HL 10: Spin-Dependent Phenomena in 2D (joint session MA/HL)

Time: Monday 15:00–17:15 Location: H19

HL 10.1 Mon 15:00 H19

Magnetoelectric behavior of breathing kagomé monolayers of Nb3(Cl,Br,I)8 from first-principles calculations — •John Mangeri — Technical University of Denmark, Kongens Lyngby, Denmark

We apply density functional theory to explore the magnetoelectric (ME) properties of two-dimensional Nb3(Cl,Br,I)8. These compounds have recently been proposed to exhibit coupled ferroelectric and ferromagnetic order leading to a switchable anomalous valley Hall effect (AVHE). Using both spin-spiral and self-consistent spin-orbit coupled calculations, we predict an in-plane 120 degree cycloid of trimerized spins as the ground state for Nb3Cl8. For Nb3Br8 and Nb3I8 we find long period incommensurate helical order. We calculate a number of magnetic properties such as the exchange constants, orbital magnetization, and Weiss temperatures. It is then shown that, despite having both broken inversion and time-reversal symmetry, the proposed AVHE and linear ME response are forbidden by the presence of helical order in the ground state. In addition, the computed switching trajectory demonstrates that it is unlikely that the polar state of the monolayers can be switched with a homogeneous electric field due to an unusual equation of state of the out-of-plane dipole moment. Nevertheless, we highlight that in the presence of a strong electric field, the trimerized spins in Nb3Cl8 will exhibit a magnetic phase transition from the 120 degree cycloid to out-of-plane ferromagnetic order, which restores the symmetry required for both AVHE and linear ME effects.

HL 10.2 Mon 15:15 H19

Ab-initio Investigation of two-dimensional Fe-Sn Kagome lattice with Nb doping — •Gérald Kämmerer[1,2] and Sinéad Griffin[2] — [1]Faculty of Physics, University of Duisburg-Essen — [2]Lawrence Berkeley National Laboratory (LBNL), Berkeley

This research investigates Fe-Sn-based kagome compounds for green energy applications, focusing on their magnetic and electronic properties, particularly in spintronics and phononics. We are investigating tunable properties in Fe_3Sn. We aim to control spin states in 2D magnetic systems by studying doped variants (Nb) in Kagome lattices to uncover topological electronic states, including Dirac fermions and flat bands.

Using first-principles calculations, we analyse impurity interactions in 2D lattices using VASP. By comparing experimental data with our computational results, this study aims to provide insights into dopant-controlled quantum states and improve material performance in electronic applications.

The financial support of the DFG within the SFB 1242 and the computational time on the LBNL supercomputer system are gratefully acknowledged.

HL 10.3 Mon 15:30 H19

Spin polarization of the two-dimensional electron gas at the $EuO/SrTiO_3$ interface — •Paul Rosenberger[1,2], Andri Darmawan[3], Olena Fedchenko[1], Olena Tkach[1], Serhii V. Chernov[4], Dmitro Kutnyakhov[4], Moritz Hoesch[4], Markus Scholz[4], Kai Rossnagel[4,5], Rossitza Pentcheva[3], Gerd Schönhense[1], Hans-Joachim Elmers[1], and Martina Müller[2] — [1]JGU Mainz, Germany — [2]Uni Konstanz, Germany — [3]UDE, Duisburg, Germany — [4]DESY, Hamburg, Germany — [5]CAU Kiel, Germany

Spin-polarized two-dimensional electron gases (2DEGs) are of particular interest for functional oxide electronics applications. Here, we use magnetic circular dichroism in the angular distribution (MCDAD) of photoemitted electrons to investigate whether and how the induced spin polarization of the redox-created 2DEG at the $EuO/SrTiO_3$ (001) interface depends on the dimensionality of the strongly ferromagnetic ($7\,\mu_B/f.u.$) EuO layer [1]. Samples with EuO thicknesses ranging from one to four monolayers were studied. We show that the EuO/STO interfacial 2DEG becomes spin-polarized starting from a threshold EuO thickness of only two monolayers. Experimental data are complemented by DFT+U calculations. Our results, and the potential to enhance the magnetic order of EuO by other proximity effects [2], indicate that the EuO/STO interface is an ideal template for creating functional spin-polarized 2DEGs for application in oxide electronics.

[1] Rosenberger *et al.*, arXiv:2410.23804 (2024).

[2] Rosenberger *et al.*, Sci. Rep. **14**, 21586 (2024).

HL 10.4 Mon 15:45 H19

***Ab initio* calculation of Spin-Orbit torques in 2D magnets** — •Gusthavo Brizolla and Jaroslav Fabian — Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

The interplay of spin-orbit coupling and magnetism in two-dimensional materials and their heterostructures presents exciting opportunities for advancing next-generation spintronic devices. In this work, we investigate the role of proximity effects in generating spin-orbit torques (SOTs) in Fe_3GeTe_2 (FGT) and FGT-based van der Waals heterostructures. Using a tight-binding Hamiltonian derived from first-principles calculations via the Wannierization procedure, we evaluate the torkances within the linear response regime using the Kubo formalism. Our results reveal key mechanisms underlying the generation of torques driven by spin accumulation, elucidating the fundamental physics of SOTs in these systems.

This research has been supported by 2D SPIN-TECH.

HL 10.5 Mon 16:00 H19

Unveiling Long-range Magnetic Textures in Twisted Moiré Antiferromagnets — •King Cho Wong[1], Ruoming Peng[1], Xiaodong Xu[3], Elton Santo[2], Adam Wei Tsen[4], Rainer Stoehr[1], and Joerg Wrachtrup[1] — [1]3rd Physics Institute, University of Stuttgart, Stuttgart, Germany — [2]University of Edinburgh, United Kingdom — [3]University of Washington, USA — [4]University of Waterloo, Canada

Stacking two-dimensional (2D) materials offers a controllable and versatile platform to engineer interlayer interactions, unveiling numerous intriguing correlated and topological states. Recent progresses in twisted 2D magnets have revealed periodic ferromagnetic domains due to the local Moiré stacking. In this study, we employed scanning quantum microscopy to investigate local magnetic responses of twisted double bilayer chromium triiodide (tDB CrI3). We observed unexpected antiferromagnetic textures with periods more than 300 nm at the 1.1° twisted devices, which are significantly exceeding the corresponded Moiré size of about 30 nm. These periodic magnetic textures are setting atop randomly distributed ferromagnetic domains with net two-layer magnetization of 30 uB/nm^2 and antiferromagnetic domains with magnetization of 0 uB/nm^2. Our findings suggest that strong magnetic competition at small twisted angles ($<2°$) can extend magnetic textures beyond the Moiré size, leading to the emergence of Néel skyrmions after field cooling.

HL 10.6 Mon 16:15 H19

Spin model of graphene triangulenes embedded in hexagonal boron nitride — •Dániel Tibor Pozsár[1,3,4,5], László Oroszlány[1,2,3], and Viktor Ivády[1,4,5,6] — [1]Department of Physics of Complex Systems, Eötvös Loránd University, Egyetem tér 1-3, H-1053 Budapest, Hungary — [2]Wigner Research Centre for Physics, Konkoly-Thege M. út 29-33, H-1121 Budapest, Hungary — [3]TRILMAX Consortium, Twinning, Horizon Europe, Budapest, Hungary — [4]QUEST projec, Twinning, Horizon Europe, Budapest, Hungary — [5]MTA*ELTE Lendület "Momentum" NewQubit Research Group, Pázmány Péter, Sétány 1/A, 1117 Budapest, Hungary — [6]Department of Physics, Chemistry and Biology, Linköping University, SE-581 83 Linköping, Sweden

We are investigating triangulene shaped substitutional defects in hexagonal boron nitride filled with carbon atoms. We show how the triangulene shaped defects encompass magnetic moments and with ab initio methods we build Heisenberg like classical spin models representing their interactions. We show how different lattice terminations and sizes impact the magnetic properties of the system.

HL 10.7 Mon 16:30 H19

Realizing Spin-3/2 AKLT State for Quantum Computation with Tetrapod Architectures — •Claire Benjamin[1], László Oroszlány[1,2], Dániel Varjas[3], and Gábor Széchenyi[1] — [1]Department of Physics of Complex Systems, Eötvös University, Pázmány Péter sétány 1/A, H-1117 Budapest, Hungary — [2]Wigner Research Centre for Physics, Konkoly-Thege M. út 29-33, H-1121 Budapest, Hungary — [3]Department of Theoretical Physics, Institute

of Physics, Budapest University of Technology and Economics, Muegyetem rkp. 3., H-1111 Budapest, Hungary

Using a novel tetrapod (5-site cluster) architecture, we implement spin-3/2 degrees of freedom in a semiconductor quantum bit platform. This framework enables us to construct a tunable artificial spin system that can realize the two-dimensional Affleck-Kennedy-Lieb-Tasaki (AKLT) state on a honeycomb lattice, known to be a universal resource for measurement-based quantum computation. We assess the model's robustness and feasibility for measurement based quantum computing using semi-analytic perturbation theory and numerical calculations.

HL 10.8 Mon 16:45 H19

Anomalous quantum oscillations from boson-mediated interband scattering — •Léo Mangeolle[1,2] and Johannes Knolle[1,2,3] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany — [3]Blackett Laboratory, Imperial College London, London SW7 2AZ, United Kingdom

Quantum oscillations (QO) in metals refer to the periodic variation of thermodynamic and transport properties as a function of inverse applied magnetic field. QO frequencies are normally associated with semi-classical trajectories of Fermi surface orbits but recent experiments challenge the canonical description. We develop a theory of composite frequency quantum oscillations (CFQO) in two-dimensional Fermi liquids with several Fermi surfaces and interband scattering mediated by a dynamical boson, e.g. phonons or spin fluctuations. Specifically, we show that CFQO arise from oscillations in the fermionic self-energy with anomalous frequency splitting and distinct strongly non-Lifshitz-Kosevich temperature dependencies. Our theory goes beyond the framework of semi-classical Fermi surface trajectories highlighting the role of many-body effects. We provide experimental predictions and discuss the effect of non-equilibrium boson occupation in driven systems.

HL 10.9 Mon 17:00 H19

Identifying the Origin of Thermal Modulation of Exchange Bias in $Fe_3GeTe_2/MnPS_3$ van der Waals Heterostructures — Aravind Puthirath Balan[1], •Aditya Kumar[1], Patrick Reiser[2], Joseph Vimal Vas[3], Thibaud Denneulin[3], Rafal E. Dunin-Borkowski[3], Patrick Maletinsky[2], and Mathias Kläui[1] — [1]Institute of Physics, Johannes Gutenberg University Mainz, Staudinger Weg 7, 55128 Mainz, Germany — [2]Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland — [3]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons and Peter Grünberg Institute, Forschungszentrum Jülich, 52425 Jülich, Germany

This study investigates the origin of exchange bias in $Fe_3GeTe_2/MnPS_3$ vdW heterostructures. A substantial 170 mT exchange bias is observed at 5 K, one of the largest values reported for vdW heterostructures, despite the compensated interfacial spin configuration of $MnPS_3$. This exchange bias is linked to unexpected weak ferromagnetic ordering in $MnPS_3$ below 40 K that we reveal by NV center imaging. A 1000% variation in the magnitude of exchange bias is obtained through thermal cycling linked to changes in the vdW gap during field cooling. Detailed interface analysis reveals atom migration between layers, forming amorphous regions on either side of the vdW gap. These findings underscore the robust and tunable nature of exchange bias in vdW heterostructures but also challenge the often assumed pristine nature of vdW interfaces calling for in-depth interface characterization.

[1] A. P. Balan et al., Advanced Materials 36, 2403685 (2024).