

## DS 36: Spins in Organic Materials (jointly with MA)

Time: Thursday 16:45–19:00

Location: H 1012

DS 36.1 Thu 16:45 H 1012

**Tunneling anisotropic magnetoresistance in organic spin valves** — •M. GRÜNEWALD<sup>1,3</sup>, M. WAHLER<sup>1,3</sup>, F. SCHUMANN<sup>3</sup>, C. GOULD<sup>1</sup>, R. SCHMIDT<sup>2</sup>, F. WÜRTHNER<sup>2</sup>, L.W. MOLENKAMP<sup>1</sup>, and G. SCHMIDT<sup>1,3</sup> — <sup>1</sup>Physikalisches Institut (EP3) Universität Würzburg, Am Hubland, 97074 Würzburg — <sup>2</sup>Institut für Organische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg — <sup>3</sup>Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, von-Danckelmann-Platz 3, 06120 Halle

Over the past years a number of spin valves (SV) based on various organic semiconductors (OSCs) and contact materials have been demonstrated. Although some experiments indicate injection of spinpolarized carriers and some clearly show tunneling, it is still unclear for a number of other results whether their data show tunneling magnetoresistance (TMR) or actual spin injection and consequently giant magnetoresistance (GMR). We report the observation of tunneling anisotropic magnetoresistance (TAMR) in an organic SV-like structure with only one ferromagnetic electrode. The device is based on a new perylene diimide-based n-type OSC. The effect originates from the tunneling injection from the bottom contact ( $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ ). Magnetoresistance measurements show a clear SV signal, with the typical two-step switching pattern caused by the magnetocrystalline anisotropy of the epitaxial magnetic electrode. TAMR so far has not been considered when interpreting the results of organic SVs. Our results imply that careful measurements on any organic SV are necessary in order to distinguish between TAMR and true SV-operation (TMR/GMR).

DS 36.2 Thu 17:00 H 1012

**Spin properties of the Alq<sub>3</sub>-cobalt oxide (CoO) interface** — •NORMAN HAAG, SABINE STEIL, NICOLAS GROSSMANN, MIRKO CINCHETTI, and MARTIN AESCHLIMANN — Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, Erwin-Schrödinger-Str. 46, D-67663 Kaiserslautern

The effect of cobalt oxidation is crucial for the understanding of the performance of organic spin valves with Co electrodes [1], as it is expected that cobalt will partly oxidize during sample production. For this reason, we analyzed the spin properties of the interface formed between tris(8-hydroxyquinoline)aluminium (III) (Alq<sub>3</sub>) and cobalt oxide. We deposited 30 ML of Co(100) and exposed the sample to an oxygen atmosphere with varying pressure. The degree of oxidation is extracted by evaluating the changes in the work function according to Wang *et al* [2]. Subsequently, Alq<sub>3</sub> was grown on the oxidized cobalt. The resulting interface was characterized by means of spin-resolved ultraviolet photoemission spectroscopy. We detected the energy level alignment and the spin polarization in the region of a few eV below  $E_F$ , both as a function of degree of oxidation. The most striking result is the shift of the Alq<sub>3</sub> molecular orbitals of up to 1 eV (for strong oxidation) away from the Fermi level. This behavior could change the character of spin and carrier conduction (from holes to electrons) in spintronics devices.

[1] Dediu *et al.*, Nature Materials **8**, 707 (2009)[2] Wang *et al.*, Surface Science **124**, 51 (1983)

DS 36.3 Thu 17:15 H 1012

**Spin-filtering at hybrid organic-inorganic interfaces** — •SABINE STEIL, NICOLAS GROSSMANN, NORMAN HAAG, MIRKO CINCHETTI, and MARTIN AESCHLIMANN — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany.

Organic semiconductors have demonstrated their potential as a new class of materials for spintronics applications [1]. They are expected to constitute a new building block for advanced spintronics devices. One of their most intriguing properties is that they form hybrid interfaces with ferromagnetic metals [2]. As an example, we have recently shown that the spin-injection efficiency at the cobalt-copper phthalocyanine interface can be tailored by electron doping [3]. Here, we will show our recent experiments on the interface between cobalt(001) and tris(8-hydroxyquinoline)aluminium(III) (Alq<sub>3</sub>). Interface formation was studied by means of spin-resolved ultraviolet photoemission spectroscopy, while the spin- and time-resolved two-photon photoemission spectroscopy was used to measure the spin-dependent lifetime of hot charge carriers excited in an unoccupied hybrid interface state.

The magnitude of the lifetime, gives information about the degree of hybridization of the considered state. More importantly, we found that the lifetime in such state is spin-dependent, providing direct evidence that hybrid organic-inorganic interfaces can be employed as a novel kind of spin-filter.

[1] V. A. Dediu, *et al.*, Nat. Mater. **8**, 707(2009) [2] S. Sanvito, Nat. Phys. **6**, 562-564(2010) [3] M. Cinchetti *et al.*, PRL **104**, 217602(2010)

DS 36.4 Thu 17:30 H 1012

**Theoretical study of dynamical switching of a single spin by exchange forces** — •ROBERT WIESER<sup>1</sup>, VASILE CACIUC<sup>2</sup>, CESAR LAZO<sup>3</sup>, HENDRIK HÖLSCHER<sup>4</sup>, ELENA Y. VEDMEDENKO<sup>1</sup>, ROLAND WIESENDANGER<sup>1</sup>, and STEFAN HEINZE<sup>3</sup> — <sup>1</sup>Institut für Angewandte Physik, Universität Hamburg, D-20355 Hamburg, Germany — <sup>2</sup>Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — <sup>3</sup>Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — <sup>4</sup>Institut für Mikrostrukturtechnik, Forschungszentrum Karlsruhe, P.O. Box 36 70, D-76021 Karlsruhe, Germany

We demonstrate the possibility to dynamically switch the spin of a single atom or molecule with the magnetic tip of an atomic force microscope due to the acting exchange forces. We choose a single transition metal benzene molecule as model system and calculate the exchange interaction with an Fe tip using density functional theory. The exchange energy displays a Bethe-Slater type behavior with ferromagnetic coupling at large tip-sample distance and antiferromagnetic coupling at closer proximity. The exchange energies reach maximum values of a few 10 meV which allows to switch single spins by overcoming the energy barrier due to the magneto-crystalline anisotropy. The spin dynamics of the system was explored by solving the time dependent Schrödinger equation with additional relaxation term. We discuss six possible scenarios, defined by the occurrence of quantum tunneling, relaxation, and tip-sample distance.

DS 36.5 Thu 17:45 H 1012

**Nanoscale assembly and order of paramagnetic organic radicals** — SABINE-ANTONIA SAVU<sup>1</sup>, INDRO BISWAS<sup>1</sup>, MATHIAS GLASER<sup>1</sup>, LORENZO SORACE<sup>2</sup>, MATTEO MANNINI<sup>2</sup>, ANDREA CANESCHI<sup>2</sup>, THOMAS CHASSÉ<sup>1</sup>, and •MARIA BENEDETTA CASU<sup>1</sup> — <sup>1</sup>IPTC, University of Tübingen, Tübingen, Germany — <sup>2</sup>LAMM, University of Florence, Florence, Italy

Nitronyl nitroxide radicals are a class of paramagnetic compounds that are of interest not only because of their magnetic properties but also because of their use as a building block in more complex magnetic structures. A crucial aspect is the possibility to grow thin films, down to the submonolayer regime, investigating their chemical, physical, and morphological properties. In this work we present X-ray photoelectron spectroscopy (XPS), near edge X-ray absorption fine structure (NEXAFS), atomic force microscopy (AFM), and electron paramagnetic resonance (EPR) investigations of thin films of a pyrene derivative of the nitronyl nitroxide radical (nitpyrene). Nitpyrene was deposited on Au(111) single crystals, using strictly controlled evaporation conditions. The electronic structure and the interaction with the surface are discussed, as well as the growth mode. The persistence of the paramagnetic character of the molecules has been proved by EPR measurements.

DS 36.6 Thu 18:00 H 1012

**Electronic structure and magnetic properties of metallocene multiple-decker sandwich nanowires** — CRISTIAN MORARI<sup>1</sup>, FLORIAN BEIUSEANU<sup>2</sup>, and •LIVIU CHIONCEL<sup>3</sup> — <sup>1</sup>National Institute for Research and Development of Isotopic and Molecular Technologies, 65-103 Donath, RO-400293 Cluj Napoca, Romania — <sup>2</sup>Department of Physics, University of Oradea, RO-410087 Oradea, Romania — <sup>3</sup>Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany

We present a study of the electronic and magnetic properties of the multiple-decker sandwich nanowires (CP-M) composed of cyclopentadienyl (CP) rings and 3d transition metal atoms (M=Ti to Ni) using Density Functional Theory first-principles techniques. We demonstrate that structural relaxation is an important effect in determin-

ing the magnetic ground-state of the system. Notably, the computed magnetic moment is zero in CP-Mn, while in CP-V a significant turn-up in magnetic moment is evidenced. CP-Fe/Cr show a half-metallic ferromagnetic ground state with a gap within minority/majority spin channel. In order to study the effect of electronic correlations upon the half-metallic ground states in CP-Cr, we introduce a simplified three-bands Hubbard model which is solved within the Variational Cluster Approach. We discuss the results as a function of size of the reference cluster and the strength of average Coulomb  $U$  and  $J$  exchange parameters. For range of studied parameters  $U=2-4\text{eV}$  and  $J=0.6-1.2\text{eV}$  the half-metallic character is not maintained in the presence of local Coulomb interactions.

DS 36.7 Thu 18:15 H 1012

**Metal-organic hybrid interface states of a ferromagnet/organic semiconductor hybrid junction as basis for engineering spin injection in organic spintronics** — STEFAN LACH<sup>1</sup>, ANNA ALTENHOF<sup>1</sup>, KARTIK TARAFDER<sup>2</sup>, FELIX SCHMITT<sup>1</sup>, MD. EHESAN ALI<sup>2,3</sup>, MICHAEL VOGEL<sup>1</sup>, JENS SAUTHER<sup>1</sup>, PETER OPPENEER<sup>2</sup>, and CHRISTIANE ZIEGLER<sup>1</sup> — <sup>1</sup>Dep. of Physics and Research Center OPTIMAS, University of Kaiserslautern, D-67663 Kaiserslautern — <sup>2</sup>Dep. of Physics and Astronomy, Uppsala University, S-75120 Uppsala — <sup>3</sup>Center for Theoretical Chemistry, Ruhr-University Bochum, D-44801 Bochum

Hybrid spintronic devices that combine organic semiconductors (OSC) with ferromagnetic (FM) substrates are expected to provide a route to devices with improved and new functionalities. A crucial role is played by the FM-OSC interface. State-of-the-art DFT+ $U$  calculations in combination with UPS and XPS as well as spin-resolved UPS directly demonstrate the formation of new hybrid interface states (HIS), induced by chemisorption of CuPc, CoPc, and FePc at Co [1]. Whereas FePc and CoPc have only weakly spin-polarized levels at the Fermi level, CuPc shows strong spin-polarization directly at EF. On the other hand, the interaction leads to a vanishing magnetic moment in case of CuPc and a strong ferromagnetic coupling in case of CoPc and FePc. The difference is explained by the symmetry of the d-orbitals which are massively involved in the hybridization. [1] S. Lach, A. Altenhof, K. Tarafder, F. Schmitt, Md. E. Ali, M. Vogel, J. Sauther, P. M. Oppeneer, Ch. Ziegler, Adv. Funct. Mat., in press

DS 36.8 Thu 18:30 H 1012

**Theoretical modelling of electronic structure and exchange interactions for metal-phthalocyanines** — WEI WU<sup>1,2</sup>, AN-

DREW FISHER<sup>2</sup>, NIC HARRISON<sup>3</sup>, SANDRINE HEUTZ<sup>1</sup>, TIM JONES<sup>4</sup>, and GABRIEL AEPPLI<sup>2</sup> — <sup>1</sup>Department of Materials and London Centre for Nanotechnology, Imperial College London — <sup>2</sup>UCL Department of Physics and Astronomy and London Centre for Nanotechnology, University College London — <sup>3</sup>Department of Chemistry, Imperial College — <sup>4</sup>Department of Chemistry, Warwick University

The theoretical understanding of exchange interactions in organics provides a key foundation for quantum molecular magnetism. Recent SQUID magnetometry of a well known organic semiconductor, copper-phthalocyanine [1,2] (CuPc) shows that it forms quasi-one-dimensional spin chains. Green's function perturbation theory and density functional theory simulations [3,4] are used to calculate exchange interactions and electronic structure for CuPc, CobaltPc, LithiumPc, and ChromiumPc. The exchange interactions depend strongly on stacking angles, but weakly on sliding angles. Our results qualitatively agree with the experiments and can guide experimentalists to synthesis novel materials.

[1] S. Heutz, et. al., Adv. Mat., 19, 3618 (2007) [2] Hai Wang, et. al., ACS Nano, 4, 3921 (2010) [3] Wei Wu, et. al., Phys. Rev. B 77, 184403 (2008) [4] Wei Wu, et. al., Phys. Rev. B 84, 024427 (2011)

DS 36.9 Thu 18:45 H 1012

**Uncovering the electronic structure of manganese phthalocyanine** — RICO FRIEDRICH<sup>1</sup>, TORSTEN HAHN<sup>1</sup>, JENS KORTUS<sup>1</sup>, FRANCISC HAIDU<sup>2</sup>, MICHAEL FRONK<sup>2</sup>, GEORGETA SALVAN<sup>2</sup>, BENJAMIN MAHNS<sup>3</sup>, and MARTIN KNUPFER<sup>3</sup> — <sup>1</sup>Institut für Theoretische Physik, TU Bergakademie Freiberg, 09596 Freiberg — <sup>2</sup>Institut für Physik, TU Chemnitz, 09107 Chemnitz — <sup>3</sup>Institut für Festkörper- und Werkstofforschung, IFW Dresden, 01171 Dresden

Manganese phthalocyanine is a magnetic transition metal complex, that exhibits organic semiconducting behavior in the bulk. Because of its high thermal and chemical stability it is a promising candidate for molecular spintronics applications. However this compound shows extraordinary electronic structure properties which can be investigated by various spectroscopic techniques as for instance EELS, PES and Ellipsometry. Here we want to present the results of our ab initio density functional calculations on this system and show how they can help to understand the significant influences on the experimentally observed electronic properties. For this purpose also environmental influences as air exposure need to be considered since they will be of decisive character in view of real applications. In particular the change of magnetic properties is crucial as this directly affects spin transport phenomena.