O 107: Poster Session VIII: Poster to Mini-Symposium: Manipulation and control of spins on functional surfaces IV

Time: Thursday 13:30–15:30 Location: P

O 107.1 Thu 13:30 P

First Principles modelling of Supramolecular Spin-valves — •Jorge Olivares, Artem Fediai, and Wolfgang Wenzel — Karlsruhe Institute of technology, Institute of Nanotechnology, Karlsruhe, Germany

Molecular spintronics uses the spin degree of freedom to develop technology that can control electrical currents in nanodevices. A good understanding of the underlying physics in nanoscale systems and reliable technical tools for simulating them are required to exploit the full capacity of the spin degree of freedom in molecules. Experimental setups have shown a remarkable spin-dependent behaviour of the current (Magnetoresistance) through a carbon nanotube decorated with single molecular magnets (SMMs). We present results of ab-initio simulations on Carbon nanotubes (CNT) decorated by two terbium phthalocyanine (SMMs). The transmission coefficient and density of states were calculated using the Non-Equilibrium Green's function (NEGF) formalism. We show the dependence of the transmission coefficient with respect to the relative spin orientation of the SMMs. Our results show how the different spin states of the system CNT+SMMs affects the transmission through a CNT as well as the advantages and limitations of an non-interactive approach. The system under study, allows us to extend our approach to any periodic sytem and different types of SMMs, opening a field of ab-initio studies of nano-electronic spintronic devices in the non-interacting and possibly to the interacting regimes.

O 107.2 Thu 13:30 P

Inducing carbon magnetism in nanographenes — •Elia Turco[1], Shantanu Mishra[1], Pascal Ruffieux[1], and Roman Fasel[1,2] — [1]Empa-Swiss Federal Laboratories for Materials Science and Technology, Dubendorf, Switzerland — [2]Department of Chemistry and Biochemistry, University of Bern, Bern, Switzerland.

Magnetism is historically associated to d- and f-block elements of the periodic table, which form the basis for modern information storage technologies. However, recent advances on the bottom-up synthesis of low-dimensional materials revealed the emergence of non-trivial magnetic states in all-carbon compounds. The low spin-orbit and hyperfine couplings in carbon, along with the possibility of electric-field control of magnetism, provides unique opportunities in emerging technologies such as quantum computation. The electronic structure of nanographenes can be selectively controlled through variation in size, shape and edge structure, allowing to experimentally realize new quantum properties, including magnetism. In this contribution, we investigate the on-surface synthesis of z-shaped nanographenes belonging to the zethrene family. Single molecule scanning probe measurements reveal the transition from a closed-shell to an open-shell singlet ground state with increasing zethrene length. In the longest analogue, singlet to triplet spin excitation are detected via inelastic electron tunneling spectroscopy, unveiling a magnetic exchange coupling of 50 meV. These results open new perspectives for the realization of organic magnetic devices operating at practical temperatures.

O 107.3 Thu 13:30 P

Supercurrent Reversal through Atomic Scale Yu-Shiba-Rusinov States — •Christian R. Ast[1], Sujoy Karan[1], Haonan Huang[1], Ciprian Padurariu[3], Björn Kubala[3], Gonzalo Morrás[2], Alfredo Levy Yeyati[2], Juan Carlos Cuevas[2], Joachim Ankerhold[3], and Klaus Kern[1,4] — [1]MPI für Festkörperforschung, Stuttgart — [2]Universidad Autónoma de Madrid, Spain — [3]Universität Ulm — [4]EPFL, Lausanne, Switzerland

Magnetic impurities on superconductors give rise to discrete bound states inside the superconducting gap known as Yu-Shiba-Rusinov (YSR) states. Varying the impurity-superconductor coupling induces a quantum phase transition (QPT) as the YSR state energy passes through zero. The concomitant sign change in the Josephson current – a long sought for hallmark of this QPT – has remained elusive so far. Using scanning tunneling microscopy (STM), we demonstrate such a 0 to π transition of a Josephson junction through a YSR state as we continuously change the impurity-superconductor coupling. We detect the sign change in the Josephson current by exploiting a second transport channel as a reference in analogy to a superconducting quantum interference device (SQUID), which provides a rudimentary phase sensitivity for the STM. The change in the Josephson current through the QPT is significant and demonstrates the role of the impurity spin as well as the parity change across the QPT.

O 107.4 Thu 13:30 P

Spin dependent transmission of nickelocene-Cu contacts probed with shot noise — Michael Mohr[1], Ricarda Reuter[1], Manuel Gruber[1], David Jacob[2], Paula Abufager[3], Nicolás Lorente[4], •Alexander Weismann[1], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [2]Departamento de Física de Materiales, Universidad del País Vasco UPV/EHU, E-20018 San Sebastián, Spain — [3]Instituto de Física de Rosario, Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), Universidad Nacional de Rosario, 2000 Rosario, Argentina — [4]Centro de Física de Materiales CFM/MPC (CSIC-UPV/EHU), E-20018 Donostia-Sebastián, Spain

The current I through nickelocene molecules and its noise are measured with a low-temperature scanning tunneling microscope on Cu(100). DFT and many-body calculations are used to analyze the data. During contact formation, two types of current evolution are observed, namely an abrupt jump to contact and a smooth transition. These data along with dI/dV spectra are interpreted in terms of a transition from a spin-1 to a spin-$\frac{1}{2}$ state that is Kondo-screened. Many-body calculations show that the smooth transition is also consistent with a renormalization of spin excitations of a spin-1 molecule by Kondo exchange coupling. The shot noise is significantly reduced compared to the Schottky value of $2eI$. The noise can be described in the Landauer picture in terms of the spin polarization of the transmission of $\approx 35\,\%$ through two degenerate d_π-orbitals of the nickelocene molecule.

O 107.5 Thu 13:30 P

Power optimization for spin-orbit torque induced magnetization switching in a monodomain magnetic particle — •Sergei Vlasov[1], Igor Lobanov[1], Grzegorz Kwiatkowski[2], Valery Uzdin[1], and Pavel F. Bessarab[1,2] — [1]ITMO University, St. Petersburg, Russia — [2]University of Iceland, Reykjavik, Iceland

The discovery of the spin-orbit torque (SOT) has opened a wide range of opportunities for the efficient manipulation of the magnetization, which is advantageous for spintronics applications. In particular, SOT produced by an in-plane current in a heavy-metal layer can be used to induce magnetization switching in a supported ferromagnetic element, thus providing means for bit operations in nonvolatile magnetic memories.

In this study, we demonstrate employing the optimal control theory that the energy cost of the SOT-induced magnetization switching can be reduced by properly tuning the current pulse. We present a complete analytical solution to the energy-efficient reversal of a macrospin under SOT. We calculate optimal control paths (OCPs) of the magnetization reversal and reconstruct the time-dependent amplitude and frequency of both components of the in-plane current. We also demonstrate the stability of calculated optimal switching protocols with respect to perturbations in materials properties and temperature.

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O 107.6 Thu 13:30 P

Spin-polarized photoelectron emission from chiral cobalt oxide layers — •Onur Gül[1], Paul Möllers[1], Daniel Nürenberg[1], Koyel Banerjee Ghosh[2], Wenyan Zhang[2], Francesco Tassinari[2], Yitzhak Mastei[2], Ortal Lidor-Shalev[2], Simon Wei[3], Emil Wierzbinski[3], David Waldeck[3], Ron Naaman[2], and Helmut Zacharias[1] — [1]Center for Soft Nanoscience, Westfälische Wilhems-Universität, 48149 Münster, Germany — [2]Department of Chemical and Biological Physics, Weizmann Institute of Science, 76100 Revohoz, Israel — [3]Chemistry Department, University of Pittsburgh, Pittsburgh, PA 15260, United States

Chiral catalyst surfaces were recently shown to enhance the chemical selectivity of an electrocatalytic water splitting reaction by aligning the electron spins in the laboratory frame. [1] [2]

In this contribution we present results of spin-resolved photoemission experiments conducted with chiral cobalt oxide thin films. The photoelectrons were excited with laser pulses at $\lambda = 213\,\mathrm{nm}$, generated as the fifth harmonic of a Nd:YVO_4 laser, and the average spin polarization was determined in a Mott scattering apparatus. While only unpolarised electrons were emitted from the achiral layers, the electrons emitted from chiral layers exibit up to 30 percent spin polarization, suggesting that the spin polarization is indeed a consequence of the chirality of the layers.

[1] S. Ghosh et al,, J. Phys. Chem. C, 123 (2019) [2] K. B. Ghosh et al., J. Phys. Chem. C, 124 (2020)

O 107.7 Thu 13:30 P

Chiral cupric oxide layers as spin-polarizing water splitting catalysts — •Paul Möllers[1], Daniel Nürenberg[1], Koyel Banerjee Ghosh[2], Wenyan Zhang[2], Francesco Tassinari[2], Yitzhak Mastai[2], Ortal Lidor-Shalev[2], Simon Wei[3], Emil Wierzbinski[3], David Waldeck[3], Ron Naaman[2], and Helmut Zacharias[1] — [1]Center for Soft Nanoscience, Westfälische Wilhelms-Universität, 48149 Münster, Germany — [2]Department of Chemical and Biological Physics, Weizmann Institute of Science, 76100 Rehovot, Israel — [3]Chemistry Department, University of Pittsburgh, Pittsburgh, PA 15260, United States

Spin-polarized catalytic surfaces can greatly enhance the selectivity of chemical reactions, e.g., in an electrocatalytic water splitting process. The spin polarization can be can be generated by the introduction of a chiral catalyst surface. [1,2] Here, we confirm that spin-polarized photocurrents can be obtained from chiral cupric oxide (CuO) films, and explore the underlying mechanism. Chiral CuO films were electrochemically deposited on polycrystalline gold substrates using a method pioneered by Switzer et al [3]. Photoelectrons were excited with laser pulses at 213 nm, and their average spin polarization was measured in a Mott scattering apparatus. The polarization exceeds $P = +10\,\%$ for 20 nm thin CuO films with 'L' chirality and, notably, is reversed for oxide films of opposite 'D' chirality.

[1] S. Ghosh et al., J. Phys. Chem. C, 123, 3024-3031 (2019)

[2] K. B. Ghosh et al., J. Phys. Chem. C, 124, 22610-22618 (2020)

[3] Kothari et al., Chem. Mater. 16, 4232-4244 (2004)