some transition metal phthalocyanines are not fully understood and have been intensely debated over the last years. A particularly broad complexity of the electronic structure is expected for Fe(II) phthalocyanines and porphyrins. In our XPS, XAS and XMCD studies, we compare thin films of FePc with their perfluorinated counterpart FePcF₁₆. The results indicate that the magnetic and electronic properties of the central Fe atom depend distinctly on the arrangement of the molecules in thin films. Compared to FePcF₁₆, FePc shows an unusually large XMCD signal at the Fe L_{3,2}-edge pointing to collective magnetic properties that do not seem possible in FePcF₁₆ due to a different molecular arrangement.

O 110.3 Thu 15:30 WIL A317

Kondo effect of a singly occupied molecular orbital in bis(phthalocyaninato)-dysprosium double decker molecules — ●TIMO FRAUHAMMER¹, TIMOFEY BALASHOV^{1,2}, GABRIEL DERENBACH¹, SVETLANA KLYATSKAYA³, EUFEMIO MORENO-PINEDA³, MARIO RUBEN³, and WULF WULFHEKEL^{1,3} — ¹Physikalisches Institut, Karlsruhe Institute of Technology, Germany — ²II. Physikalisches Institut, RWTH Aachen, Germany — ³Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany

Double decker bis(phthalocyaninato)-dysprosium single molecule magnets adsorbed on Au(111) have been investigated using low temperature STM. No direct magnetic signal by the 4f electrons could be detected in STS. However, a clear Kondo resonance located on the ligands of the molecules can be observed. This indicates an odd number of electrons residing in the molecular orbitals of the ligands. Interestingly, a splitting of this Kondo resonance has been observed even in the absence of external magnetic fields, which can be attributed to a ferromagnetic exchange coupling between the unpaired spin on the ligands and the 4f angular momentum of the Dy central ion. Using spin-polarized tips, this might enable the readout of the 4f spin of Dy.

O 110.4 Thu 15:45 WIL A317

Real-time susceptibility measurements of CoTMPP on magnetic Ni/Cu(110)-(2x1)O thin films — ●GIZEM MENDIREK¹,

ALEKSANDER BROZYNIAK¹, MICHAEL HOHAGE¹, MARIELLA DENK¹, ANDREA NAVARRO-QUEZADA^{1,2}, and PETER ZEPPENFELD¹ — ¹Institut für Experimentalphysik, Johannes Kepler Universität Linz, Altenberger Str. 69, 4040 Linz, Österreich — ²Institut für Halbleiter und Festkörperphysik, Johannes Kepler Universität Linz, Altenberger Str. 69, 4040 Linz, Österreich

The magneto-optic signal of organic molecular thin films is expected to be rather small. Therefore, a high sensitivity is required to measure the magnetic susceptibility of thin molecular layers. In this work we present the implementation of a sinusoidal modulation of the magnetic field to a Reflectance Difference Magneto-Optical Kerr Effect (RD-MOKE) setup with increased sensitivity that allows detecting of variations of the Kerr rotation angle below 1 μ rad/mT at applied fields of a few mT. We illustrate the capabilities of the setup for Ni thin films grown on Cu(110)-(2x1)O surfaces, which exhibit a sharp spin reorientation transition (SRT) of the magnetic easy axis from in-plane to out-of-plane at a coverage of 9 ML. Subsequent deposition of cobalt tetramethoxyphenylporphyrin (CoTMPP) on Ni/Cu(110)-(2x1)O surface induces characteristic changes in the magnetic properties that can be monitored in real-time during the growth of the organic layer. Our results demonstrate the potential of the setup for studying ultrathin organic/ferromagnetic interfaces.

O 110.5 Thu 16:00 WIL A317

Emergence of on-surface molecular magnetism by non-magnetic impurity doping — ●ROBERTO ROBLES¹, WE-HYO SOE², CARLOS MANZANO³, NICOLÁS LORENTE^{1,4}, and CHRISTIAN JOACHIM² — ¹Centro de Física de Materiales CFM/MPC (CSIC-UPV/EHU), San Sebastián, Spain — ²Centre d'Elaboration de Matériaux et d'Études Structurales (CEMES), CNRS, Université de Toulouse, Toulouse, France — ³Institute of Material Research and Engineering (IMRE), Agency for Science, Technology and Engineering (A*STAR), Singapore — ⁴Donostia International Physics Center (DIPC), San Sebastián, Spain

Using a low-temperature scanning tunneling microscope (LT-STM) combined with density functional theory (DFT) calculations we show how non-magnetic organic molecules on a metallic surface can become magnetic by doping them with light metal atoms. By single atom/molecule manipulation we construct a complex formed by two aluminum atoms doping a phenanthrazine molecule on an Au(111) surface. We use the Kondo effect to characterize the magnetic moment and confirm the emergence of a localized magnetic moment in the 2(Al)-phenanthrazine complex. DFT calculations allow us to describe the electronic and magnetic properties of the new system. This procedure opens a new way to design light magnetic molecular complexes without the need of transition metal atoms.

O 110.6 Thu 16:15 WIL A317

Probing intramolecular metal-ligand spin coupling by STM — ●YUQI WANG¹, SOROSH ARABI¹, KLAUS KERN^{1,2}, and MARKUS TERNES^{3,4} — ¹Max Planck Institute for Solid State Research, D-70569 Stuttgart, Germany — ²École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland — ³RWTH Aachen University, Institute of Physics, D-52074 Aachen, Germany — ⁴Peter-Grünberg-Institute, Forschungszentrum Jülich, D-52425 Jülich, Germany

The bonding of metal-organic molecules to a substrate induces molecular ligand spin states, which lead to an intramolecular conductance and spin dynamics [1]. However, the intramolecular spin coupling has not been studied in detail at molecular scale yet. Here we use a low-temperature scanning tunneling microscope (STM) to study cobalt phthalocyanine (CoPc) molecules on a 2H-NbSe₂ substrate. We observe that there are two kinds of adsorbed CoPc molecules due to two slightly different adsorption geometries. While one behaves like a $S = 1/2$ system which introduces Yu-Shiba-Rusinov states in the superconducting gap of the substrate [2], the other behaves like an effective $S = 0$ system which shows a singlet-triplet transition at about 23 meV due to the antiferromagnetic coupling between the central Co atom of the metal-organic complex and its ligands. [1] A. Mugarza, *et al.*, *Nat. Comm.* **2**, 490 (2011). [2] S. Kezilebieke, *et al.*, *Nano Lett.* **18**, 2311 (2018).

O 110.7 Thu 16:30 WIL A317

Mapping magnetic anisotropies in molecular junctions — ●CRISTINA MIER¹, LEONARD GARNIER², BENJAMIN VERLHAC², ROBERTO ROBLES¹, LAURENT LIMOT², NICOLÁS LORENTE¹, and DEUNG-JANG CHOI¹ — ¹Centro de Física de Materiales (MPC) CSIC-EHU, San Sebastián, Spain — ²Université de Strasbourg, CNRS, IPCMS, UMR 7504, Strasbourg, France

The ability to control the spin of single molecules is of great interest for the development of quantum technologies. Nickelocene ((Ni(C₅H₅)₂NiCp₂) is a magnetic molecule with spin S=1, which shows a big electronic inelastic signal due to the excitation of its spin state [1]. We studied this molecule on a superconducting surface and used a superconducting tip which allows us having a higher energy resolution than the one with normal metallic tips. We found peaks in the differential conductance due to the spin excitations, permitting us to determine the magnetic anisotropy energy (MAE) of the system. The energy position of peaks is slightly shifted at different molecules, which indicates differences in magnetic anisotropy energies for each molecules. This study gives us more parameters to tune the MAE in a molecular junction.

[1] M. Ormaza, N. Bachellier, M. N. Faraggi, B. Verlhac, P. Abufager, P. Ohresser, L. Joly, M. Romeo, F. Scheurer, M.-L. Bocquet, N. Lorente, and L. Limot. Efficient spin-flip excitation of a nickelocene molecule. *Nano Letters*, 17(3):1877*1882, 2017. PMID: 28199115.

O 110.8 Thu 16:45 WIL A317

Organic radical functionalisation of a gold surface — ●TOBIAS JUNGHÖFER, EWA MALGORZATA NOWIK-BOLTYK, and MARIA BENEDETTA CASU — Eberhard Karls Universität Tübingen, Institut für Physikalische und Theoretische Chemie, 72076 Tübingen, Germany

Organic radical thin films are of great interest for organic electronics such as spin filtering devices, data storage devices, and as quantum bits for quantum computing devices. Here we present the functionalisation of a gold substrate by using a derivative of the perchlorotriphenylmethyl (PTM) radical. PTM is a very chemically and thermally stable radical. We investigate the gold/PTM derivative interface by using soft X-ray techniques, such as X-ray photoelectron spectroscopy (XPS) and near-edge X-ray absorption fine structure (NEXAFS) spectroscopy. Our results show that the functionalisation is successful under specific preparation conditions. The radical is still intact and keeps its magnetic character at the interface. Our findings are a significant step forward on the implementation of organic radicals in molecular-based devices with different properties and applications as energy, sensing, imaging, memories, and spintronics.

O 110.9 Thu 17:00 WIL A317

Spin-polarized photoelectron emission from chiral cupric oxide layers — ●PAUL MÖLLERS¹, DANIEL NÜRENBERG¹, KOYEL BANERJEE GHOSH², WENYAN ZHANG², FRANCESCO TASSINARI², YITZHAK MASTAI², ORTAL LIDOR-SHALEV², SIMON WEI³, EMIL WIERZBINSKI³, DAVID WALDECK³, RON NAAMAN², and HELMUT ZACHARIAS¹ — ¹Center for Soft Nanoscience, Westfälische Wilhelms-Universität, 48149 Münster, Germany — ²Department of Chemical and Biological Physics, Weizmann Institute of Science, 76100 Rehovot, Israel — ³Chemistry Department, University of Pittsburgh, Pittsburgh, PA 15260, United States

The chirality-induced spin selectivity (CISS) effect introduces a coupling between the linear and the spin angular momentum of electrons moving through a chiral molecule [1]. Chiral cupric oxide (CuO) layers can be grown by electrodeposition from a solution containing chiral precursor molecules such as tartaric acid [2]. The choice of the enantiomer of this precursor determines the chiral crystal structure and the preferential crystallographic orientation.

Here, we present results from spin-resolved photoemission experiments performed with chiral CuO layers to investigate the presence of CISS. We demonstrate that the spin polarization observed in these layers can be exploited to enhance the chemical selectivity of an electrocatalytic water splitting reaction [3].

[1] R. Naaman et al., *Nat Rev Chem* 3, 250 (2019) [2] Kothari et al., *Chem. Mater.* 16, 4232 (2004) [3] K. B. Gosh et al., *J. Phys. Chem. C* 123, 3024 (2019)

O 110.10 Thu 17:15 WIL A317

Quantifying exchange forces of a spin spiral on the atomic scale — NADINE HAUPTMANN¹, SOUMYAJYOTI HALDAR², TZU-CHAO HUNG¹, ●WOUTER JOLIE¹, LORENA NIGGLI^{1,3}, MARA

GUTZEIT², DANIEL WEGNER¹, STEFAN HEINZE², and ALEXANDER A. KHAJETOORIANS¹ — ¹Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands — ²Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität, Kiel, Germany — ³Physik Institut, University of Zurich, Switzerland

Chiral magnetic structures are stabilized by an interplay between competing exchange interactions at the atomic scale. Spin-polarized scanning tunneling microscopy (SP-STM) has achieved great success in investigating the magnetization of such structures, but faces a number of limitations in being able to directly detect the underlying exchange forces, as well as delineate between structural and electronic contributions. To go beyond these limitations, we have developed a new method, which combines SP-STM and magnetic exchange force microscopy (SPEX) based on nc-AFM. Here, we utilize SPEX to investigate a monolayer of Mn on W(110), which exhibits an antiferromagnetic cycloidal spin-spiral ground state driven by the Dzyaloshinskii-Moriya interaction. We show that our force measurements are more sensitive to atomic-scale variations of the exchange force field and the local chemical environment than the current [1]. First-principles calculations explain our observations and reveal the magnetic exchange force mechanisms.

[1] N. Hauptmann et al., arXiv:1908.00959

O 110.11 Thu 17:30 WIL A317

Magnetism of valence electrons in lanthanide atoms on metallic substrates and lanthanide thin films — ●DARIA SOSTINA^{1,2}, APARAJITA SINGHA^{1,2}, CHRISTOPH WOLF^{1,2}, SAFA AHMED^{1,2}, DENIS KRYLOV^{1,2}, PIERLUIGI GARGIANI³, ALESSANDRO BARLA⁴, WOO-SUK NOH⁵, MARINA PIVETTA⁶, STEFANO RUSPONI⁶, HARALD BRUNE⁶, ANDREAS HEINRICH^{1,2}, and FABIO DONATI^{1,2} — ¹Center for Quantum Nanoscience, Institute for Basic Science (IBS), Seoul, Republic of Korea — ²Department of Physics, Ewha Womans University, Seoul, Republic of Korea — ³ALBA Synchrotron Light Source, Cerdanyola del Vallès, Catalonia, Spain — ⁴Istituto di Struttura della Materia (ISM), Consiglio Nazionale delle Ricerche (CNR), Trieste, Italy — ⁵Pohang University of Science and Technology, Pohang, Republic of Korea — ⁶Institute of Physics, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

Valence electrons in rare earth single atoms play a fundamental role in determining their magnetic stability and energy level structure [*Phys. Rev. Lett.* 121, 027201 (2018)]. Here, we investigate the occupation and magnetic moments of 5d and 6p electrons of Gd in the metallic state using X-ray magnetic circular dichroism. We observe charge transfer to occur when Gd atoms and clusters are deposited on Ag(100) surface and negligible occupation of Gd 5d orbital. Additional measurements performed on Gd films and related comparison with density functional theory allow us to understand the contribution of electron-electron correlations and hybridization of the Gd 5d orbitals to the magnetism of rare earths atomic-scale structures.

O 110.12 Thu 17:45 WIL A317

Magnetism of surface-embedded lanthanide single atoms with room temperature structural stability — ●SAFA LAMIA AHMED^{1,2}, APARAJITA SINGHA¹, DENIS KRYLOV¹, STEFANO RUSPONI³, MARINA PIVETTA³, CHRISTOPH WOLF¹, ALESSANDRO LODESANI⁴, ANDREA PICONE⁴, ALBERTO BRAMBILLA⁴, ALESSANDRO BARLA⁵, HARALD BRUNE³, ANDREAS JOACHIM HEINRICH^{1,2}, and FABIO DONATI^{1,2} — ¹Center for Quantum Nanoscience, Institute for Basic Science (IBS), Seoul 03760, Republic of Korea — ²Department of Physics, Ewha Womans University, Seoul 03760, Republic of Korea — ³Institute of Physics, Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland — ⁴Dipartimento di Fisica, Politecnico di Milano, 20133 Milano, Italy — ⁵Istituto di Struttura della Materia (ISM), Consiglio Nazionale delle Ricerche (CNR), I-34149 Trieste, Italy

We investigate surface embedded lanthanide atoms in ultra-thin MgO film on Ag(100) as a potential solution towards realizing single atom magnets [*Science* 352, 318 (2016)] with room-temperature (RT) structural stability. RT scanning tunneling microscopy images show negligible surface diffusion and nucleation of the embedded atoms. Using X-ray magnetic circular dichroism, we reveal out-of-plane anisotropy for Tm and Sm; in-plane anisotropy for Ho and Dy and negligible anisotropy for Er and Gd. All systems show paramagnetic loops at 2.5 K. Using density functional theory and multiplet calculations, we model the interaction between the 4f electrons and their ligand environment, and determine the atom's magnetic level structure.