Magnetic Interfaces and Nanostructures
Room 318 - Session MI2-MoA

Emergent Magnetism at Molecular Interfaces, Chirality Induced Spin Selectivity, Molecular Magnetoresistance

Moderators: Oliver Monti, University of Arizona, **Yonatan Dubi**, Ben Gurion University of the Negev

2:30pm **MI2-MoA-5 THz Light Emission via Inverse Chiral Induced Spin Selectivity in Chiral Perovskite***, **Matthew Beard**,* The National Laboratory of the Rockies. **INVITED**

Understanding and the interconversion between spin and charge current under chirality induced spin selectivity (CISS) is critical in leverage chiral semiconductors for developing room-temperature control over spin, charge and light. CISS phenomena arise from an interplay among structural chirality, electron spin orientation, and charge current. Steady-state observations such as magnetoresistance (MR) offer little insight into the timescales that govern the spin-charge interconversion. In contrast, inverse CISS involves the conversion of spin to a charge current. Terahertz (THz) emission spectroscopy (TES) offers a non-contact probe of the induced charge current that maps the charge current direction in three dimensions. We show how the THz emission can map the spin-to-charge conversion and study THz emission in FM/chiral perovskite heterostructures. We contrast with room temperature magnetoresistance in similar films. We show that both CISS and ICISS exhibit similar symmetry, i.e., for ICISS the current direction reverses either for changing the chirality or magnetization direction. These observations directly demonstrate the inherent coupling between spin and charge currents in chiral systems. These observations suggest constraints on the CISS mechanism. For a chiral/FM interface there is spin accumulation at the interface: injection of either charge (CISS) or spin (ICISS) drives the spin configuration out of equilibrium and movement of spin (CISS) or charge (ICISS) must compensate, thus driving the spin-to-charge interconversion.

3:00pm **MI2-MoA-7 Direction-Dependent Magnetic Conductive Atomic Force Microscopy as a Probe of the Chiral-Induced Spin Selectivity Mechanism***, **Joseph A. Albro**, Noah T. Garrett, Keerthana Govindaraj, Brian P. Blook, Nathaniel L. Rosi, David H. Waldeck,* University of Pittsburgh

The chiral-induced spin selectivity (CISS) effect is the preferential transport of one electron spin orientation through a chiral material. Most measurements of CISS in films use magnetic conductive atomic force microscopy (mc-AFM) in a vertical geometry, along the substrate normal, even when the helical axis of the material lies in the plane. In that geometry it is difficult to separate spin selection that occurs during transport from models that place it at the ferromagnetic electrode interface, such as the spinterface model or a magnetization-dependent spin injection barrier. We report an mc-AFM platform that measures spin polarization along different directions in helical fibers that straddle an in-plane magnetized ferromagnetic electrode. Because the preferred spin in a chiral material is tied to the electron momentum, current-voltage curves taken to the left and to the right of the electrode probe opposite spin directions in the lab frame, and a spin polarization is obtained without reversing the magnetization. Chiral polyaniline (PANI) fibers were used to establish the working principle. For an S-PANI fiber, the longitudinal spin polarization along the helical axis was 94 +/- 0.8% with the field along +Z and 92 +/- 3.3% with the field along -Z, while the transverse polarization measured perpendicular to the fiber axis on the same fiber was 40 +/- 4.9%. R-PANI fibers gave the opposite sign. The factor of two between the longitudinal and transverse response shows that spin filtering depends

3:15pm **MI2-MoA-8 Vibrationally-Mediated Dzyaloshinskii-Moriya Interaction as the Origin of Chirality-Induced Spin Selectivity in Donor-Acceptor Molecules***, **Leonardo Celada**, Alessandro Chiesa, D. K. Andrea Phan Huu, Arianna Cantarella,* Università degli Studi di Parma, Italy*; Michael R. Wasielewski,* Northwestern University*; Paolo Santini, Stefano Carretta,* Università degli Studi di Parma, Italy

Chirality-induced spin selectivity (CISS) in photoinduced electron transfer poses a fundamental challenge: how can sizable spin polarization emerge in molecular systems with weak spin-orbit coupling and large electronic energy gaps [1]. Here we show that low-energy torsional vibrations provide a solution to this energy-scale paradox by generating a Dzyaloshinskii-Moriya interaction between the transferred electron and the donor spin during electron transfer [2].

Starting from a microscopic vibronic model for donor–chiral bridge–acceptor molecules, we derive an effective low-energy spin Hamiltonian where vibrational modulation of hopping and spin-orbit coupling produces Dzyaloshinskii-Moriya interactions comparable to isotropic exchange. This interaction mixes singlet and triplet radical-pair states and yields large spin polarization for realistic parameters, while naturally introducing the low-energy scale required to explain the magnetic-field dependence observed in time-resolved EPR experiments [3].

Numerical simulations of the electron-transfer dynamics show that this mechanism produces sizable CISS efficiencies, predicts a non-trivial temperature dependence, and explains avoided-level-crossing features controlling the field response. In contrast to purely electronic mechanisms, the effect is amplified by low-energy vibrations and remains robust under realistic thermal conditions.

These results identify vibrationally mediated spin interactions as a microscopic origin of CISS in electron transfer, reconcile apparently conflicting experimental observations, and provide experimentally testable signatures for molecular spintronics and quantum technologies [4].

This project is supported by the Horizon Europe program through the ERC-Synergy CASTLE project (proj. n.101071533).

References

[1] Bloom, B. P.; Chem. Rev. 2024, 124, 1950–1991.
[2] Chiesa, A. et al. arXiv 2604.03210 (2026).
[3] Eckvahl, H. J. Science 2023, 382, 197–201.
[4] Chiesa, A. J. Phys. Chem. Lett. 2025, 16, 5358–5365.

3:45pm **MI2-MoA-10 Enantiomer-Dependent Chiral Transport Asymmetry in KTaO3 Based Nanowires on Direction Within the Material, and That the Response Does Not Arise Solely from the Electrode Interface***, **Sayanwita Biswas**, Joseph A. Albro, Pubudu Wijesinghe, Jiangfeng Yang, Patrick Irvin, Chang-Boem Eom, Jeremy Levy,* University of Pittsburgh

Chirality-induced spin selectivity has been studied for three decades, almost exclusively in molecules, where the handedness of the conductor is fixed by synthesis and the achiral control is a separate compound. Here we write chiral nanowires at the $LaAlO_3/KTaO_3$ interface using a conductive atomic force microscope, with a construction in which a lateral meander of the tip path and a modulation of the writing voltage share one period, and the phase between them sets the handedness. We find that the four-terminal current-voltage characteristic of such a nanowire depends on the current drive direction. This drive-direction dependence produces a difference in conductance for a helical nanowire that is absent in a straight nanowire, and also absent when current flows through two oppositely handed nanowires in series. The conductance difference has opposite sign for the two enantiomers and persists from 70 mK to 300 K and from zero to finite magnetic field. The same construction at $LaAlO_3/SrTiO_3$ shows little difference between the two drive directions. We attribute the transport asymmetry to an accumulated Berry phase that is odd in handedness.

4:00pm **MI2-MoA-11 Spin-dependent Charge Transport in Single-Molecule Junctions of a-helical Peptide Sequences***, **Ismael Diez Perez**,* King's College London, UK*; Vladimiro Mujica,* Arizona State University*; Wenzhu Kuang, Qiankun Wang,* King's College London, UK*; Mario Galante,* Arizona State University*; Albert Cortijos,* University of Barcelona, Spain **INVITED**

In this contribution, we will present our latest experimental results on spin-dependence charge transport through single-molecule electrical contacts made with chiral alpha-helical peptide backbones. We synthesize a series of a-helical peptides sequences of varying lengths, *i.e.*, from 6 to 22 amino acids and their two corresponding D- and L-optical isomer, all bearing the repeating pattern (H_2N-Cys(Acm)-**(**Glu-Ala-Ala-Ala-Lys**)**$_n$-NH-CH_2-CH_2-SH). The peptide is flanked by two axial thiol groups; an Acm (acetamidomethyl)-protected *Cys*(-SH) residue and a alkanethiol terminal group. The chosen specific sequence presents an a-helix favored conformation in the working polar mixture water : TFE (trifluoroethanol). We use a magnetic STM break-junction approach we have previously exploited to measure magnetoresistance in a single-molecule contact[1,2]. This approach allows us to trap individual a-helical peptide between two metal beads (namely, a Au and a ferromagnetic Ni electrode) oriented along the main helix axis though the two side thiol groups specifically binding to the two metal electrodes. We are then able to inject spin-polarized electrons from the ferromagnetic Ni to individual a-helical chiral structures and measure the conductance as a function of the Ni magnetization direction. The analysis of the single-peptide charge transport results provides an intuitive picture combining both CISS and spinterface effects that has enough flexibility to accommodate the description of the observed differences in magnetoresistance as a function of the peptide

chirality[3]. The latter picture is then studied as a function of well-known structural drivers of the CISS/Spinterface manifestation such as the electric dipole direction of the helical structure[4], the molecular length and the secondary structure[5]. We hope our work demonstrates the feasibility of our single-molecule platform to study fundamental mechanisms of spin-dependent transport in chiral biomolecular motifs, and proposes to expand the studies to more complex metalloproteins with redox-dependent functions where the electron spin might play a key quantum biological role.

[1] A.C. Aragonès *et al. Nano Lett.* **2016**, 16, 218

[2] A.C. Aragonès *et al. JACS* **2017***,* 139, 5768

[3] A.C. Aragonès *et al. Small* **2016***, DOI: 10.1002/smll.201602519*

[4] A.C. Aragonès*et al. JACS* **2025***,* 147, 36453

[5] W. Kuang *et al.* **2026***in preparation.*

4:30pm **MI2-MoA-13 The Role of Electron Correlations in Chirality-Induced Spin Selectivity of Molecular Junctions***, **Aadi Konidena,*** King's College London, UK

Chirality-induced spin selectivity is an exciting phenomenon where the geometry of helicoid molecules evidently determines the resulting electron spin when a current is driven through the molecule. Despite experimental backing, the details of the primary mechanism that drives spin selection is still not understood. In fact, theoretical simulations based on spin-orbit coupling alone still disagree substantially with experimental data, prompting the investigation into alternate rationales for the observed spin-polarised current. To assess the possible role of the electron-electron correlation effects in current spin polarisation, we study the quantum transport through a molecular junction with Hubbard interactions added on each site of a helical molecule alongside the spin-orbit coupling. We employ the Non-Equilibrium Green's Function formalism and Feynman diagram technique to account for the Hubbard interactions within the Second Born approximation. To calculate the spin current as a function of the temperature and the applied bias, our treatment goes beyond the simple Landauer approach and incorporates the Hubbard self-energies in the equation for the full current.

4:45pm **MI2-MoA-14 Strong Paramagnetic Correlation in Spin Crossover Molecular Complex in a Matrix of Polyaniline***, **Wai Kiat Chin***[1]*,* University of Nebraska-Lincoln, Malaysia*; Mohammad Zaid Zaz,* University of Nebraska-Lincoln, India*; Sartaz Sarkib,* University of Nebraska-Lincoln, Bangladesh*; Faruk Soso,* Tuskegee University, Nigeria*; Ignatius Ebo-Quansah,* Tuskegee University, Ghana*; Peace Ikeoluwa Adegbite,* University of Nebraska-Lincoln, Nigeria*; Gauthami Viswan,* University of Nebraska-Lincoln, India*; Arjun Subedi,* University of Nebraska-Lincoln, USA, Nepal*; Alpha T. N'Diaye,* Lawrence Berkeley National Lab*; Vijay Rangari,* Tuskegee University*; Rebecca Lai, Peter Dowben,* University of Nebraska-Lincoln, USA

To investigate the paramagnetic correlation length of a spin crossover complex, a tri-composite system of Fe(Phen)2(NCS)2 plus polyaniline plus NiCo2O4 magnetic nanoparticles were fabricated. Owing to its anti-ferromagnetic coupling nature between the Fe(Phen)2(NCS)2 and NiCo2O4, the paramagnetic correlation length can be evaluated, which is estimated to be 20.1nm. Such a long paramagnetic correlation length, in a disordered molecular system which has no free electron density to mediate the exchange, is extraordinary.

5:00pm **MI2-MoA-15 A Theoretical Model for Surface Chirality Sensors - Tribute to Vladimiro Mujica***, Vladimiro Mujica, **Oliver Monti,*** Arizona State University*; Jonatan Dubu,* Ben Gurion University, Israel

We present a theoretical approach to the design of surface chirality sensors, based on a model of spin-dependent van der Waals interactions between chiral molecules, and the physics of spinterface effects. This combination of theoretical approaches allow us to describe both the physisorption and the chemisorption regimes, and the possibility of comparing with experiments designed to achieve chiral recognition, both through measurements of absorption energies and magnetic interactions.

[1] **Falicov Student Award Finalist**

Author Index

Bold page numbers indicate presenter

— A —
Albro, Joseph A.: MI2-MoA-10, 1; MI2-MoA-7, **1**
— B —
Beard, Matthew: MI2-MoA-5, **1**
Biswas, Sayanwita: MI2-MoA-10, **1**
Blook, Brian P.: MI2-MoA-7, 1
— C —
Cantarella, Arianna: MI2-MoA-8, 1
Carretta, Stefano: MI2-MoA-8, 1
Celada, Leonardo: MI2-MoA-8, **1**
Chiesa, Alessandro: MI2-MoA-8, 1
Chin, Wai Kiat: MI2-MoA-14, **2**
Cortijos, Albert: MI2-MoA-11, 1
— D —
Diez Perez, Ismael: MI2-MoA-11, **1**
Dowben, Peter: MI2-MoA-14, 2
Dubu, Jonatan: MI2-MoA-15, 2
— E —
Ebo-Quansah, Ignatius: MI2-MoA-14, 2
Eom, Chang-Boem: MI2-MoA-10, 1
— G —
Galante, Mario: MI2-MoA-11, 1
Garrett, Noah T.: MI2-MoA-7, 1
Govindaraj, Keerthana: MI2-MoA-7, 1
— I —
Ikeoluwa Adegbite, Peace: MI2-MoA-14, 2
Irvin, Patrick: MI2-MoA-10, 1
— K —
Konidena, Aadi: MI2-MoA-13, **2**
Kuang, Wenzhu: MI2-MoA-11, 1
— L —
Lai, Rebecca: MI2-MoA-14, 2
Levy, Jeremy: MI2-MoA-10, 1
— M —
Monti, Oliver: MI2-MoA-15, **2**
Mujica, Vladimiro: MI2-MoA-11, 1; MI2-MoA-15, 2
— P —
Phan Huu, D. K. Andrea: MI2-MoA-8, 1
— R —
Rangari, Vijay: MI2-MoA-14, 2
Rosi, Nathaniel L.: MI2-MoA-7, 1
— S —
Santini, Paolo: MI2-MoA-8, 1
Sarkib, Sartaz: MI2-MoA-14, 2
Soso, Faruk: MI2-MoA-14, 2
Subedi, Arjun: MI2-MoA-14, 2
— T —
T. N'Diaye, Alpha: MI2-MoA-14, 2
— V —
Viswan, Gauthami: MI2-MoA-14, 2
— W —
Waldeck, David H.: MI2-MoA-7, 1
Wang, Qiankun: MI2-MoA-11, 1
Wasielewski, Michael R.: MI2-MoA-8, 1
Wijesinghe, Pubudu: MI2-MoA-10, 1
— Y —
Yang, Jiangfeng: MI2-MoA-10, 1
— Z —
Zaz, Mohammad Zaid: MI2-MoA-14, 2