# DS 31: Molecular Spintronics - Current Status and Challenges I (Focused Session)

Time: Thursday 10:30–12:45 Location: H2

**Topical Talk** DS 31.1 Thu 10:30 H2

**Spintronics with Organic Semiconductors** — •V. Alek Dediu — ISMN-CNR, Via Gobetti 101, 40129 Bologna

Spin electronics, in its aim to compete with conventional electronics, is always looking for new and more performing materials. Conjugated organic semiconductors represent a possible breakthrough in the discipline, due to their weak spin-orbit scattering and their chemical flexibility. The former produces extremely long spin flip times, enabling spin manipulation processes in various devices. The latter promises an enormous choice of materials. Here I propose an outlook of the main issues in the field of organic spintronics as well as I present most recent results from our laboratory on magnetic and multifunctional effects in hybrid organic-inorganic devices. Finally, I will discuss the challenges in the field and possible strategies to outcome them.

**Topical Talk** DS 31.2 Thu 11:00 H2

**Muon measurements of spin transport and dynamics in organic semiconductors** — •Alan Drew — Physics Department, Queen Mary University of London, UK

Organic semiconductors fall into a class of materials that shows significant potential for future applications and as a result, the field is becoming extremely topical. However, there is a lack of suitable techniques that can yield information on intrinsic spin and charge carrier dynamics in organic materials.

Low Energy Muon Spin Rotation can directly measure the depth resolved spin polarisation of charge carriers in organic spin injection devices [1]. Using this technique, it is possible to separate out the various contributions to spin decoherence, differentiating between interface and bulk spacer layer effects. I will present the first direct measurement of spin coherence length and initial polarisation of injected electrons in a realistic and fully functional organic spin valve. Bulk muon techniques can also be used to probe the charge carrier and spin dynamics of organic semiconductors on a molecular lengthscale [2]. I will present measurements of temperature dependent electron spin relaxation rates, on a series of organic molecules of different morphology and molecular structure, which points towards some generality of the underlying spin scattering mechanisms in organic materials [3].

[1] A. J. Drew et al., Nature Materials 8, 109 (2009) [2] A. J. Drew et al., Phys. Rev. Lett. 100, 116601 (2008) [3] L. Schulz et al., in preparation

DS 31.3 Thu 11:30 H2

**Engineering of the energy level alignment at organic semiconductor interfaces by intra-molecular degrees of freedom: transition metal phthalocyanines** — •Mandy Grobosch[1], Victor Y. Aristov[1,2], Olga V. Molodtsova[1], Christian Schmidt[1], Brian P. Doyle[3,4], Stefano Nannarone[3], and Martin Knupfer[1] — [1]IFW Dresden, D-01069 Dresden, Germany — [2]nstitute of Solid State Physics, Russian Academy of Sciences, Moscow, Russia — [3]University of Johannesburg, PO Box 524 Auckland Park — [4]TASC-INFM Laboratory Trieste, Italy

The fact, that the transition metal ion in the central cavity of the Pc's can have a magnetic moment is a characteristic feature of TMPc's, and therefore these phthalocyanines can also show fascinating magnetic properties. We have determined the energy level alignment at interfaces between various transition metal phthalocyanines and gold using photoemission spectroscopy. Our results demonstrate that the transition metal center has a strong influence on the electronic properties of the phthalocyanine films as well as their interfaces with gold. This offers a route to adjust the hole injection barrier via the choice of otherwise equivalent molecular organic semiconductors. In particular, the interfaces MnPc/Au and CoPc/Au are characterized by a small hole injection barrier, which would be advantageous for applications. These are directly related to the presence of metal 3d states closest to the chemical potential; a fact that is also reflected in smaller ionization potentials for MnPc and CoPc as compared to other phthalocyanines. For details see: M. Grobosch et al., J. Phys. Chem. C 113, 13219 (2009).

DS 31.4 Thu 11:45 H2

**Magnetic transition metal phthalocyanine thin films: electronic properties via K doping** — •Olga Molodtsova[1], Victor Aristov[1,2], Volodymyr Maslyuk[3], Denis Vyalikh[4], Alexei Preobrajenski[5], Ingrid Mertig[3], Thomas Bredow[6], and Martin Knupfer[1] — [1]IFW Dresden, Germany — [2]ISSP RAS, Russia — [3]Uni Halle, Germany — [4]TU Dresden, Germany — [5]Max-Lab Lund, Sweden — [6]Uni Bonn, Germany

Magnetic transition metal phthalocyanines (MTM-Pc's) are considered as materials for development of low dimensional molecular magnets and quantum computers. To make further progress in development such devices both the understanding and the tailoring of the physical, chemical and transport properties of the organic semiconductor components are required. Due to the exceptional ability to incorporate electron acceptors and/or donors into molecular crystals the control of their electronic properties is possible. In this work the evolution of electronic structure of the MTM-Pc's with potassium doping has been studied by means of photoemission spectroscopy, near-edge X-ray absorption fine structure and DFT calculations. The DFT calculations and detailed analysis of the core-level spectra permit us to suggest possible lattice sites for the potassium ions. The data disclosed filling of the lowest unoccupied molecular orbital upon doping and associated changes of the core level absorption spectra. None of the films prepared in our studies showed a finite electronic density of states at the Fermi level. Acknowledgements: This work was supported by the RFBR under grant no. 08-02-01170.

DS 31.5 Thu 12:00 H2

**Magnetic transition metal phthalocyanine thin films on Au(001): ordering and electronic structure** — •Victor Aristov[1,2], Volodymyr Maslyuk[3], Olga Molodtsova[1], Ingrid Mertig[3], Thomas Bredow[4], and Martin Knupfer[1] — [1]IFW Dresden, Germany — [2]ISSP RAS, Russia — [3]Uni Halle, Germany — [4]Uni Bonn, Germany

At the present time magnetic transition metal phthalocyanines (MTM - Pc's) are considered as objects for the elaboration of low dimensional molecular magnets because they are supposed as possible candidates for potential applications in high-density information storage and quantum computers. Such possible applications give a strong motivation to characterize and investigate the ordering and electronic properties of MTM-Pc thin films since this determines the performance of devices. In this presentation we report the results of investigations of the molecular ordering, as well as the core-levels, valence band and unoccupied electronic states of the organic semiconductors MTM-Pc in situ grown on Au(001) surface under UHV conditions. The studies were done using a combination of experimental and theoretical techniques, by means of quantum-chemical calculations at DFT level, direct and resonant photoemission and NEXAFS. The experimentally obtained electronic features are in a good agreement with ab initio density of state results allowing a detailed site specific insight into the system. Acknowledgments: This work was supported by the RFBR under grant no. 08-02-01170.

**Topical Talk** DS 31.6 Thu 12:15 H2

**Role of the van der Waals interaction on the adsorption of organic molecules on surfaces** — •Nicolae Atodiresei — Institut für Festkörperforschung, Forschungszentrum Jülich

The design of nanoscale molecular elements in multifunctional devices relies on a clear understanding of the physics at electrode-molecule interfaces with a particular emphasis on the functionality of specific molecules in a given organic-inorganic surface environment. Using *ab initio* simulations and appropriate methods to account for the long-range dispersion effects we have performed studies on several organic molecules adsorbed on non-magnetic and ferromagnetic surfaces. Our results show that the alignment of the molecular orbitals at adsorbate-substrate interface depends on the number of heteroatoms present in an aromatic ring and, as a direct consequence, for a flat adsorption geometry, the molecule-surface van der Waals interaction involves not only the $\pi$-like orbitals which are perpendicular to the molecular plane but also $\sigma$-like orbitals delocalized in the molecular plane. In the case of perpendicular adsorption geometries we demonstrate that the position of the heteroatoms in the aromatic rings can be used to precisely tune the HOMO-LUMO gap making possible a chemical identification of the specific molecular species embedded into a molecular layer. Furthermore, our calculations demonstrate that, for specific types of organic molecules, taking into account the non-local correlation effects responsible for the long range van der Waals interaction is essential to correctly describe the charge transfer at the interface which yields the formation of molecule-surface hybrid states.