Magnetic Interfaces and Nanostructures
Room 318 - Session MI-MoM

Advanced Magnetic Materials in Low Dimensional Structures I

Moderators: Dr. Valeria Lauter, Oak Ridge National Laboratory, **Prof. Dr. Markus Donath**, Muenster University, Germany

10:00am **MI-MoM-1 Bringing Materials-Specific Clarity to the Debate on Magnetism in RuO_2, *Bharat Jalan,*** University of Minnesota, USA **INVITED**

RuO_2, a rutile 4d-transition metal oxide, exhibits a unique crystal structure with both edge- and corner-sharing octahedra. This intrinsic anisotropy, when combined with strain engineering, provides a powerful avenue for tuning anisotropic electronic and optical properties. However, from a synthesis perspective, challenges such as variable Ru valence states, Ru/O stoichiometry control, anisotropic strain states, and structural defects can make it difficult to distinguish intrinsic properties from extrinsic effects in RuO_2 thin films – a classic trick in the pursuit of novel functionalities in quantum materials. In this talk, I will highlight our group's efforts in overcoming these synthesis challenges while demonstrating metallicity in epitaxial RuO_2 films down to the unit cell scale. Through a combination of advanced X-ray scattering, X-ray absorption spectroscopy, transmission electron microscopy, temperature-dependent transport, magneto-optical measurements, and density functional theory (DFT) calculations, we uncover robust magnetism in epitaxially strained RuO_2, consistent with an altermagnetic metallic phase [1-4]. Additionally, we reveal a novel polar phase in strained films with significant implications for electrical transport – an unexpected treat in the realm of functional oxides. I will discuss these findings in detail, emphasizing their sensitivity to material defects and structure – key ingredients that are often overlooked but crucial in determining emergent quantum phenomena.

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4. S. G. Jeong, B. Y. X. Lin, M. Jin, I. H. Choi, S. Lee, Z. Yang, S. Nair, R. Choudhary, J. Parikh, A. Santhosh, M. Neurock, K. A. Stoerzinger, J. S. Lee, T. Low, Q. Tu, J. M. LeBeau, and B. Jalan,**Strain-Stabilized Interfacial Polarization Tunes Work Function Over 1 eV in RuO_2/TiO_2Heterostructures,** *Nat. Commun. 17, 2516 (2026)*

10:30am **MI-MoM-3 Compositionally Tunable Synthesis of High-Entropy Transition Metal Dichalcogenides Exhibiting Above-Room-Temperature Magnetism*, Xiahua Zhong,*** *Chen Zhang,* University of Missouri-Columbia*; Zheng Gai, Huan Zhao,* Oak Ridge National Laboratory, USA*; Yingchao Yang,* University of Missouri-Columbia

As silicon-based electronics approach their physical limits, spintronics, leveraging electron spin rather than charge, offers a promising path for next-generation information technologies. Realizing this potential requires two-dimensional (2D) materials with robust and tunable room-temperature magnetism. Here, we report a two-step synthesis strategy for fabricating 2D high-entropy transition metal dichalcogenides (HE-TMDs) incorporating magnetic elements beyond conventional groups 4-6. High-entropy layered double hydroxides (HE-LDHs) are first synthesized via hydrothermal coprecipitation, enabling atomic-level mixing of diverse transition metals across groups 4-12. Subsequent chalcogenization yields 2D HE-TMDs while preserving homogeneous elemental distribution. This approach circumvents the constraints of high-temperature and vapor-phase methods, enabling the synthesis of compositionally complex and structurally controlled 2D magnets. Representative $V_\alpha Cr_\beta Fe_\gamma Co_\delta Ni_{1-\alpha-\beta-\gamma-\delta} S_{2-x}$ exhibits robust ferromagnetism above room temperature, demonstrating the potential of this high-entropy design strategy to expand the family of 2D magnetic materials for spintronic applications.

10:45am **MI-MoM-4 Anomalous Hall Effect in Antiferromagnetic Dirac Semimetal $EuCu_2Sb_2$, *Souvik Sasmal,*** Argonne National Lab

Magnetic Dirac semimetals—where Dirac fermions are protected by combined crystalline and magnetic symmetries—remain experimentally rare, despite intense theoretical interest. In this work, we identify EuCu2Sb2 as a promising candidate hosting Dirac-like electronic states in proximity to magnetic order. Temperature-dependent transport and magnetization measurements reveal an A-type antiferromagnetic transition at 5.1 K, accompanied by anisotropic resistivity, spin reorientation, and weak anomalous Hall features. Angle-resolved photoemission spectroscopy (ARPES) reveals linear Dirac-like band crossings at the X point, already present in the paramagnetic phase. First-principles calculations support a topological band inversion near the Fermi level and confirm the origin of the Dirac dispersion. These findings establish EuCu2Sb2 as a rare material system that bridges topological band structure with localized magnetism, offering a platform to explore symmetry-protected Dirac states in correlated magnetic materials.

11:00am **MI-MoM-5 Revisiting Altermagnetism in RuO2 and Cr-doped RuO2 Epitaxial Films through THz Spectroscopy and Neutron Scattering*, David T. Plouff, Nawsher J. Parvez,*** Department of Physics and Astronomy, University of Delaware*; Laura Scheuer,* Department of Physics and Astronomy, University of Delaware, Germany*; Shreya Shrestha,* Department of Physics and Astronomy, University of Delaware*; Weipeng Wu,* Department of Physics and Astronomy, University of Delaware, China*; subhash Bhatt,* University of Delaware*; Xinhao Wang,* University of Delaware, China*; Lars Gundlach, M. Benjamin Jungfleisch,* University of Delaware*; Xixiang Zhang,* King Abdulah University of Science and Technology, Saudi Arabia*; Adam A. Aczel,* Oak Ridge National Laboratory, USA*; Jonathan Gaudet,* National Institute for Science and Technology (NIST)*; **John Q. Xiao**,* University of Delaware **INVITED**

Altermagnetism has recently emerged as a potentially transformative concept in spintronics, offering the possibility of combining the ultrafast dynamics of antiferromagnets with spin-split electronic structures typically associated with ferromagnets. Among proposed candidates, rutile RuO_2 has attracted intense attention because of predictions of unconventional spin transport. However, despite intense activity, the existence of an intrinsic altermagnetic order in RuO_2 remains highly controversial.

In this talk, we will present our systematic experimental investigation of epitaxial RuO_2 and $Ru_{1-x}Cr_xO_2$ thin films using terahertz and neutron-scattering measurements. Time-domain THz spectroscopy measurements on RuO_2 reveal that previously reported spintronic signatures can be consistently explained by conventional mechanism, including inverse spin Hall effects and anisotropic electronic conductivity associated with the rutile crystal structure, without invoking altermagnetic order. Motivated by theoretical predictions that hole doping may stabilize an altermagnetic state, we further probed magnetic state in $Ru_{1-x}Cr_xO_2$ thin films by using neutron scattering techniques.Our measurements show no evidence of long-range magnetic ordering down to 10 K in $Ru_{0.8}Cr_{0.2}O_2$ thin films, placing important experimental constraints on current theoretical models of altermagnetism in rutile oxides.

Beyond resolving the magnetic ground state, our work also reveals a new THz emission mechanism originating from the interplay between spintronic THz generation and anisotropic electronic transport in RuO_2. This hybrid mechanism enables magnetic-field tuning of the polarization ellipticity of emitted THz radiation, opening new opportunities for functional THz emitters based on correlated oxide materials.

This research was sponsored by NSF DMR-2316664, NSF through the University of Delaware Materials Research Science and Engineering Center (MRSEC), and King Abdullah University of Science and Technology (KAUST), ORFS-2022-CRG11-5031.2.

11:30am **MI-MoM-7 Cobalt Doping on Topological Superconductor $FeTe_{0.55}Se_{0.45}$, *John Drain*[1],** University of Wyoming*; Mykola Telychko,* Oak Ridge National Laboratory*; Zheng Gai,* Oak Ridge Natinal Laboratory*; TeYu Chien,* University of Wyoming

$FeSe_xTe_{1-x}$ (FTS) is an iron-based superconductor that has been shown to have non-trivial topology with the correct relative Te/Se content ($FeTe_{0.55}Se_{0.45}$) and relatively high superconducting transition temperature,

[1] **Falicov Student Award Finalist**

T_C, of 14.5 K. Majorana zero modes (MZM), a quasiparticle needed for the development of topological quantum computing, have also been observed in magnetic vortices as well as at Fe adatom sites in FTS. Thus, the introduction of new magnetic elements to FTS is of particular interest, due to their potential to influence the formation of MZM and local topology. In this study, the effects of depositing magnetic Co atoms on the FTS surface are explored using scanning tunneling microscopy. We observe an apparent surface reconstruction after cobalt deposition with Co adatoms on top of the surface as well as defects from evident Co absorption. Areas with high concentration of Co defects show suppressed superconductivity. When superconductivity is preserved, in-gap bound states are observed at Co defect sites at either finite energy or zero energy. Furthermore, the energy of these finite energy states shifts to zero as the tunnel-barrier conductance of the STM tip is increased during spectroscopy measurements. The origins of these features as MZM, Yu-Shiba-Rusinov bound states, or Kondo effect will be discussed. These results present a potential prospect for a way to influence FTS properties locally through the introduction of Co to produce conditions ideal for Majorana zero mode and their braiding.

This work was funded by the NSF through Award #: DMR-2228841

11:45am **MI-MoM-8 Magnetic and Magnetostrictive Properties of Multilayer $Fe_{50}Co_{50}$ – Ag with Varied Ag Thickness**, ***Thomas Mion,*** US Naval Research Laboratory*; Margo Staruch,* US naval Research Laboratory*; Zoey Warecki,* us naval Research Laboratory*; Konrad Bussmann, Peter Finkel,* US Naval Research Laboratory

Temperature stable high magnetostrictive materials are required for microelectromechanical systems (MEMS) devices that seek to function reliably at high temperatures. Due to the immiscibility of Ag with Fe and Co, multilayers of $Fe_{50}Co_{50}$ – Ag will not alloy up to at least 700 C allowing for a stable high magnetostrictive material for MEMS platforms. $Fe_{50}Co_{50}$ is known to be moderately magnetostrictive and with a curie temperature ~1,000 C and a high saturation magnetization. Previous studies have shown with ~10nm $Fe_{50}Co_{50}$ and ~3nm Ag layers the multilayer system remains up to 400 C where higher temperatures cause breakdown of the Ag interlayer. This investigation seeks to improve the thermal stability of the FeCo-Ag multilayer system through varied Ag thickness and understand the mechanism of the nonmagnetic layer breakdown. Transmission Electron Microscopy investigations reveal the Ag layer is coherent up to 77 multilayers (~930 nm) even with increased roughness as the thickness increases resulting in the restricted in-plane magnetization and subsequent lower coercive field.

Magnetic Interfaces and Nanostructures
Room 318 - Session MI1-MoA

Advanced Magnetic Materials in Low Dimensional Structures II

Moderators: Prof. Dr. Markus Donath, Muenster University, Germany, **Dr. Valeria Lauter**, Oak Ridge National Laboratory

1:30pm **MI1-MoA-1 Observation of Mirror-Odd and Mirror-Even Spin Texture in Ultra-Thin Epitaxially-Strained RuO_2 Films**, *Ming Yi,* Rice University*; **Yichen Zhang**,* Caltech **INVITED**

Recently, rutile RuO_2 has attracted renewed interest due to expectations of prominent altermagnetic spin-splitting. However, accumulating experimental evidence suggests that in its bulk and thick-film forms, RuO_2 does not display any form of magnetic ordering. Despite this, the spin structure of RuO_2 remains largely unexplored in the ultra-thin limit, where substrate-imposed epitaxial strain can be substantial. Here, we employ spin-resolved angle-resolved photoemission spectroscopy, supported by ab-initio calculations, to reveal the electronic structure of 2.7~nm-thick epitaxial RuO_2 heterostructures. We observe an unconventional spin texture characterized by the coexistence of mirror-even and mirror-odd momentum-dependent components. A comprehensive symmetry analysis rules out nonmagnetic origins of this spin texture. These findings suggest an emergent non-relativistic spin structure enabled by epitaxial strain in the ultra-thin limit, marking a distinct departure from the behavior of relaxed or bulk RuO_2. Our work opens new perspectives for exploring symmetry-breaking mechanisms and spin textures in oxide heterostructures.

2:00pm **MI1-MoA-3 On the Sign of the Rashba Parameter in Image-Potential States**, ***Markus Donath***, *Fabian Schöttke,* University of Münster, Germany*; Kaishu Kawaguchi,* University of Tokyo, Japan*; Kenta Kuroda,* Hiroshima University, Japan*; Peter Krüger, Thorsten Deilmann,* University of Münster, Germany*; Ayumi Harasawa, Shuntaro Tani, Yohei Kobayashi, Takeshi Kondo,* University of Tokyo, Japan

For spintronic devices, spin manipulation without external magnetic fields is highly desirable. At surfaces and two-dimensional materials, the spin degeneracy of electronic states can be lifted by the Rashba effect. The Rashba effect in surface states at high-*Z* materials is related to both the strong spin-orbit interaction in heavy atoms and the orbital angular momentum arising from the inversion-symmetry breaking at the surface. Image-potential surface states are simple model systems, where spin-dependent effects can be studied in view of spintronic applications. Our study on Bi_2Se_3 and Bi_2Te_3 showcases that the orbital angular momentum causes an intrinsically reversed Rashba parameter $\alpha_R \approx -100$ meV Å, i.e., a reversed spin splitting compared with the prototypical Rashba-split Au(111) crystal-induced surface state [1] or the image-potential state at Re(0001) [2]. The sign of α_R is decisive for controlling the absolute spin directions in view of spintronic devices. We present a consistent picture of spin-resolved experimental data from inverse photoemission and three-photon photoemission together with calculations from density-functional theory and many-body perturbation theory.

[1] M. Hoesch *et al.*, Phys. Rev. B **69**, 241401(R) (2004); S. N. P. Wissing *et al.*, New J. Phys. **15**, 105001 (2013).
[2] F. Schöttke *et al.*, Phys. Rev. B **105**, 155419 (2022).

2:15pm **MI1-MoA-4 High Magnetocrystalline Anisotropy-Driven Fuel Cell Electrocatalysis in PtPdFe Intermetallic Alloys**, *Muhammad Irfansyah Maulana,* ***Jong-Sung Yu***, DGIST, Republic of Korea

Ordered Pt-based intermetallic alloys are emerging as efficient oxygen reduction reaction (ORR) electrocatalysts in hydrogen fuel cells, outperforming their disordered counterparts. However, the intrinsic role of atomic ordering in governing ORR catalytic performance remains unclear. In this work, we report ferromagnetic PtPdFe ternary intermetallics with structurally ordered tetragonal $L1_0$ and cubic $L1_2$ phases (Figure 1a), each featuring distinct crystal structures and atomic arrangements. Our study highlights magnetocrystalline anisotropy as a key structure-dependent descriptor that governs ORR activity in these alloys. Electrochemical half- and single-cell tests reveal that $L1_0$-PtPdFe magnetic intermetallic catalysts (MICs) deliver higher ORR activity than their $L1_2$ counterparts (Figure 1b). Combined experimental and theoretical analyses attribute this enhancement to the unique tetragonal $L1_0$ structure, where strong 5d–3d orbital interactions along the c-axis induce ferromagnetic ordering and elevate magnetocrystalline anisotropy energy, thereby accelerating ORR kinetics. Furthermore, membrane electrode assemblies fabricated by $L1_0$-PtPdFe cathode MICs sustain fuel cell performance beyond the 2025 US Department of Energy stability targets under H_2–O_2, H_2–air, and H_2–N_2 conditions. These findings establish a new design principle for Pt-based intermetallic catalysts, demonstrating that magnetic anisotropy arising from ferromagnetic ordering can be strategically harnessed to optimize fuel cell performance.

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.

References:

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2. B. Kilic, S. Alvarruiz, E. Barts, B. van Dijk, P. Barone, J. Sławińska, *Universal symmetry-protected persistent spin textures in nonmagnetic solids*, Nature Communications 16, 7999 (2025)
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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).
[3] Eckvahl, H. J. Science 2023, 382, 197–201.
[4] Chiesa, A. J. Phys. Chem. Lett. 2025, 16, 5358–5365.

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)
4. X. Duan et al., Phys. Rev. Lett. 134, 106801 (2025)
5. Z. Zhu et al., Phys. Rev. Lett. 136, 186702 (2026)

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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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**

Magnetic Interfaces and Nanostructures
Room Ballroom A - Session MI-ThP

Magnetic Interfaces and Nanostructures Poster Session

MI-ThP-1 Wilson Loop as a Tool to Investigate Chirality-Induced Spin Selectivity: Role of Vibrations and Multiple Channels, ***Leonardo Celada***, *D. K. Andrea Phan Huu, Alessandro Chiesa, Paolo Santini, Luca Griguolo, Stefano Carretta,* Università degli studi di Parma, Italy

Chirality-induced spin selectivity (CISS) has been observed in a wide range of chiral molecular systems, yet the minimal microscopic ingredients required for spin polarization remain debated [1]. Here we introduce the Wilson loop as a general theoretical criterion to identify when spin polarization can emerge in model Hamiltonians relevant to CISS.

Using open tight-binding models with spin-orbit coupling, we show that the Wilson loop provides a gauge-invariant characterization of spin-dependent interference and recovers the known absence of CISS in single-channel purely electronic models, where a local spin gauge transformation removes all spin dependence. By contrast, non-trivial Wilson loops arise in systems with multiple transport channels, providing a direct symmetry-based criterion for finite spin polarization, consistent with previous theoretical studies of CISS mechanisms [2].

We then extend this framework to electron-vibration models and show that vibronic pathways can generate non-trivial Wilson loops even in nominally single-channel systems. In particular, Peierls-type coupling creates spin-dependent interference in vibronic space and enables CISS, whereas Holstein coupling preserves a trivial Wilson loop and cannot induce spin polarization. This establishes a distinction between vibrational mechanisms proposed in the literature [3].

Beyond reproducing known results, the Wilson-loop formulation provides a unifying path-based picture connecting gauge structure, interference, and spin selectivity across electronic and vibronic mechanisms. The framework can be generalized to arbitrary molecular architectures and offers a tool to identify necessary conditions for CISS in transport and electron-transfer settings, including systems where spin selectivity has recently been observed experimentally [4].

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

References

[1] Naaman, R. Nat. Rev. Chem. 2019, 3, 250.
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[4] Eckvahl, H. J. Science 2023, 382, 197–202.

MI-ThP-2 Experimental Insights into Spin-Driven Correlated Phase Transitions in CrN, ***Khan Alam***, Department Of Physics, Kfupm, Saudi Arabia*; Arthur Smith,* Department of Physics

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Abstract

Chromium nitride (CrN) is an important transition metal nitride that serves as a model system for studying correlated structural, electronic, and magnetic phase transitions. The coupling among these transitions makes CrN a compelling example of a correlated material in which magnetic spin ordering plays a central role in driving the observed transformations. Upon cooling, CrN undergoes a first-order transition involving antiferromagnetic spin ordering, along with structural and electronic transitions. These structural, electronic, and magnetic transitions are not independent but strongly intertwined, offering insight into the mechanisms of magnetostructural coupling in correlated electron systems.

Our experimental investigations of these coupled transitions in CrN include neutron diffraction, reflection high-energy electron diffraction, variable-temperature x-ray diffraction, electronic transport measurements, and scanning tunneling microscopy, we probe the evolution of structural symmetry, magnetic spin order, and electronic states across the transition. The results elucidate how spin ordering triggers and stabilizes the structural and electronic phase transitions, highlighting the cooperative nature of these coupled phenomena. These findings not only deepen our understanding of CrN but also shed light on the broader class of correlated transition metal nitrides that exhibit intertwined spin-lattice-charge interactions.

Acknowledgements

This work was supported by the Deanship of Research Oversight and Coordination of King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia under grant No. INSE2615.

MI-ThP-3 Utilizing MOKE Magnetometry to Observe Properties of Magnetic Thin Films, ***Ivan Gray***, *Seth Woodwyk, Femi Akinrinola, Raj Bhandari, Jeremy Fanelli, Mikel Holcomb,* West Virginia University

In the study of thin film materials, magnetometry can be a powerful tool for understanding the magnetic properties and interactions of materials, though most widely available magnetometers are designed for bulk materials, so surface level probing at a focused point can be difficult. The magneto-optical Kerr effect (MOKE), however, offers a surface-sensitive alternative to bulk magnetometry techniques. MOKE is a magneto-optic phenomenon that results from interactions between light and the magnetization of a material. A magnetized material will experience differing refractive indices for left and right-circularly polarized light due to the off-diagonal tensorial elements of the dielectric constant of the material. As light reflects from this material, the two circularly polarized components are reflected with varying amplitudes and phase shifts, resulting in a changed polarization state of the reflected light. This is described by both the Kerr rotation, the angle in which the original polarization is rotated, and the Kerr ellipticity, describing the resulting elliptical polarization. Changes in these properties can be observed over a range of applied fields, showing the magnetic hysteresis of the material, noted as Kerr magnetometry. We are using this method to explore the mechanisms behind spontaneous magnetization reversal (SMR) in single layer thin films of $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) grown on $SrTiO_3$ (STO). SMR is more commonly seen in multilayer systems, while it has only been reported in a few single layer systems. In SMR, competing magnetic interactions under a cooling or applied field can result in the net magnetization reversing direction relative to the field. In particular, LSMO exhibits SMR both at low applied magnetic fields and near room temperature, allowing for potential real-world applications. Understanding how the mechanisms driving SMR in LSMO work will inform the design of future devices that exploit SMR under practical operating conditions.

MI-ThP-4 Early-Stage Experimental Training in Magnetism: A Hands-On Freshman Research Course as a Gateway to Advanced Magnetic Materials, ***Mikel Holcomb***, West Virginia University*; Femi Akinrinola,* West Virginia University, USA*; Robbyn Trappen, Seth Woodwyk, Ivan Gray, Tap Raj Bhandari, Jeremy Fanelli, Dorian Davis, Nethmi Kankanamge, John Stewart,* West Virginia University

The development of advanced magnetic materials and low-dimensional magnetic systems relies critically on a skilled experimental workforce capable of integrating measurement and data interpretation at early stages of training. I describe a hands-on freshman-level research course designed to introduce students to experimental magnetism through direct engagement with measurement techniques and a variety of magnetic systems. In this course, students perform studies on magnetic materials, with an emphasis on data acquisition and physical interpretation. Projects are structured to connect fundamental concepts—such as magnetic anisotropy, hysteresis and types of magnetism—to experimental observables, providing an entry point into phenomena central to modern magnetism research. Students develop experimental intuition through open-ended investigations that reflect the uncertainty and exploratory nature of contemporary research, with each project structured as a potentially extensible research direction. I will discuss course design, representative experiments, and evidence for improved student readiness for research in physics and materials science. This model suggests a pathway for broadening participation and accelerating training in areas aligned with emerging challenges in magnetic interfaces and nanostructures. This work is supported by NSF DUE 2417349.

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