

## TT 43: Focus Session: Spin Phenomena in Chiral Molecular Systems II (joint session O/TT)

Time: Wednesday 10:30–12:30

Location: MA 141

**Topical Talk** TT 43.1 Wed 10:30 MA 141  
**Chiral-induced Spin Selectivity in Hybrid Chiral Molecule/Metal Systems** — ASHISH MOHARANA<sup>1</sup>, YAEL KAPON<sup>2</sup>, FABIAN KAMMERBAUER<sup>1</sup>, DAVID ANTHOFER<sup>1</sup>, SHIRA YOCHELIS<sup>2</sup>, YOSSI PALTIEL<sup>2</sup>, and ANGELA WITTMANN<sup>1</sup> — <sup>1</sup>Johannes Gutenberg University Mainz, Germany — <sup>2</sup>Hebrew University Jerusalem, Israel

The chiral-induced spin selectivity (CISS) effect has recently gained significant attention in the field of spintronics. The remarkably high polarization efficiency of chiral molecules via the CISS effect paves the path toward novel, sustainable hybrid chiral molecule magnetic applications. While research has predominantly focused on transport properties so far, in our work, we explore spintronic phenomena at hybrid chiral molecule magnetic interfaces to elucidate the underlying mechanisms of the chiral-induced spin selectivity effect. For this, we investigate the interfacial spin-orbit coupling in chiral molecule/metal thin film heterostructures by probing the chirality and spin-dependent spin-to-charge conversion. Our findings validate the central role of spin angular momentum for the CISS effect, paving the path toward the functionalization of hybrid molecule-metal interfaces via chirality.

**Topical Talk** TT 43.2 Wed 11:00 MA 141  
**Chirality-induced spin selectivity at the single-molecule scale** — DANIEL EMIL BÜRGLER<sup>1</sup>, MOHAMMAD REZA SAFARI<sup>1</sup>, FRANK MATTHES<sup>1</sup>, NICOLAE ATODIRESEI<sup>1</sup>, CLAUD MICHAEL SCHNEIDER<sup>1</sup>, and KARL-HEINZ ERNST<sup>2</sup> — <sup>1</sup>Peter Grünberg Institut, Forschungszentrum Jülich, Germany — <sup>2</sup>Molecular Surface Science Group, Empa, Dübendorf, Switzerland

Chirality-induced spin selectivity (CISS) leads to spin-selective electron transport in chiral molecules and enantiospecific adsorption on magnetic surfaces. To advance the development of theoretical models, well-defined single-molecule experiments are needed. Here, we report CISS effects for single chiral heptahelicene molecules that are sublimed under ultra-high vacuum onto uncoated single-crystalline and perpendicularly magnetized Co nanoislands. We use spin-polarized scanning tunneling microscopy (SP-STM) to (i) determine the handedness of individual heptahelicenes and the magnetization direction of the underlying Co nanoisland and (ii) measure spin-polarized transport through single molecules. Analysis of more than 740 molecules provides unequivocal evidence for enantioselective adsorption and reveals that enantioselection must occur in a physisorbed transient precursor state.  $I-V$  curves of two enantiomers under otherwise identical conditions show at 5 K magnetochiral conductance asymmetries of up to 50% when either the molecular handedness is exchanged or the magnetization of the STM tip or Co substrate is reversed. The results demonstrate that CISS is a single-molecule effect and rule out electron-phonon coupling and ensemble effects as its primary mechanisms.

TT 43.3 Wed 11:30 MA 141  
**Spin polarization through a helical molecule- functionalized tip dependence on the tip-sample distance observed by ambient STM** — THI NGOC HA NGUYEN<sup>1</sup>, LECH TOMASZ BACZEWSKI<sup>2</sup>, OLAV HELLMIG<sup>3</sup>, and CHRISTOPH TEGENKAMP<sup>1</sup> — <sup>1</sup>Analysis of Solid Surfaces, Nanostructures and Quantum Materials, Chemnitz University of Technology, Germany — <sup>2</sup>Institute of Physics, Polish Academy of Sciences, Warszawa, Poland — <sup>3</sup>Functional Magnetic Materials, Chemnitz University of Technology, Chemnitz, Germany

Polyalanine (PA) with an alpha-helix conformation has gathered recently a lot of interest as the propagation of electrons along the helical backbone structure comes along with spin polarization of the transmitted electron. However, studies on a molecular scale are still rare, although this length scale provides direct insight into the role of molecular properties. We studied now in detail with a PA molecule-functionalized Au tip on magnetic Au/Co/Au/Pt/Al<sub>2</sub>O<sub>3</sub> substrates and probed the transmission by local spectroscopy (STS). Because of the high spatial resolution, our setup allows to study this CISS effect on the nanoscale and probe the importance of cooperative effects. Using this functionalized tip, we found that the spin polarization (SP) significantly varies with tip-sample distance. Interestingly, the SP through the self-assembled film of PA on the same substrate at different non-functionalized Au tip-sample distance doesn't show significant change. Our observation provides that the overlapping tip and sample orbitals, the coupling as well as the electric field strength in the close proximity

of tip - sample surface take the main roles on this SP variation.

TT 43.4 Wed 11:45 MA 141  
**Chirality-induced spin selective quantum capacitance** — THEILER PIUS MARKUS — ETH Zürich, Zürich, Switzerland

The absence of symmetries has a significant impact on physics, particularly in chiral molecules or crystals lacking mirror symmetry. When an electric charge interacts with such chiral materials, the spin of the charge aligns even at room temperature. This spin polarization is known as chirality-induced spin selectivity (CISS). Although the exact mechanism behind the effect remains unclear, it may have played a role in the origin of life and significantly impacted biological processes. The effect has potential applications in chemical catalysis, renewable energy, and quantum technologies. This work aims to elucidate the key mechanism behind CISS surface potential changes upon toggling the enantiomer or magnetic polarization of the substrate. For the first time, chiral  $\alpha$ -helical polypeptide films are investigated with time-resolved Kelvin-probe atomic force microscopy to probe the dynamics of the surface potential and a CISS quantum capacitance. This discovery of the CISS quantum capacitance leads to the conclusion that CISS is a persistent effect and paves the way to a fundamental reinterpretation of the CISS effect.

TT 43.5 Wed 12:00 MA 141  
**Magnetization generation in helical molecular junctions** — RICHARD KORYTÁR<sup>1</sup>, JAN VAN RUITENBEEK<sup>2</sup>, and FERDINAND EVERS<sup>3</sup> — <sup>1</sup>Univerzita Karlova, Prague, Czech Republic — <sup>2</sup>Leiden University — <sup>3</sup>University of Regensburg

Despite extensive experimental and theoretical literature on the spin-selective transport in helical molecules [1], a satisfactory theoretical explanation of the effect is lacking [2]. We present analytical calculations of charge and spin conductances in a minimal model of a helical molecule with spin orbit coupling attached to non-magnetic leads. The calculations extend previous studies, which focused on spin-polarization [5,3]. The band-structure of the model exhibits spin-momentum locked bands analogous to the edge modes of a quantum spin Hall system. The spin currents in the left and right lead carry opposite signs and consequently both leads pick up parallel magnetizations (in linear response). We discuss the feedback of resulting spin accumulations in the leads to the charge current [4].

[1] Ron Naaman, Yossi Paltiel & David H. Waldeck, *Nature Reviews Chemistry*, volume 3, pages 250\*260 (2019)

[2] Evers et al., *Adv. Mater.* 2022, 34, 2106629

[3] J. M. van Ruitenbeek, R. Korytár, F. Evers, *J. Chem. Phys.* 159, 024710 (2023)

[4] R. Korytár, J. M. Ruitenbeek, F. Evers, in preparation

[5] K. Michaeli and R. Naaman, *J. Phys. Chem. C* 123, 17043 (2019)

TT 43.6 Wed 12:15 MA 141  
**Study of magneto-optical properties of cobalt-layers by adsorption of  $\alpha$ -helical polyalanine self-assembled monolayers** — LOKESH RASABATHINA<sup>1</sup>, APOORVA SHARMA<sup>1</sup>, JULIA KRONE<sup>1</sup>, ANNIKA MORGENSTERN<sup>1</sup>, THI NGOC HA NGUYEN<sup>1</sup>, MARKUS GÖSSLER<sup>2</sup>, KARIN LEISTNER<sup>2</sup>, CHRISTOPH TEGENKAMP<sup>1</sup>, GEORGETA SALVAN<sup>1</sup>, and OLAV HELLMIG<sup>1</sup> — <sup>1</sup>Institute of Physics, Chemnitz University of Technology, 09126 Chemnitz, Germany — <sup>2</sup>Institute of Chemistry, Chemnitz University of Technology, Chemnitz, 09111, Germany

High spin polarization in helical polyalanine molecules enables selective electron transport with a defined spin direction, a phenomenon known as Chirality Induced Spin Selectivity (CISS). This discovery holds promising implications for organic spintronic devices. Furthermore, the adsorption of pure enantiomers of  $\alpha$ -helical polyalanine on a gold-covered ferromagnetic thin film, termed Magnetism Induced by the Proximity of Adsorbed Chiral molecules (MIPAC), can influence the magnetization of the ferromagnetic thin film. In our ongoing research, we are delving into the magnetic properties of thin films and attempt to increase the size of atomically smooth terraces at the Au(111) surface. By varying parameters such as deposition pressure and annealing temperature, we aim to understand how alterations in the Au surface affect the arrangement of molecules and how the molecule adsorption at the Au surface depends on the magnetic properties and state of the underlying magnetic thin film.