DS 7: Spins in Molecular Systems: Strategies and Effects of Hyperpolarization

Time: Wednesday 9:30–11:45 Location: H14

Invited Talk DS 7.1 Wed 9:30 H14

Enhancing Organic Spin Valves Through Spinterface Engineering — •Shuaishuai Ding and Wenping Hu — Institute of Molecular Aggregation Science, School of Science, Tianjin University, Tianjin, China

Organic spin valves hold immense promise for efficient spintronic devices, driving advancements in information processing and storage technologies. The spinterface, the interface between an organic semiconductor and a ferromagnetic electrode, plays a crucial role in the performance of these devices. However, the inherent instability of the spinterface poses challenges that must be addressed to fully realize this potential. To tackle these issues, we have developed a comprehensive approach that combines innovative fabrication techniques and material engineering. Electrode transfer technology enhances interfacial properties by enabling the precise deposition of high-quality ferromagnetic electrodes onto organic semiconductors, while doping with F4-TCNQ effectively improves spin injection efficiency through modulation of electronic and magnetic characteristics. Moreover, the engineering of controllable bottom spinterfaces allows for precise regulation of spin injection, resulting in highly tunable device performance. By leveraging the spinterface, we have achieved in-situ control of device tunability, significantly expanding the multilevel resistance modulation of organic spin valves. These advancements not only address key challenges of unstable spinterface but also establish novel methods for device modulation, marking an important leap forward in organic spintronics.

DS 7.2 Wed 10:00 H14

Hyperpolarised electron spins as a sensitive probe for investigating structure–function relationship in organic energy materials — •Till Biskup — Universität Rostock, Rostock, Germany

Energy conversion and storage is of paramount importance, and organic functional materials are increasingly being used for this purpose. Hyperpolarised electron spins as created, e.g., by light excitation act as sensitive probe of their environment. This allows to investigate the structure–function relationship of these materials by using time-resolved electron paramagnetic resonance (TREPR) spectroscopy. Insights range from morphology and details of the aggregation behaviour in both, film and solution to triplet routes to the electronic structure of these materials far beyond exciton delocalisation. Here, we focus particularly on the effects of conjugation break and systematic backbone variation on exciton delocalisation as well as solvent and cooling rate on aggregate formation. TREPR spectroscopy provides insight into these effects with molecular resolution that is not available by and complementary to other methods.

DS 7.3 Wed 10:15 H14

The CISS magnetoresistance effect for polyalanine and polyproline molecules studied by ambient STM — •Thi Ngoc Ha Nguyen[1], Lech Tomasz Baczewski[2], Tobias Theiss[3], Tanja Gulder[3], and Christoph Tegenkamp[1] — [1]Solid Surface Analysis, Institute of Physics, Chemnitz University of Technology, Chemnitz, Ger- many — [2]Reichenhainerstr., 70 — [3]Institute of Organic Chemistry, Faculty of Chemistry and Mineralogy, Leipzig University, Leipzig, Germany

The chirality induced spin selectivity (CISS) effect has been up to now measured in a wide variety of systems but its exact mechanism is still under debate. Whether the spin polarization occurs at an interface layer or builds up in the helical molecule is yet not clear. We investigated the current transmission through helical polyalanine molecules, revealing a strong and length dependent dipole moment, as a part of a tunnel junction realized with a scanning tunneling microscope. Depending on whether the molecules were chemisorbed directly on the magnetic Au/Co/Au substrate or at the STM Au-tip, the magnetizations of the Co layer had been oriented in the opposite direction in order to preserve the symmetry of the IV-curves. These results show that besides the helicity also the electric dipole play a crucial role. Latest experiments with polyproline with a small electric dipole moment showed that the CISS effect is almost vanishing. Our results can be explained by a spin-polarized or spin-selective interface effect, induced and defined by the helicity and electric dipole orientation of the molecule at the interface.

session break

DS 7.4 Wed 10:45 H14

Analysis of polaron pair lifetime dynamics and secondary processes in exciplex driven TADF OLEDs using organic magnetic field effects (MFE) — •Annika Morgenstern[1], Dominik Weber[2], Lukas Hertling[1,3], Konstantin Gabel[1], Ulrich T. Schwarz[1], Daniel Schondelmaier[2], Dietrich R.T. Zahn[1,3], and Georgeta Salvan[1,3] — [1]Institute of Physics, TU Chemnitz — [2]Physical Engineering and Computer Science, WH Zwickau — [3]MAIN, TU Chemnitz, Chemnitz

MFE in TADF materials have been shown to influence the reverse intersystem crossing and to impact on electroluminescence and conductivity. Here, we present a novel model combining Cole-Cole and Lorentzian functions to describe low and high MFE originating from hyperfine coupling, the Δg mechanism, and triplet processes. We applied this approach to organic light-emitting devices of third generation based on TCTA and TPBi, exhibiting blue emission, to unravel their loss mechanisms. The quality of the regression function was evaluated using k-fold cross-validation. The scoring was compared to various alternative fitting functions, which were previously proposed in literature. Density functional theory calculations, photoluminescence, and electroluminescence studies validated the formation of a TADF exciplex system. Furthermore, we propose successful encapsulation using a semi-permeable polymer, showing promising results for magnetic field sensing applications. This study provides insights into the origin of MFE in exciplex-TADF materials, with potential applications in optoelectronic devices and sensing technologies.

DS 7.5 Wed 11:00 H14

Employing CISS for Modification of Skyrmion Diffusion and Size — •Fabian Kammerbauer[1], Yael Kapon[2], Theo Balland[1], Shira Yochelis[2], Yossi Paltiel[2], and Mathias Kläui[1] — [1]Institut für Physik, Johannes-Gutenberg-Universität Mainz, 55099 Mainz, Germany — [2]Institute of Applied Physics, Faculty of Sciences, The Hebrew University of Jerusalem, Jerusalem 9190401, Israel

Chirality-induced spin selectivity (CISS) is a phenomenon that has garnered significant attention due to its ability to generate large spin polarizations in organic molecules and its associated effects, such as the magnetic switching of ferromagnets induced by chiral molecules [1]. In hybrid systems, these chiral molecules have been found to influence magnetic properties, including changes in the magnetization [2]. This study explores the interaction between chiral molecules, specifically alpha-helix polyalanine, and chiral spin structures such as magnetic skyrmions. The skyrmions are stabilized in ferromagnetic/heavy metal multilayers via the Dzyaloshinskii-Moriya interaction [3]. Through magneto-optic Kerr effect imaging, we demonstrate that chiral polypeptides can alter the stability of skyrmions by shifting the temperature and magnetic field ranges where they remain stable. Furthermore, we reveal the impact of chiral molecules on skyrmion size and thermal skyrmion diffusion.

[1] R. Naaman et al. Nat. Rev. Chem. 3, 250 (2019)
[2] Y. Kapon et al. J. Chem. Phys. 159, 064701 (2023)
[3] K. Everschor-Sitte et al. J. Appl. Phys. 124, 240901 (2018)

DS 7.6 Wed 11:15 H14

Microscopic and Macroscopic CISS Effect Characterization: Moving from MBE to Sputter-Deposited Au/Co/Au Substrates — •Lokesh Rasabathina[1], Thi Ngoc Ha Nguyen[1], Julia Krone[1], Annika Morgenstern[1], Franziska Schölzel[1,2], Markus Gössler[1], Karin Leistner[1], Aleksandr Kazimir[4], Jannik Knoche[4], Christina Lamers[4], Irene Coin[4], Lech Thomasz Baczewski[5], Christoph Tegenkamp[1], Georgeta Salvan[1,2], and Olav Hellwig[1,2,3] — [1]Chemnitz University of Technology, Chemnitz, Germany — [2]Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology,Chemnitz, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [4]Leipzig University, Leipzig, Germany — [5]Polish Academy of Sciences, Warszawa, Poland.

Adsorption of alpha-helical polyalanine molecules on metallic substrates enables interfacial selective electron transport with a defined spin direction, a phenomenon known as Chirality Induced Spin Se-

lectivity (CISS). We combine microscopic STM/STS of hybrid spin-valve structures with macroscopic MOKE magnetometry for CISS effect characterization on Au/Co/Au substrates. Microscopically we observe magneto resistance changes across the hybrid spin-valve structure and macroscopically we find a coercivity enhancement of the Co layer after exposure to molecules. To use more complex systems, we moved from MBE to sputterd substrates and discuss the challenges related to this transition.

DS 7.7 Wed 11:30 H14

Towards a quantum sensing approach to single-cell chemical and mechanical analysis using nanoscale NMR — •Baha Sakar[1], Sirswa Kuldeep Shree Ram[1], Maximilian Püllmann[1], Frank Sauer[2], Rustem Valiullin[1], Josef A. Käs[2], and Nabeel Aslam[1] — [1]Felix-Bloch-Institut für Festkörperphysik - Universität Leipzig, Leipzig, Deutschland — [2]Peter-Debye-Institut für Physik der weichen Materie - Universität Leipzig, Leipzig, Deutschland

Understanding single-cell mechanical and chemical properties is key to exploring cellular behavior and dysfunction, influencing processes like development, immune response, and disease progression, including cancer metastasis. While fluorescence microscopy enables structural insights and tracking, it lacks the chemical specificity of conventional NMR. The latter is however limited to ensemble measurements and cannot resolve single-cells. In this study, we utilize a quantum sensing platform based on NV centers in diamond, which are atomic-scale spin defects capable of detecting nuclear spins with sensitivities up to fifteen orders of magnitude higher than conventional NMR, enabling single-cell resolution. By applying resonant microwave pulse sequences and specially designed magnetic fields, we probe the NMR signal of the cells' nuclear spins. In this talk, we will discuss the steps towards studying the micromechanical and chemical properties of single cells, distinguishing between intracellular and extracellular molecular diffusion processes. Furthermore, we will present initial results of correlating fluorescence microscopy and NMR spectroscopy with the goal to investigate the link between cell mechanics and tumor aggressiveness.