DS 18: Spins in Molecular Systems

Time: Thursday 15:00–17:30 Location: REC/C213

DS 18.1 Thu 15:00 REC/C213

The forgotten sister of the CISS effect: spin polarization induced via proximity of adsorbed chiral molecules — •Franziska Schölzel[1], Aybüke Gülkaya[2], Dominik Hornig[1], Rico Ehrler[1], Lokesh Rasabathina[1], Aleksandr Kazimir[3], Christina Lamers[3], Olav Hellwig[1], Michael Mehring[1], Shuxia Tao[2], and Georgeta Salvan[1] — [1]Chemnitz University of Technology, Chemnitz, Germany — [2]Eindhoven University of Technology, Eindhoven, the Netherlands — [3]Leipzig University, Leipzig, Germany

Within the past years a new research field around chirality induced spin selectivity (CISS) has emerged and gains increasing attention. The central part is often played by complex chiral or helical molecules; ferromagnetic, gold capped, sometimes structured substrates and electrical transport measurements [1]. An aspect most often forgotten within this framework is the effects static equivalent [2]. We observed the Spin Polarization Induced via the Proximity of Adsorbed Chiral Molecules (SPIPAC) effect in nickel thin films for various chiral molecules. This study probes the resulting magneto-optical signal of the Ni substrate using Circular Dichroism spectroscopy. Furthermore, the impact of film thickness of the substrate, molecule density on the surface and the chirality of the molecules is explored. [1] B. Bloom et al., Chem. Rev. 124, 4, 1950-1991 (2024) [2] O. Ben Dor et al., Nat Commun 8, 14567 (2017)

DS 18.2 Thu 15:15 REC/C213

Understanding interface-controlled CISS-MR (magnetoresistance) via electric dipole inversion using ambient STM — •T. N. Ha Nguyen[1], Lech Tomasz Baczewski[2], Aleksandr Kazimir[3], Christina Lamers[3], and Christoph Tegenkamp[1] — [1]Analysis of Solid Surfaces, Nanostructures and Quantum Materials, Technische Universität Chemnitz, Germany — [2]Reichenhainerstr., 70 — [3]Institute for Drug Discovery, Medical Faculty University of Leipzig, Leipzig, Germany

Recent studies have highlighted the significant influence of electric dipole moment orientation in chiral molecules on spin polarization. When chiral molecules with strong dipole moments adsorb onto a surface, their orientation breaks the interfacial symmetry, leading to enhanced spin-polarized currents. Using scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS), we measured spin-polarized electron transport through polyalanine molecules, which possess substantial dipole moments. Notably, inverting the dipole moment while maintaining the molecule*s chirality results in a reversal of the chiral-induced spin selectivity magnetoresistance (CISS-MR). Our findings not only highlight the crucial role of electric dipole moments in chiral molecules but also provide insights into the CISS mechanism, particularly regarding the interface effect.

DS 18.3 Thu 15:30 REC/C213

Effect of adsorbed chiral molecules on the magnetic properties of skyrmion-hosting multilayers — •Mariam Hassan[1,2], Ivan Saldatov[3], Lokesh Rasabathina[4], Franziska Schölzel[1,2], D.R.T Zahn[1,2], Olav Hallwig[1,4], and Georgeta Salvan[1,2] — [1]Research Center for Materials, MAIN, Chemnitz University of Technology, Germany — [2]Semiconductor Physics, Institute of Physics, Chemnitz University of Technology, Germany — [3]Institute for Metallic Materials, IFW, Dresden — [4]Functional Magnetic Materials, Institute of Physics, Chemnitz University of Technology, Germany

Chirality-induced spin selectivity (CISS) and Magnetism Induced by Proximity of Adsorbed Chiral molecules (MIPAC) effects are phenomena that caught significant interests over the last few decades because of the large spin polarizations generated by organic molecules and the alteration of the surface's magnetism upon the adsorption of chiral molecules respectively [1,2]. On the other hand, magnetic skyrmions have emerged as a promising path for next-generation information storage and processing technologies. Thus, tuning skyrmion properties is of increasing interest for application in future spintronic devices. In light of the CISS and MIPAC effects, the use of chiral molecules might represent an attractive approach to address the challenge of tuning skyrmion properties [3]. In this work, we aim to investigate how adsorbed chiral molecules interact with magnetic skyrmions that are stabilized in [Co/Ni]N ferromagnetic multilayers with PMA. We observe that the adsorbed chiral molecules locally change the magnetic properties of the film, affecting the density of skyrmion nucleation sites.

DS 18.4 Thu 15:45 REC/C213

Self-Assembly of Helical Molecular Monolayers Using a Coarse-Grained Chiral Patchy Model — •Hadis Ghodrati Saeini[1], Faezeh Shabani[1], Sibylle Gemming[1], Christoph Tegenkamp[1], Florian Günther[2], and Jeffrey Kelling[1,3] — [1]Technische Universität Chemnitz, Chemnitz, Germany — [2]São Paulo State University, Rio Claro, Brazil — [3]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

The Chiral-Induced Spin Selectivity (CISS) effect makes helical molecules promising for spintronic applications, yet their surface self-assembly remains poorly understood due to experimental and computational constraints. Although Density-Functional Tight-Binding (DFTB) potentials accurately describe polyalanine (PA) α-helix SAMs, their high computational cost limits large-scale and kinetic investigations.

We introduce a coarse-grained chiral patchy model parameterized to fit the PA-specific DFTB potential, capturing its essential chiral symmetry and interaction features while remaining computationally efficient. Validation is achieved by comparing low-energy configurations obtained from annealing Monte Carlo simulations using the DFTB-based potential with dynamic pathways from coarse-grained molecular dynamics. Dynamic simulations made feasible by this model successfully reproduce the final assembled morphologies and allow explorations of potential metastable states, demonstrating its reliability and versatility for studying the kinetics of helical molecular self-assembly.

DS 18.5 Thu 16:00 REC/C213

Exploring the Origins of Helical Bundle Stability and Their Role in the CISS Effect — •Faezeh Shabani[1], Sibylle Gemming[1], Georg Kuenze[2], Paul Kluge[2], and Florian Guenther[3] — [1]Technische Universität Chemnitz, Chemnitz, Germany — [2]Universität Leipzig, Leipzig, Germany — [3]Instituto de Geociências e Ciências Exatas, Universidade Estadual Paulista, Rio Claro, Brazil

Helical bundles provide a highly regular and tunable chiral environment, making them ideal model systems for investigating the principles of the CISS effect and exploring possibilities for generating electronic hyperpolarization through (super)helical geometries. Beyond their relevance to chiral-induced spin selectivity, helix bundles also play important roles in nature: they consist of two or more α-helices supercoiled around a central axis and function as essential structural motifs in many biological systems. In this talk, we explore these characteristics using DFTB+ calculations. This computational approach allows us to analyze the energetic origins of specific bundling motifs, assess the role of dispersion interactions, and ultimately understand why certain helix bundle architectures are favored in nature.

15 min. break

DS 18.6 Thu 16:30 REC/C213

Unwinding the Helicity-Driven Electronic Properties in Polyproline I and II Chains — •Saba Arshad, Faezeh Shabani, and Sibylle Gemming — TU Chemnitz, Chemnitz, Germany

Polyproline is a polypeptide that adopts two distinct helical conformations, polyproline I (PPI) and polyproline II (PPII), with identical primary sequence but markedly different helicities and structural behavior, providing a valuable platform for examining electronic properties and their potential impact on CISS (Chirality-Induced Spin Selectivity) effects. Here, we employed density-functional approaches for chains with different numbers of monomers to investigate how helical geometry influences the electronic properties of both conformers. Our results reveal significant differences in the HOMO-LUMO gap and density of states between PPI and PPII, with the gap consistently narrowing as additional monomers are incorporated. Dipole moments calculated for chains of increasing length display distinct scaling trends for PPI and PPII helices, highlighting how both chain length and topology govern emerging molecular electronic applications.

DS 18.7 Thu 16:45 REC/C213

Modelling spin particles in an infinite helical box —

Alex Mureşan[1,2], Fabian Prasse[1], and •Sibylle Gemming[1] — [1]Institute of Physics, TU Chemnitz, Germany — [2]Faculty of Physics, Babes-Bolyai University, Cluj-Napoca, Romania

Calculating the electronic states of a quantum mechanical particle in a potential well with infinitely high walls is probably the most readily accessible, still analytically solvable textbook example of quantisation via spatial confinement. As such, it is an ideal starting point for including additional terms to the Hamiltonian in order to adapt the model to a specific experimental setting, e.g. by introducing multiple particles or external fields. Here we present an extension that assumes an externally given spatial modulation of the potential well with helical characteristics as boundary condition. We derive analytical solutions for the motion of classical, Newtonian particles on a helical path, for charged Schrödinger-type quantum particles in a one-dimensional helical confinement, and quantum-mechanical spin 1/2-particles in a helical spin-orbit-split environment, which is encountered in investigations of the chirality-induced spin selectivity effect. We show that the model extension steps successively refine the eigenspectra of the simplest case, and that the spin-orbit interaction term leads to an extra splitting within the helical confinement.

Invitied Talk DS 18.8 Thu 17:00 REC/C213

Insights from Quantum Dynamics Simulations: From Molecules to Organic-Material Interfaces — •Frank Ortmann — Technical University of Munich, Munich, Germany

Understanding charge, exciton and spin dynamics in molecular systems is critical for advancing organic semiconductor-based technologies. We present insights from our work addressing distinct yet complementary aspects of these phenomena for organic-electronics materials. First, we explore charge-transfer dynamics in electron-phonon coupled model systems, identifying regimes such as polaron transport and transient localization, emphasizing their seamless transitions across vibrational modes and temperatures. Second, a comparative analysis of the Matrix Product State (MPS) and Multilayer Multiconfiguration Time-Dependent Hartree (MCTDH) methods demonstrates their efficacy in modeling non-adiabatic exciton dissociation, revealing specific sensitivities to electronic-vibrational entanglement in complex systems. Lastly, we introduce current work toward a general quantum mechanical treatment of spin transport in donor-acceptor systems. These works underline the theoretical advances in capturing the interplay of various degrees of freedom in molecular optoelectronics and spintronics.