

## DS 28: Spins in Organic Materials I (Focused Session, jointly with MA – Organisers: Salvan, Hess, Timm)

Time: Wednesday 11:00–13:00

Location: GER 37

### Topical Talk DS 28.1 Wed 11:00 GER 37

**Selective spin-blockade in interacting molecular interferometers** — ●MILENA GRIFONI, ANDREA DONARINI, and GEORG BEGEMANN — Institut für Theoretische Physik, Universität Regensburg, Regensburg, Germany

We consider molecular junctions in the single-electron tunneling regime which, due to a high degree of spatial symmetry, have a degenerate many-body spectrum. As a consequence, interference phenomena which cause a current blocking can occur at specific values of the bias and gate voltage. We present here necessary and sufficient conditions for interference blockade also in the presence of spin-polarized leads. As an example we analyze a benzene single-electron transistor. For a setup with parallel polarized leads, we show how to exploit the current blocking to selectively prepare the system in a defined spin state without application of any external magnetic field.

References:

A. Donarini, G. Begemann and M. Grifoni, *Nano Lett.* 9, 2897 (2009)

A. Donarini, G. Begemann and M. Grifoni, *Phys. Rev. B* 82, 125451 (2010)

### Topical Talk DS 28.2 Wed 11:30 GER 37

**Charge and Spin Transport through Single-Atom and Single-Molecule Junctions** — ●JÖRG KRÖGER — Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany

The tip of a scanning tunnelling microscope is used to controllably contact single atoms and molecules adsorbed to surfaces. Owing to atomically precise imaging, the conductance dependence of a single-C<sub>60</sub> junction on the C<sub>60</sub> orientation has been unambiguously demonstrated. Time-resolved measurements of these junctions show two-level variations of the conductance and indicate an enhanced coupling of electrons to molecular vibrations. Orders-of-magnitude modifications of single-molecule contact conductances have been achieved by dehydrogenating tin-phthalocyanine molecules on Ag(111). Concomitant calculations visualize the current flow through the molecule and highlight the importance of chemical bonds to the electrodes. Spin valve effects have been observed at the ultimate size for magnetic single-atom contacts, which exhibit spin-dependent conductance in the ballistic electron transport regime.

### Topical Talk DS 28.3 Wed 12:00 GER 37

**The strange life of a molecular spin observed under a microscope** — ●GERMAR HOFFMANN — University of Hamburg, Germany — Academia Sinica, Taiwan

The 90ies saw the emerging of a new and fascinating class of magnetic materials based on molecules [1]. Although, the spin density is low, spin information can be efficiently stored in and transmitted by spatially and energetically well defined molecular orbitals. These orbitals can be experimentally precisely addressed. The internal and external spin interaction through molecular orbitals can be engineered by the molecular design. This opens also new concepts for spintronic devices through the combination of the molecular spin with additional functionality - on a length scale not accessible by classical systems. Though, the further development lacks of precise experimental access to understand the behavior of the individual molecular spin in a given environment and to guide toward an improved design of molecular spin-systems.

Here, I will present and discuss recent results on molecular magnetism. By means of spin-polarized scanning tunneling microscopy, scanning tunneling spectroscopy, and local manipulation, single mag-

netic molecules are locally and energetically investigated in different environments. Thereby, molecular systems cover commercially available [2], specially synthesized, and on-surface synthesized systems.

[1] R. Sessoli et al., *JACS* 115, 1804 (1993); M. Tamura et al., *Chem. Phys. Lett.* 186, 401 (1991). [2] J. Brede et al., *Phys. Rev. Lett.* 105, 047204 (2010); N. Atodiresei et al., *Phys. Rev. Lett.* 105, 066601 (2010).

### DS 28.4 Wed 12:30 GER 37

**Design of the Local Spin-Polarization at Hybrid Organic-Ferromagnetic Interfaces** — ●NICOLAE ATODIRESEI<sup>1</sup>, PREDRAG LAZIĆ<sup>2</sup>, VASILE CACIUC<sup>1</sup>, and STEFAN BLÜGEL<sup>1</sup> — <sup>1</sup>Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425-Jülich, Germany — <sup>2</sup>Massachusetts Institute of Technology, Cambridge, 02139-Massachusetts, USA

Combining molecular electronics with spintronics represents one of the most exciting avenues in building future nanoelectronic devices. In this context, a clear understanding of the physics at magnetic electrode-molecule interfaces is highly desirable and, in particular, first principles simulations are used to elucidate and design the functionality of specific molecules in a given organic-metal surface environment. We will present a conceptual study to understand the manipulation of the local spin-polarization present at the interface for several single organic molecules adsorbed on a ferromagnetic surface. The generality of the concept predicted by the theoretical calculations on model systems is further strengthened by the spin-polarized scanning tunneling microscopy (SP-STM) experiments. In this study it is demonstrated that, by an appropriate selection of the adsorbed molecules, the electrons of different spin [i.e. up and down] can selectively be injected from the same ferromagnetic surface by locally controlling the spin-polarization. [1] N. Atodiresei *et al.* *Phys. Rev. Lett.* 102, 136809 (2009); [2] J. Brede *et al.* *Phys. Rev. Lett.* 105, 047204 (2010); [3] N. Atodiresei *et al.* *Phys. Rev. Lett.* 105, 066601 (2010).

### DS 28.5 Wed 12:45 GER 37

**Structural and magnetic properties of trinuclear-Cu(II)-complexes** — ●TORSTEN HAHN<sup>1</sup>, TOBIAS RUEFFER<sup>2</sup>, and VLADISLAV KATAEV<sup>3</sup> — <sup>1</sup>Institute for Theoretical Physics, TU Bergakademie Freiberg, Germany — <sup>2</sup>Department of Chemistry, Chemnitz University of Technology, Germany — <sup>3</sup>Leibniz Institute for Solid State and Materials Research Dresden, Germany

The magnetic super-exchange interactions in Cu(II) bis(oxamato) and bis(oxamidato) complexes [1] are shown to be highly sensitive to structural modifications coordinating close to the central copper. This work presents a detailed theoretical investigation of the influence of such modifications of the molecular structure on the magnetic coupling by means of DFT using the broken symmetry approach. The relation between structural parameters, the local spin density and the corresponding magnetic exchange parameters is discussed and compared to experimental results from EPR studies and magnetic measurements. Special attention was paid to the relationship between the spin population of the monomeric building blocks and the trends of the exchange interaction in case of the corresponding trinuclear complexes. Furthermore, the use of a simplified transport model based on the Non-Equilibrium-Green-Functions formalism delivers first insights into transport properties of these complexes for possible spintronic applications.

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[1] B. Brauer, *et. al.*, *Inorg. Chem.* 47, 6633 (2008)