Magnetic Interfaces and Nanostructures
Room 318 - Session MI2-MoA

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

Moderators: Prof. Oliver Monti, University of Arizona, **Prof. 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 Toward Spin Selectivity in Solids - Efficient Charge-to-Spin Conversion and Long Spin Lifetimes in Chiral Crystals***, **Jagoda Slawinska**,* University of Groningen, Netherlands

Chiral crystals, which lack inversion and mirror symmetries, offer unique ways for controlling electron spin using purely electrical means. In these systems, chirality gives rise to charge-to-spin conversion in which spin accumulation aligns parallel or antiparallel to the applied current, resembling the chirality-induced spin selectivity (CISS) observed in molecular systems.

Our recent studies have shown that in semiconducting tellurium, chirality leads to remarkably efficient charge-to-spin conversion accompanied by long-range spin transport. These two properties, traditionally viewed as mutually exclusive, are reconciled through the emergence of slow collective relaxation modes (“slow relaxons”), which suppress spin dephasing despite strong spin-orbit coupling.

Building on these results, we explore how chirality impacts spin accumulation across a broader class of chiral materials. In both semiconducting and metallic chiral systems, including Te, $TaSi_2$, OsSi, and $NiTa_3S_6$, symmetry-enforced persistent spin textures remain robust over large regions of the Brillouin zone, enabling efficient spin generation and enhanced spin lifetimes.

These findings establish chiral crystals as a solid-state platform for CISS-like spin physics and highlight chirality as a powerful approach for achieving efficient spin generation and robust spin transport in quantum materials.

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Acknowledgment

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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

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[2] Chiesa, A. et al. arXiv 2604.03210 (2026).
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3:30pm **MI2-MoA-9 Unconventional Spintronics from Chiral Perovskites to Altermagnets***, **Igor Zutic**,* University at Buffalo

With the growing class of materials that support spin-polarized carriers, current, and excitations, it is possible to envision emerging spintronic applications that are not limited to net magnetization and magnetoresistance. Here we focus on chiral perovskites with no net magnetization where the space-inversion and mirror symmetries are broken to induce chiral structure. The known importance of these perovskites is further expanded by the demonstration of the chiral-induced spin selectivity (CISS). However, the generation of the spin-polarized carriers across the interface with these chiral perovskites remains to be fully understood. Our first-principles studies for two-dimensional PbBr4-based chiral perovskites provide their electronic structure and an orbital-based symmetry analysis, which allows us to establish an effective Hamiltonian to elucidate the underlying origin of their chirality [1]. The resulting chiral proximity effect can be viewed as an equilibrium precursor to CISS and an element in materials design through proximity effects [2]. We also use this analysis for electrical generation of the nonequilibrium spin polarization in many materials, which in chiral perovskites could be a mechanism contributing to CISS. To accurately obtain optical properties and

excitonic energies in these materials, we combine quasi-particle self-consistent Green function framework for calculating the self-energy of the many-body from first principles together with the Bethe-Salpeter equations [1,3]. Furthermore, by examining optical properties of chiral perovskites and the opportunity to use them to realize tunable altermagnets [4], another class of zero-magnetization spintronic materials, we put forth a versatile materials platform for unconventional spintronics and proximity effects [5].

1. Y. Liu et. al, Adv. Funct Mater. 35 e09127 (2025)

2. I. Zutic et al., Mater. Today 22, 85 (2019)

3. D. Pashov et al., Comput. Phys. Commun. 249,107065 (2020)

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3:45pm **MI2-MoA-10 Chiral Nanoparticles as a Platform for Probing the CISS Effect***, **Elizabeth Shiby**, Brian Bloom,* University of Pittsburgh, USA

The chiral-induced spin selectivity (CISS) effect, which links molecular chirality and electron spin, holds considerable promise for next-generation room-temperature spintronic devices, quantum computing, and beyond. Despite significant progress, the factors governing this phenomenon and its full range of applications remain incompletely understood. Using chiral nanoparticles as a versatile material platform, we present two studies that, together, identify key factors controlling the CISS response. In the first study, we employ chiral CdSe quantum dots to show that the chiral strength of a material is a critical determinant of the CISS response, which we experimentally validate using a combination of spin-polarized charge current measurements via magnetic conductive atomic force microscopy (mcAFM) and pure spin current measurements via ferromagnetic resonance (FMR). Building on this, the second study demonstrates that dopants can further modulate the CISS response beyond the effect of chirality alone, using lanthanide-doped CdS quantum dots as a model system; crucially, this modulation is strongly governed by the nature of the electronic and magnetic coupling between the dopant and the host lattice.

Collectively, these studies advance our understanding of the structural and chemical factors that govern the CISS effect and highlight its potential to enable new classes of functional nanomaterials.

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,* King's College Lonodon, UK*; 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.

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[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 Electron Spin, Chiral Symmetry Breaking, and Life's Homochirality***, **Furkan Ozturk**,* Caltech **INVITED**

Electron spin couples strongly to molecular chirality through the recently discovered phenomenon of chiral-induced spin selectivity. As such, spin-polarized magnetic surfaces can function as robust chiral reagents and facilitate asymmetric processes. I will discuss recent experiments that exploit the strong coupling between electron spin, molecular chirality, and chiral phonons, as well as explain their relation to life's homochirality—one of the grandest challenges in origin-of-life research since Pasteur's discovery of molecular chirality more than 175 years ago.

5:30pm **MI2-MoA-17 A Theoretical Model for Surface Chirality Sensors***, **Vladimiro Mujica**,* Arizona State University

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