

DS 4: Magnetic / Organic Interfaces, Spins in Organics and Molecular Magnetism (jointly with MA)

Time: Monday 15:00–17:45

Location: CHE 91

Invited Talk DS 4.1 Mon 15:00 CHE 91
Interfaces of archetype magnetic molecules: from interface dipoles to charge and spin transfer — ●MARTIN KNUFFER — IFW Dresden and TU Dresden, Germany

The active control and the manipulation of spin degrees of freedom in organic electronic devices - often called organic spintronics - is anticipated to enable the fabrication of future electronic systems. One way to incorporate the spin degree of freedom is the use of magnetic molecules. For the understanding and development of devices, detailed knowledge on the interaction of such molecules at various interfaces, that are present in devices, is required. We have studied archetype magnetic molecules, the transition metal phthalocyanines, at a number of interfaces to e.g. simple metals, ferromagnetic materials or other organic compounds using spectroscopic methods. These studies provided detailed insight into interactions at such interfaces ranging from interface dipoles to charge and even spin transfer.

The work presented in this contribution has been carried out within the DFG research unit 1154 (Towards molecular spintronics).

DS 4.2 Mon 15:30 CHE 91
Interface and thin film properties of metal-free organic magnets — ●REZA KAKAVANDI, SABINE-ANTONIA SAVU, THOMAS CHASSÉ, and MARIA BENEDETTA CASU — Institute of Physical and Theoretical Chemistry, Tübingen, Germany

Metal-free organic-based magnets are relatively new materials with open-shell structure that offer tremendous opportunity in information storage and processing technology, based on the presence of spatially delocalized unpaired electrons. Essential tools such as X-ray Photoelectron Spectroscopy (XPS) and Near Edge X-ray Absorption Fine structure (NEXAFS) Spectroscopy are utilized to study the electronic structure and the paramagnetic character of nitronyl nitroxide radicals deposited on well-defined metal-oxide surfaces. The molecule-substrate interface and the thin film properties are investigated, focusing on their impact on the magnetic character of the systems. In particular, the transitions related to the singly occupied molecular orbitals, expected for this class of materials, are investigated using NEXAFS spectroscopy.

DS 4.3 Mon 15:45 CHE 91
Investigation of the magnetic exchange coupling between MnTPPCL molecules and a ferromagnetic cobalt substrate by X-ray photo-emission electron microscopy — ●JAN GIROVSKY¹, MICHELE BUZZI¹, CHRISTIAN WAECKERLIN¹, DOROTA SIEWERT², JAN NOWAKOWSKI¹, PETER M. OPPENEER³, FRITHJOF NOLTING¹, THOMAS A. JUNG¹, NIRMALYA BALLAV⁴, and ARMIN KLEIBERT¹ — ¹Paul Scherrer Institut, Switzerland — ²University of Basel, Switzerland — ³Uppsala University, Sweden — ⁴Indian Institute of Science Education and Research, Pune, India

Adsorption of spin bearing metallo-porphyrins and -phthalocyanines on ferromagnetic substrates leads to an exchange induced magnetic moment on the molecules [1]. The magnetic coupling across the magneto-organic interface can be further modified by the introduction of a non-magnetic spacer layer [2]. In this contribution we use X-ray photo-emission electron microscopy combined with X-ray magnetic circular dichroism to study the magnetic exchange coupling between Mn-porphyrin molecules and a ferromagnetic cobalt substrate through a Cr spacer layer with increasing thickness. Our spectro-microscopic correlation enables us not only to study the local magnetic coupling of the molecules, but also their chemical state and the spatial distribution of the respective elements on the sample [3].

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

[2] C. F. Hermanns et al., Adv. Mater. 25, 3473 (2013).

[3] J. Girovsky et al., Chem. Commun., accepted (2013).

DS 4.4 Mon 16:00 CHE 91
Determination of spin polarized hybridization states of C60 on a ferromagnetic Co(001) surface and its importance for spintronic applications — ●STEFAN LACH¹, OLIVER RUDEN¹, ANNA ALTENHOF¹, SHENWEI SHI², MATS FAHLMAN², and CHRISTIANE ZIEGLER¹ — ¹Technical University of Kaiserslautern and state research centre OPTIMAS — ²Linköping University, SE-58183 Linköping, Swe-

den

It is both the high electron affinity resulting in small energy barriers for electron injection at the interfaces with 3d transition metal ferromagnets and its lack of hydrogen and hence no spin dephasing by hyperfine coupling, which makes C60 an important candidate for organic spintronic devices. We present the identification of spin polarized hybrid interface states (sp-HIS) for the C60/Co(001) organic-inorganic interface. Supported by IPES measurements for the unoccupied states and XPS core level spectroscopy, we will show that the also observed Interface dipoles and the spin-split can be explained by covalent bond formation associated with a p-d hybridization between the Co atoms and the C60. Our results provide further insight into the rehybridization reactions of C60 on ferromagnetic substrates beyond a simple charge transfer. This explains the observed interface dipoles and determines the spin-split behavior. The latter is of high importance for spin filtering effects at the C60/Co(001) interface and thus for spintronic devices.

DS 4.5 Mon 16:15 CHE 91
Vertical organic spin-valves with sub-micrometer lateral dimensions — ●ROBERT GÖCKERITZ¹, BODO FUHRMANN², NICO HOMONNAY¹, TIM RICHTER¹, ALEXANDER MÜLLER¹, and GEORG SCHMIDT^{1,2} — ¹Inst. f. Physik, FG Nanostrukturierte Materialien, Martin-Luther-Universität Halle-Wittenberg, Halle (Saale) — ²Interdisziplinäres Zentrum für Materialwissenschaften, Martin-Luther-Universität Halle-Wittenberg, Halle (Saale)

To get a deeper insight to the underlying physics of spin transport in vertical organic spin-valve devices a promising approach is to go to smaller active device areas. A new fabrication process is presented which offers the possibility to achieve active device areas less than 100nm and which is flexible in terms of material choice for the active layers. As proof of principle magnetoresistance measurements of devices are shown with a large active area of 200x100 micrometer as well as scaled-down device with dimensions of about 500 nm using the organic semiconductor AlQ3 and LSMO and cobalt as ferromagnetic electrodes.

DS 4.6 Mon 16:30 CHE 91
Resistive switching in organic TAMR devices — ●MATTHIAS GRÜNEWALD, NICO HOMONNAY, JOHANNES KLEINLEIN, and GEORG SCHMIDT — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Von-Danckelmann-Platz 3, 06120 Halle

Resistive switching (RS), i.e. the remanent (reversible) change of a device's resistance, is a widely investigated phenomenon as it holds the prospect for realizing high density memory devices. A lot of reports are available in the literature showing results for metal-insulator-metal structures where the insulating layer (often an oxide, rarely an organic semiconductor) is modified and hence the resistance changed. Especially for the oxide based devices a lot of models exist explaining the physics behind the effect. They are prevalently emphasizing the role of oxygen stoichiometry in these materials for their physical properties.

Here we present results showing RS in organic tunneling anisotropic magnetoresistance (TAMR) devices, in which one electrode is a complex oxide (La_{0.7}Sr_{0.3}MnO₃) and the organic semiconductor tris-(8-hydroxyquinoline) aluminium (AlQ₃) is used. In contrast to similar studies that demonstrate an interplay of RS and a magnetoresistance effect (MR), the latter is unambiguously identifiable as TAMR in the present devices and allows for probing the tunnel barrier between the oxide electrode and the AlQ₃ layer. This barrier is found to be changed during RS. In order to analyze the RS dynamics the barrier's modification is determined by employing I/V characterization and appropriate fitting procedures in several experiments.

DS 4.7 Mon 16:45 CHE 91
Tailoring the energy level alignment at the Co/AlQ₃ interface by controlled cobalt oxidation — ●NORMAN HAAG, SABINE STEIL, NICOLAS GROSSMANN, ROMAN FETZER, MIRKO CINCHETTI, and MARTIN AESCHLIMANN — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schroedinger-Strasse 46, 67663 Kaiserslautern, Germany

We have studied the influence of oxygen exposure at the pro-

tototypical interface between cobalt and the organic semiconductor tris(8-hydroxyquinoline)aluminum (III) (Alq_3) by photoemission spectroscopy. We find that oxidation of the cobalt leads to a gradual suppression of hybrid interface states, to a progressive change in the work function and to a continuous energetic shift of the molecular orbitals towards higher binding energies. Based on these observations, we propose controlled oxidation of the ferromagnetic electrode as an easy and effective possibility to tune the performance of organic spintronics devices. Besides this method yields insight into possible origin of the interfacial dipole.

DS 4.8 Mon 17:00 CHE 91

Detailed analysis of sharp nonreactive interface formation in soft-landing conditions: ferromagnetic metallic top contacts onto model wide-gap organic semiconductor using rare-gas condensed at 30K. — ●SERGEY BABENKOV¹, OLGA MOLODTSOVA¹, JENS VIEFHÄUS¹, MATTHIAS KALLÄNE², ERIC KRÖGER², ARNDT QUER², CRISTOPH SEIBEL⁴, FRANK SCHOLZ¹, JÖRN SELTMANN¹, LEIF GLASER¹, and VICTOR ARISTOV^{1,3} — ¹DESY, Hamburg, Germany — ²CAU, Kiel, Germany — ³ISSP RAS, Chernogolovka, Russia — ⁴UW, Würzburg, Germany

The present work studies the formation of sharp non-reactive metal-organic interfaces at soft landing conditions. In previous work it has been shown that at low coverage of Fe on copper-phthalocyanine (CuPc) there is a strong chemical reaction under room temperature (RT) conditions. In contrast, the results of investigation of size selected clusters in condensed rare gas matrices show almost no diffusion or agglomeration of metal atoms into the organic substrate. In our present investigation by XPS using the PETRA III synchrotron radiation facility at DESY, the formation of interfaces between well-ordered thin film of CuPc with iron and nickel at room and low temperatures (LT) and in condensed Xe matrix were studied. The observed XPS spectra show a strong chemical reaction of the metal with the organic film at RT conditions both for iron and for nickel while at LT with Xe a sharp non-reactive interface formation is observed. This sharp metal-organic interface formation obtained at soft landing conditions can be used for spin injection in spintronic devices.

DS 4.9 Mon 17:15 CHE 91

Fermi level engineering in organic semiconductors for controlled manufacturing of charge and spin transfer materials — ●RICO FRIEDRICH^{1,2}, BERTHOLD KERSTING³, and JENS KORTUS¹ — ¹Institute of Theoretical Physics, TU Bergakademie Freiberg,

Leipziger Str. 23, D-09596 Freiberg, Germany — ²Present address: Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany — ³Institut für Anorganische Chemie, Universität Leipzig, Johannisallee 29, D-04103 Leipzig, Germany

The rational design of materials for organic electronics and spintronics has been a long-standing challenge. In this presentation it will be demonstrated by theoretical means how to achieve Fermi level engineering in an organic semiconductor like for instance a metal phthalocyanine. It turns out that substitution of the peripheral hydrogen atoms by either fluorine atoms or methoxy groups allows to tune the Fermi level by about 1.5 eV [1]. Finally, we show how such tuning could be exploited to achieve a systematic way to manufacture charge and spin transfer materials by studying the system $(\text{MeO})_8\text{CoPc}/\text{F}_{16}\text{CoPc}$ and compare its electronic and magnetic properties to the first representative of this materials class namely $\text{MnPc}/\text{F}_{16}\text{CoPc}$ [2].

[1] R. Friedrich, B. Kersting, and J. Kortus, *Physical Review B* **88**, 155327 (2013).

[2] S. Lindner, M. Knupfer, R. Friedrich, T. Hahn, and J. Kortus, *Physical Review Letters* **109**, 027601 (2012).

DS 4.10 Mon 17:30 CHE 91

Magnetic Exchange Coupling of Iron-Porphyrin to $c(2 \times 2)$ Oxygen-reconstructed $\text{Co}(100)$ Surfaces: Insights from Ab initio Theory — ●MD. EHESAN ALI and PETER OPPENEER — Department of Physics and Astronomy, Uppsala University, Box 516, S-751 20 Uppsala, Sweden

The spin-interface magnetic properties of Fe-porphyrins adsorbed on $c(2 \times 2)$ oxygen-reconstructed $\text{Co}(100)$ surfaces have been studied applying density functional theory.[1,2] The electrostatic interaction between electronegative oxygen atoms and the pi-electron cloud of the porphyrin plays a vital role in the binding mechanism of porphyrins to the oxygen-reconstructed surfaces. We have investigated this using various dispersion interactions included functionals in combination with the on-site Coulomb correlation corrected DFT+U method. The surface diffusion of porphyrin molecules is determined from finite-temperature ab initio molecular dynamics simulations, which reveal a promising possibility of controlling the interface magnetic properties upon controlling the molecule-surface dynamics.[3]

References: [1] M. Bernien, J. Miguel, C. Weis, Md. E. Ali et al., *Phys. Rev. Lett.* **102**, 047202 (2009). [2] A. P. Weber, A. N. Caruso, E. Vescovo, Md. E. Ali et al., *Phys. Rev. B* **87**, 184411 (2013). [3] Md. E. Ali and P. M. Oppeneer, Submitted.