

Magnetic Interfaces and Nanostructures Room 121 - Session MI+2D+AC+TF-WeM

Altermagnetism and Spin-Dependent Systems

Moderators: Markus Donath, Muenster University, Germany, Valeria Lauter, Oak Ridge National Laboratory

8:00am **MI+2D+AC+TF-WeM-1 Twisted Electrons in Momentum Space: A Photoemission Perspective on Spin and Orbital Angular Momentum in Quantum Materials**, Maximilian Ünzelmann, University of Würzburg, Germany; B. Geldiyev, University of Würzburg, Germany; T. Figgemeier, University of Würzburg, Germany; H. Bentmann, NTNU Trondheim, Norway; F. Reinert, University of Würzburg, Germany

INVITED

Beyond the spin, electronic states in crystalline solids can exhibit finite expectation values of orbital angular momentum (OAM). This phenomenon has attracted considerable attention in recent years and can particularly be traced back to the following key applications: (i) Since OAM is formed solely by inversion symmetry breaking (ISB) – and thus can also be present without magnetism or strong spin-orbit coupling (SOC) – it appears as an interesting quantum degree of freedom raising the potential of orbital analogs to spintronic phenomena, i.e. the field of *orbitronics*. (ii) OAM has been proposed to be a useful observable to assess nontrivial topology in the band structure of topological quantum matter. Lastly, if the atomic SOC strength is sizable, OAM is coupled to the electron spin giving rise to rich spin and orbital momentum space textures.

In this talk, I will shed light on those textures from the perspective of angle-resolved photoemission spectroscopy (ARPES). Combining ARPES with light-polarization-dependent and spin-resolved measurements allows us to address the momentum-dependent properties of the spatial and spin part of the wave functions, respectively. I will present experimental results on model-like monolayer systems and topological quantum materials and show that – as well as how – the complex interplay of ISB and SOC forms striking spin-orbital textures. Based on these findings, I will discuss the potential of utilizing OAM (i) towards orbitronic transport and (ii) to detect unexpected topological features.

8:30am **MI+2D+AC+TF-WeM-3 Falicov Student Award Finalist Talk: Gap Tuning by Hole Doping in EuZn₂As₂ Semimetal**, Deji Kong¹, University of Virginia; S. Karbasizadeh, University of South Carolina; G. Narasimha, Oak Ridge National Laboratory; P. Regmi, University of South Carolina; C. Tao, Oak Ridge National Laboratory; S. Mu, University of South Carolina; R. Vasudevan, Oak Ridge National Laboratory; I. Harrison, University of Virginia; R. Jin, University of South Carolina; Z. Gai, Oak Ridge National Laboratory

EuZn₂As₂ is an ideal candidate for topological magnetism study in comparison to other europium-based semimetals that exhibit a similar type of magnetic transition from the antiferromagnetic phase to the ferromagnetic phase at a low temperature. ¹ Theoretical calculations predict gapped and flatter bands in EuZn₂As₂ but a gapless Γ point in EuCd₂As₂. ² In this work, a low-temperature cleaved EuZn₂As₂ crystal is studied using scanning tunneling microscopy/spectroscopy (STM/S) and density functional theory (DFT). A group of triangular-shaped defects in combining with the DFT calculations are used to identify the existence of the europium-terminated and arsenic-terminated surfaces at the cleavage. Large bandgaps are observed on the two pristine terminations. However, the bandgap width is found to be very sensitive to local heterogenous, like defects and step edges. Two defect groups that create local electron deficiency, i.e. substitutional defect of As replacing Zn, and Zn vacancy, can drastically lower the bandgap. Furthermore, the modification of the bandgap width shows a discrepancy on the two terminations, bigger on Eu termination but much smaller on As-Zn termination. So, we predict that purposely hole doping the system during the crystal growth stage may create a new topological semimetal material with a gapless europium layer sandwiched by a gapped As-Zn lattice.

Reference:

¹ Blawat, J. *et al.* Unusual Electrical and Magnetic Properties in Layered EuZn₂As₂. *Adv Quantum Technol* **5** (2022).

² Wang, Z. C. *et al.* Anisotropy of the magnetic and transport properties of EuZn₂As₂. *Phys Rev B* **105** (2022).

8:45am **MI+2D+AC+TF-WeM-4 Characterization of LaMnO₃/SrTiO₃ Thin Films and Its Mn Valence State Correlated with Ferromagnetism**, Ghadendra Bhandari, P. Tavazohi, V. Dewasurendra, M. Johnson, M. Holcomb, West Virginia University

Thin films of LaMnO₃ (LMO) / SrTiO₃ (STO) perovskite have gained interest for their abilities to be an essential component of some heterostructures while still exhibiting an interesting magnetic phase diagram. We have grown LaMnO₃ thin films on SrTiO₃ using pulsed laser deposition and deposition has been monitored by reflection high energy electron diffraction (RHEED) to verify layer-by-layer growth. Structure and magnetic properties have been characterized by X-ray diffractometry (XRD), and vibration sample magnetometry (VSM). LaMnO₃ thin films exhibit ferromagnetic FM phases whereas bulk LaMnO₃ is antiferromagnetic A-type. All thin films are coherently strained, forcing them to have the in-plane lattice parameter of the STO substrate (3.905 Å), but the out-of-plane parameter varies (3.89-3.93 Å). The variation in the c-lattice is developed from O₂ growth pressure and consequently the Mn cation is in mixed valence state Mn^{3+/4+}. The valence state of the Mn cation is realized from XPS and XAS study. The ferromagnetic magnetization is originated by the double exchange of Mn³⁺-O-Mn⁴⁺. The thickness averaged magnetizations from PNR measurements are comparable with magnetization obtained from VSM. The strength of magnetization correlates with content of Mn⁴⁺.

9:00am **MI+2D+AC+TF-WeM-5 Altermagnetism: From Spintronics to Unconventional Magnetic Phases**, Libor Šmejkal, Uni Mainz, Germany

INVITED

The search for unconventional quantum phases that break the symmetries of the crystal lattice has been a focus in physics since the early days of quantum theory, driven by both fundamental interest and potential applications. Prominent examples include cuprate superconductors, which are known for their unconventional d-wave Cooper pairing, and dissipationless transport.

In this presentation, we will discuss our recent discovery^[1] of an unconventional magnetic phase motivated by our earlier predictions and observations of unconventional spintronics effects ^[2,3,4]. This unconventional phase, altermagnetism (see Figure), unlike common ferromagnetism and antiferromagnetism, breaks the symmetries of the crystal lattice, and features d, g, or i-partial wave characteristics simultaneously in its spin and electronic structure^[1]. D-wave altermagnetism thus represents magnetic analogue of d-wave superconductivity.

We identified altermagnetism by employing and developing a symmetry framework that considers paired transformations involving electron spin and the crystal lattice. This framework is emerging as a new paradigm in the study of magnetic crystals. We will demonstrate its usefulness by discussing (i) the altermagnetic band structure of the semiconductor MnTe, which we recently experimentally observed through collaborative work using photoemission spectroscopy^[5], and (ii) our identification of more than 240 realistic altermagnetic candidates.

Additionally, we will explore the rapid expansion of altermagnetic concepts to many fields with focus on ultrafast spintronics memories^[6], dissipationless transport ^[2-4] and two-dimensional band topology ^[7]. Finally, we will outline the latest developments in the field, including the theoretical identification of the magnetic analog of superfluid helium-3 and we will propose transport experiments which can be used for its detection^[8].

[1] L. Šmejkal, J. Sinova, and T. Jungwirth, *Phys. Rev. X* **12**, 031042 (2022)

[2] L. Šmejkal, et al., *Sci. Adv.* **6**, eaaz8809 (2020)

[3] I. Mazin, et al., *PNAS* **118**, e2108924118 (2021)

[4] H. Reichlová, et al., *Nature Communications* **15**, 4961 (2024)

[5] J. Krempasky*, L. Šmejkal*, S. Souza*, et al., *Nature*, **626**, 517 (2024)

[6] L. Šmejkal et al., *Phys. Rev. X* **12**, 011028 (2022)

[7] I. Mazin, R. Gonzalez-Hernandez, and L. Šmejkal, arXiv:2309.02355 (2023)

[8] Birk Hellenes, et al., arXiv:2309.01607v2 (2024)

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9:30am **MI+2D+AC+TF-WeM-7 Growth Study of Kagome-structured Mn₃Sn on Gallium Nitride (000-1) Using Molecular Beam Epitaxy**, *H. Hall, S. Upadhyay, T. Erickson, A. Shrestha, A. Abbas, Arthur Smith*, Ohio University
Over the past few years, there has been a large amount of interest in Kagome-structured magnetic materials with non-collinear antiferromagnetic ordering [1]. Such materials show interesting magnetic properties including anomalous Hall effect and topological Hall effect [2]. In recent work, we have reported growth of Mn₃Sn on sapphire (0001) which resulted in either *a*-plane or *c*-plane film orientations [3,4]. The substrate however was not ideal, and frequently we observed the disappearance of the diffraction pattern upon opening the Mn and Sn shutters with the pattern reappearing after some amount of resting time. In the case of the *c*-plane orientation, theory suggested this could be due to interfacial disordering of the lattice. This might be due to the ~19% lattice mismatch which also is one reason for the preferred growth of *a*-plane oriented Mn₃Sn on sapphire (0001) due to the much smaller lattice mismatch (<5%) along that direction. Nonetheless, high quality films prove difficult to obtain on sapphire (0001), and a better substrate is desirable. As such, we have investigated the growth of Mn₃Sn films on freshly grown gallium nitride surfaces. The Mn₃Sn growth follows immediately after the growth of N-polar GaN (000 $\bar{1}$), thus giving a perfectly clean and well-ordered substrate surface with only ~2.66% lattice mismatch along the 30° line to the high symmetry axis of GaN. We have investigated this as a function of substrate temperature and find an optimal temperature range in which streaky and clear RHEED patterns are obtained from the beginning of the growth. Next plans include studying of this surface with high-resolution STM and spin-polarized STM. This research has been supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award No. DE-FG02-06ER46317.

- [1] H. Yang *et al.*, *New J. of Physics* **19**, 015008 (2017).
[2] S. Nakatsujii, N. Kiyohara, and T. Higo, *Nature* **527**, 212 (2015).
[3] S. Upadhyay *et al.*, *J. Vac. Sci. & Technol. A* **41**, 042710 (2023).
[4] S. Upadhyay *et al.*, *Surfaces and Interfaces* **42**, 103379 (2023).

9:45am **MI+2D+AC+TF-WeM-8 Exchange Bias Effect in Single-Layer Antiferromagnetic Mn₃GaN Films**, *Ali Abbas, A. Shrestha*, Ohio University; *D. Russell, F. Yang*, The Ohio State University; *A. Smith*, Ohio University
Strain-induced spin structures in non-collinear antiferromagnetic materials like Mn₃GaN can be controlled by an external magnetic field[1][2]. In this work, we report the intrinsic exchange bias in the “single” antiferromagnetic Mn₃GaN films fabricated by epitaxial growth of Mn₃GaN on MgO (001) substrate using molecular beam epitaxy under *in-plane* tensile and *out-of-plane* compressive strain. Scanning transmission electron microscopy confirms significant strain at the Mn₃GaN/MgO interface due to substrate induced tetragonal distortion. Superconducting quantum interference device measurements reveal an exchange bias field (H_{eb}=1225 Oe) and a vertical magnetization shift below 300 K. Furthermore, magnetization M vs. the applied field H measurements from 300K down to 50K reveal the consistent horizontal and vertical shift of the hysteresis loop, which are usually observed only in ferro-/antiferromagnetic bilayers. Here, the exchange bias effect may be attributed to strain, leading to canted and uncompensated Mn spins coupled with an upper antiferromagnetic region, as reported in another system [2][3]. The findings of strain-induced exchange bias in antiferromagnetic Mn₃GaN films may open a new route/ novel system for spintronic properties by design. This research has been supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award No. DE-FG02-06ER46317 (work done at Ohio University, not including XRD) and under award No. DE-SC0001304 (XRD and SQUID measurements done at The Ohio State University).

References:

- [1] X.F. Zhou *et al.*, “Exchange Bias in Antiferromagnetic Mn₃Sn Monolayer Films,” *Physical Review Applied*, 14(5), 054037 (2020).
[2] B. Cui *et al.*, “Strain engineering induced interfacial self-assembly and intrinsic exchange bias in a manganite perovskite film”. *Scientific reports*, 3(1), 2542, (2013).
[3] L. Wanget *et al.*, “Exchange bias and vertical shift of the magnetic hysteresis loop in Co/BiFeO₃ bilayers. *Ferroelectrics Letters Section*, 48(4–6), 65–71, (2021).

11:00am **MI+2D+AC+TF-WeM-13 L-Gap Surface Resonance at Pt(111): Influence of Atomic Structure, d Bands, and Spin-Orbit Interaction**, *Markus Donath, F. Schöttke, P. Krüger*, University of Münster, Germany; *L. Hammer, T. Kiblinger, M. Schneider*, University of Erlangen-Nürnberg, Germany

Pt(111) hosts a surface resonance with peculiar properties concerning energy vs momentum dispersion and spin texture. At variance with the free-electronlike behavior of the L-gap Shockley-type surface states on the fcc(111) surfaces of Au, Ag, and Cu, it splits into several branches with distinct spin polarization around the center of the surface Brillouin zone. Theoretical predictions based on density-functional theory vary depending on the particular functionals used. To clarify this issue, we investigate the atomic structure of Pt(111) by low-energy electron diffraction and the unoccupied electronic structure by spin- and angle-resolved inverse photoemission. The experimental results are backed by theoretical studies using different functionals which show that the characteristics of the surface band depend critically on the lattice constant. We identified a delicate interplay of several contributions: Lattice constant, hybridization with d bands, and the influence of spin-orbit interaction are critical ingredients for understanding the peculiar energy dispersion and spin character of the unoccupied surface resonance.

11:15am **MI+2D+AC+TF-WeM-14 Substrate-Induced Strain Effects on SrFeO₃ Thin Films**, *Lucas Barreto*, University of Pennsylvania; *P. Rogge, J. Wang, B. Lefler*, Drexel University; *D. Puggioni, J. Rondinelli*, Northwestern University; *S. Koroluk, R. Green*, University of Saskatchewan, Canada; *S. May*, Drexel University

Materials with non-trivial magnetic ordering give rise to exotic topological phenomena that can enhance spin-based devices' performance. In this scenario, the cubic perovskite SrFeO₃ exhibits a rich magnetic ordering, described by a multi-*q* magnetic arrangement. In this work, we evaluate how in-plane lattice stress influences the structural, magnetic, and electronic of SrFeO₃ films. We grow epitaxial SrFeO₃ films on different substrates to induce compressive and tensile strains, characterize them using X-ray diffraction, and probe the electronic transport as a function of temperature. The experimental data are supported by density functional theory calculations, from which we obtain the structural and electronic properties of the strained SrFeO₃ structure. We map the magnetic ordering via resonant x-ray magnetic diffraction and observe shifts in the projection of the magnetic wavevector *q* along the [111] direction. Our results indicate that the lattice strain can tune the magnetic propagation vector on the films while maintaining the SrFeO₃ metallic behavior.

11:30am **MI+2D+AC+TF-WeM-15 Tunable Localized Currents at Crystallographic Domain Boundaries in Altermagnet RuO₂**, *Gina Pantano, E. Thareja*, University of South Florida; *L. Šmejkal*, the Czech Academy of Sciences and Johannes Gutenberg Universität Mainz, Germany; *J. Sinova, Johannes Gutenberg Universität Mainz, Germany; J. Gayles*, University of South Florida

Research on interfacial phenomena in condensed matter physics has garnered significant interest over the last few decades due to the discovery of new properties and phases distinct from the bulk, enabling the manipulation of materials for technological applications. In this work, we investigate the novel effects that arise from the presence of a locally chiral crystallographic domain boundary in the altermagnet ruthenium dioxide (RuO₂). Altermagnets are characterized by having a substantial non-relativistic spin splitting comparable to ferromagnetic materials but with compensated magnetic ordering. The spin splitting originates from the Heisenberg exchange interaction combined with the anisotropic octahedral crystal field from the surrounding nonmagnetic O atoms, which reduces the symmetry relating the two opposite spin sublattices to an antiunitary rotation or mirror symmetry. This introduces a new mechanism for controlling spin-dependent transport phenomena by altering the crystal configuration, specifically through its local chirality, such as the crystal Hall effect. Thus, looking at an interface where the local chirality reverses allowed for a more detailed analysis of how the change of symmetry affects electronic transport. RuO₂ was chosen for this study due to its high Néel temperature, metallic nature, and exhibiting one of the largest spin splittings in this new material class. We use first-principle calculations to characterize the interfacial states and their contribution to electronic transport. We observe an induced magnetization at the domain boundary and enhanced anomalous transport along the interface when spin-orbit coupling is considered, due to the change of symmetry. We theorize the localized currents are tunable by the direction of the magnetization at the interface. Our findings will contribute to the understanding of how altermagnetic properties evolve toward interfaces with the reduction in

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dimensionality and symmetry and contribute to advancements toward the design of sustainable, energy-efficient devices.

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