O 69: Poster: Spin Phenomena in Chiral Molecular Systems

Time: Wednesday 18:00–20:00 Location: Poster C

O 69.1 Wed 18:00 Poster C

Self-assembly of the chiral donor-acceptor molecule DCzDCN on Cu(100) — Robert Ranecki, •Stefan Lach, and Christiane Ziegler — RPTU Kaiserslautern - Landau and Research Center OPTIMAS, Erwin-Schrödinger-Str. 56, 67663 Kaiserslautern, Germany

The twisted donor-acceptor molecule DCzDCN (5-(4,6-diphenyl-1,3,5-triazine-2-yl)benzene-1,3-dinitrile) shows an interesting self-assembly behavior on Cu(100). This D-A molecule is of particular interest as a system that uses reverse intersystem crossing (rISC) to massively increase the fluorescence yield. The orientation of the molecules with the donor part towards the substrate results in a chiral resolution at the interface, forming only homochiral phases. It ranges from tetramers in the submonolayer region to 1D structures near monolayer coverage, with a slight excess of the M-(-) dimer-determined phases. Using a multi-method approach with STM/STS and photoelectron spectroscopy, the topography and the molecular electronic properties of the DCzDCN/Cu(100) system are studied globally and locally. The appearance of hybrid interface states (HIS) will be discussed [2].

[1] Y. J. Cho et al. Adv. Mater. 26, 4050 (2014) [2] R. Ranecki et al. arXiv:2310.19534 [cond-mat.mtrl-sci]

O 69.2 Wed 18:00 Poster C

Multi-scale simulation of structural motifs in assemblies of helical molecules — Kevin Preis[1], •Sibylle Gemming[1], Jeffrey Kelling[1], and Florian S. Günther[2] — [1]Instute of Physics, TU Chemnitz, Chemnitz, Germany. — [2]UNESP, Rio Claro, Brazil.

Helical polypeptide molecules sparked interest as candidate materials for studying spintronic effects on the nano-scale. As charge carriers are transmitted through assemblies of helical molecules, spin polarization of the transmitted current has been detected by scanning tunneling spectroscopy and attributed to a polarization dependent tunneling resistance or a spin-selective propagation along the backbone of the helical molecule. For single molecules there is, however, debate, whether the helical symmetry break alone or also the adsorption-induced surface polarization for films on metallic substrates decisively influences the polarization direction [1]. The present simulations, address potentially beneficial effects of aggregate formation from helical molecules depending on the type of helicity, the orientation on the surface and the type and strength of the molecule-surface interaction. For polyalanine (PA) we studied the lateral*ordering between PA homo- and heterochiral pairs by van-der-Waals-corrected DFT-based tight binding calculations. Denser packing geometries can be reached by heterochiral PA pairs. Furthermore, coarse-grained classical potentials were derived from the DFTB data, and the different PA phases seen in STM were also successfully obtained from Monte-Carlo simulations. [1] Aragones et al., small 2017, 13, 1602519.

O 69.3 Wed 18:00 Poster C

Pinning of magnetic domains and skyrmions by adsorption of chiral polypeptides — Yael Kapon[1], •Theo Balland[2], Fabian Kammerbauer[2], Mathias Kläui[2], Shira Yochelis[1], Mathias Kläui[2], and Yossi Paltiel[1] — [1]Institute of Applied Physics, Faculty of Sciences, The Hebrew University of Jerusalem,Jerusalem 9190401, Israel — [2]Institute of Physics, Johannes Gutenberg University, Staudingerweg 7, 55128 Mainz, Germany

Spin currents are of intrinsic interest to the magnetism community due to its ability to influence magnetic states. A high degree of spin polarization can be achieved by chirality-induced spin selectivity (CISS) [1]. Here we investigate the impact of adsorbed chiral polypeptides on the pinning of magnetic domains [2]. The examined structure comprises chiral polypeptide α-helix polyalanine adsorbed on a Ta(5)/CoFeB(0.9)/MgO(2)/Ta(2)/Au(5) thin film, exhibiting perpendicular magnetic anisotropy, along with a Ti(2)/Ni(80)/Au(5) thin film. Utilizing Magneto-Optic Kerr Effect microscopy, the magnetic structures are visualized, and the surface magnetization is quantified. Magnetic imaging of domain walls unveils distinctions between chiral and achiral molecules adsorbed on the surface. Comparative analysis of the in-plane magnetization curves of Ti/Ni/Au/chiral molecules enables the observation of the rotation of the easy axis of magnetization. This rotation is attributed to the alignment of magnetization with the spatial orientation (tilt angle) of the molecules [2].

[1] R. Naaman et al., Nat. Rev. Chem. 3, 250-260 (2019)

[2] Y. Kapon et al., J. Chem. Phys. 159, 064701 (2023)

O 69.4 Wed 18:00 Poster C

Theory for phonon-mediated chirality-induced spin selectivity — •Namgee Cho, Thibaut Lacroix, James Lim, Susana F. Huelga, and Martin B. Plenio — Institut für Theoretische Physik, Universität Ulm, D-89081 Ulm, Germany

Chirality-induced spin selectivity (CISS) is an intriguing phenomenon where the chirality of organic molecules induces significant spin selectivity in various electronic processes, such as bound electron transport, photoelectron transmission and chemical reactions. Although the CISS effects have been demonstrated in various experiments, the underlying mechanism is still unknown. Recently, the influence of electron-phonon interaction on CISS has attracted considerable interest. However, the previous theoretical studies have considered simplified models where phonon degrees of freedom are treated classically or approximately described by a single quantum harmonic oscillator. In this work, we consider a pseudo-mode theory where multiple quantum harmonic oscillators under Lindblad noise effectively describe non-Markovian phonon baths inducing fluctuations in electronic parameters of chiral molecules. We investigate how the electron-phonon interaction leads to CISS effects in charge separation and how the degree of spin polarization depends on environmental parameters.

O 69.5 Wed 18:00 Poster C

Chiral-Induced Spin Selectivity and Non-equilibrium Spin Accumulation in Molecules and Interfaces: A First-Principles Study — •Sumit Naskar[1], Vladimiro Mujica[2], and Carmen Herrmann[1] — [1]Institute for Inorganic and Applied Chemistry HARBOR Bldg. 610 Luruper Chaussee 149, 22761 Hamburg, Germany — [2]Arizona State University, School of Molecular Sciences, PO Box 871604, Tempe, Arizona 85287-1604, USA

Electrons moving through chiral molecules are selected according to their spin orientation and the helicity of the molecule, an effect known as chiral-induced spin selectivity (CISS)[1-2]. To help elucidate the underlying mechanism, a non-equilibrium Green's function method, combined with a Landauer approach and density functional theory, is applied to carbon helices contacted by gold electrodes, resulting in spin polarization in the non-equilibrium electronic structure of the junctions[3]. While this spin polarization is small calculated with a pure exchange-correlation functional, its sign changes with the direction of the current and with the handedness of the molecule[3]. Previous studies as well as our results suggest that computationally more expensive hybrid functionals may lead to considerably larger spin polarization in the electronic structure[4]. Thus non-equilibrium spin accumulation could be a key component in understanding the CISS mechanism.

References: [1] Goehler B. et. al., Science 2011, 6019, 894.; [2] Naaman R. et al., J. Phys. Chem. Lett. 2020, 11, 3660. [3] Naskar S. et al., J. Phys. Chem. Lett. 2023, 14, 694. [4] Zoellner M. et al., J. Chem. Theo. Comput. 2020, 16, 7357