2024 Swiss Workshop on Materials with Novel Electronic Properties Basic research and applications





August 14th - 16th, 2024



Program & Abstracts

2024 Swiss Workshop on Materials with Novel Electronic Properties Basic research and applications

Les Diablerets

Switzerland



August 14th - 16th, 2024

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August 14th - 16th, 2024

Sponsors





PROGRAM OVERVIEW

Wed, Aug 14, 2024				
11:30	Registration & Drinks at			
	the Hotel Victoria			
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Superconductivity				
	Manfred Sigrist			
13:45	Elena Hassinger			
14:15	Zurab Guguchia			
14:45	Menghan Liao			
15:00	Aline Ramires			
15:15	Ilaria Maccari			
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Andrea Caviglia				
16:00	Libor Smejkal			
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16:45	Debarghya Dutta			
17:00	Pratyay Ghosh			
17:15	David Santos-Cottin			
17:30	1'Poster session			
	Claude Monney			
18:00	Poster session 1 &			
	commercial exhibit			
20:30	Dinner			

Thu, Aug 15, 2024			
Oxide interfaces / Nickelates			
Jean-Marc Triscone			
08:30	Berit Goodge		
09:00	Meng Wang		
09:30	Clémentine Thibault		
09:45	Subhrangsu Sarkar		
10:00	Giacomo Sala		
10:15	Coffee break		
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	Felix Baumberger		
10:45	Matteo Mitrano		
11:15	Martin Eckstein		
11:45	Corinna Burri		
12:00	Frédéric Chassot		
12:30	lunch		
	Materialgrowth		
	Marisa Medarde		
13:45	Bharat Jalan		
14:15	Lucia Varbaro		
14:45	Anastasiia Lukovkina		
15:00	Lucia Varbaro		
15:15	Coffee break		
Qı	antum materials 3D		
	Fabian von Rohr		
15:45	Leslie M Schoop		
16:15	Hiroki Ueda		
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17:00	Volodymyr Multian		
17:15	Jens Oppliger		
17:30	Sandy Adhitia Ekahana		
17:45	1' Poster session Bruce Normand		
18:15	Poster session 2 & commercial exhibit		
20:30	Conference Dinner		

Fri, Aug 16, 2024		
Quantum materials 2D		
	Christoph Renner	
08:30	Mathias Scheurer	
09:00	Xiadong Xu	
09:30	Louk Rademaker	
09:45	Julia Issing	
10:00	Ishita Pushkarna	
10:15	Giacomo Morpurgo	
10:30	Coffee break	
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	Stefano Gariglio	
11:00	Franck Peauger	
11:30	Celia Lucas Esparseil	
11:45	Ludovica Tovaglieri	
12:15	Lunch	

DETAILED PROGRAM

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		Lunch	12:00 - 13:40
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13:45 – 14:15	Controlling two-phase superconduc Elena Hassinger (TU Dresden/Max Pla	tivity in CeRh2As2 with anck Institute Dresden)	pressure
14:15 – 14:45	Time-Reversal Symmetry-Breaking i Muon Spin Rotation Zurab Guguchia (Paul Scherrer Institu	in Charge-Ordered Kago	ome-Lattice Systems Probed with
14:45 – 15:00	Spectroscopic evidence for a firs Ovchinnikov state Menghan Liao (DQMP, University of G	t-order transition to	the orbital Fulde-Ferrell-Larkin-
15:00 – 15:15	Improper orders in nonsymmorphic Aline Ramires (Paul Scherrer Institut)	e systems	
15:15 – 15:30	Nonunitariy superconductivity from Ilaria Maccari (Institute for Theoretica	a competing electronic o al Physics, ETH Zürich)	rders in multiorbital systems

Coffee 15:30 - 16:00August 14 (Wed) 16:00 - 17:30

Session 2: Quantum magnetism

Chair: Andrea Caviglia (University of Geneva)

16:00 – 16:30	Altermagnetism and spin symmetries Libor Smejkal (Universität Mainz/Czech Academy of Sciences/Max Planck I	Institute Dresden)
16:30 – 16:45	Hidden order in the kagome magnet Co3Sn2S2 probed by RIXS Tianlun Yu (Paul Scherrer institut)	
16:45 – 17:00	Investigating Phase Transitions in Van Der Waals Magnets using a Quar Debarghya Dutta (University of Basel)	ntum Sensor
17:00 – 17:15	Spin liquid and deconfined criticality in maple-leaf quantum magnet Pratyay Ghosh (Institute of Physics, EPFL)	
17:15 – 17:30	EuCd2As2: a magnetic semiconductor David Santos-Cottin (Department of Physics, University of Fribourg)	
1' poster pre	sentations	17:30 - 18:00

1' poster presentations

Chair: Claude Monney (University of Fribourg)

Poster session 1 & commercial exhibit

18:00 - 20:30

20:30

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Dinner
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August 15 (Thu)

August 15 (Thu)

8:30 - 10:15

10:15 - 10:45

10:45 - 12:15

Session 3: Oxide interfaces / Nickelates

Chair: Jean-Marc Triscone (University of Geneva)

- 8:30 9:00 **Resolving the polar interface in superconducting nickelate thin films** Berit Goodge (Max Planck Institute Dresden / Cornell University)
- 9:00 9:30 **Discovery of high-Tc superconductivity in a nickelate under pressure** Meng Wang (School of Physics, Sun Yat-sen University)
- 9:30 9:45 **The role of oxygen octahedra connectivity in orthorhombic perovskite heterostructures** Clémentine Thibault (DQMP, University of Geneva)
- 9:45 10:00 Altermagnetic property at a cuprate/manganite interfacet Subhrangsu Sarkar (Department of Physics and Center for Nanomaterials, University of Fribourg)

Coffee

10:00 – 10:15 **Quantum metric and nonlinear magnetotransport from spin-momentum locking** Giacomo Sala (DQMP, University of Geneva)

August 15 (Thu)

Session 4: Out of equilibrium physics

Chair: Felix Baumberger (University of Geneva)

- 10:45 11:15 An X-ray view of light-driven quantum materials Matteo Mitrano (Department of Physics, Harvard University)
- 11:15 11:45 **Long-lived non-thermal phases of strongly correlated electrons** Martin Eckstein (University of Hamburg)
- 11:45 12:00 **Direct detection of nonthermal phase switching in a 1T-TaS2 memory device** Corinna Burri (Paul Scherrer Institut / Department of Physics and Quantum Center, ETH Zürich)
- 12:00 12:15 Unveiling the Electronic Properties of α-SnTe: From Ferroelectric Distortion to Unexpected Topological Surface State
 Frédéric Chassot (University of Fribourg)

assot (Oniversity of Pribourg)

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Session 5: Material growth

Chair: Marisa Medarde (Paul Scherrer Institut)

- 13:45 14:15 Unlocking the Promise and Simplicity of Atomically Precise Synthesis for 4d and 5d Metal **Oxides through Hybrid MBE** Bharat Jalan (Department of Chemical Engineering and Materials Science, University of Minnesota)
- 14:15 14:45 Synthesis of Electronic-Grade Quantum Heterostructures by Hybrid PLD Chang-Beom Eom (University of Wisconsin-Madison)
- 14:45 15:00 Controlling the Magnetic Properties of the van der Waals Multiferroic Crystals Co_{1?x}Ni_xI₂ Anastasiia Lukovkina (DQMP, University of Geneva)
- 15:00 15:15 Turning a metal into an insulator Lucia Varbaro (DQMP, University of Geneva)

Coffee	15:15 – 15:45

August 15 (Thu)

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Chair: Fabian von Rohr (University of Geneva)

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16:45 – 17:00	Interplay of electronic orders in kagome metals Mark H Fischer (Cornell University)	
17:00 – 17:15	New approach for nonlinear optical tensor determination. Application to Rare ear lates microcrystals Volodymyr Multian (Department of condensed matter physics, Weizmann Institute of Sci	r th nicke- ience)
17:15 – 17:30	Discovery of Giant Unit-Cell Super-Structure in PrNiO2 Jens Oppliger (Physik-Institut, Universität Zürich)	
17:30 – 17:45	Anomalous electrons in a metallic kagome ferromagnet Sandy Adhitia Ekahana (Paul Scherrer Institut)	
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1' poster presentation

Chair: Bruce Normand (Paul Scherrer Institut)

Poster session 2 & commercial exhibit

18:15 - 20:30

Conference dinner

20:30

August 16 (Fri)

August 16 (Fri)

Session 7: Quantum materials 2D

Chair: Christoph Renner (University of Geneva)

- 8:30 9:00 **Exotic superconducting states in 2D materials and moiré engineering at oxide interfaces** Mathias Scheurer (Institute for Theoretical Physics III, University of Stuttgart)
- 9:00 9:30 **Observation of fractional quantum anomalous hall effect** Xiadong Xu (Department of Physics, Department of Materials Science and Engineering University of Washington)
- 9:30 9:45 Moiré is Different: Metal-Insulator Transitions, Kondo Lattice Physics and Chiral Spin Liquids in TMD Bilayers Louk Rademaker (DQMP, University of Geneva)
- 9:45 10:00 Electronic structure of encapsulated mono-, bi- and trilayer T_d -MoTe₂ Julia Issing (DQMP, University of Geneva)
- 10:00 10:15 Tuning electronic characteristics of MoS₂-Au heterostructures via twist angle manipulation: STM insights Ishita Pushkarna (DQMP, University of Geneva)
- 10:15 10:30 Low-density Hall response of two-dimensional electrons with a local and energy-dependent self-energy Giacomo Morpurgo (DQMP, University of Geneva)

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Chair: Stefano Gariglio (University of Geneva)

- 11:00 11:30 **New superconducting radiofrequency materials serving the future FCC collider** Franck Peauger (CERN)
- 11:30 11:45 **Towards the development of superconducting joints between REBCO coated conductors: a thermomechanical study** Celia Lucas Esparseil (DQMP, University of Geneva)
- 11:45 12:00 **Controlling and investigating domain and domain walls in PbTiO**₃ **ferroelectric thin films and heterostructures** Ludovica Tovaglieri (DQMP, University of Geneva)

Lunch

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August 14 (Wed)

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ABSTRACTS

of the

oral presentations

Controlling two-phase superconductivity in CeRh2As2 with pressure

Elena Hassinger,^{1,2} Konstantin Semeniuk,² Meike Pfeiffer,^{1,2} Javier Landaeta,^{1,2} and Seunghyun Khim²

¹ TU Dresden Technical University, Institute for Solid State and Materials Physics, 01062 Dresden
² Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

CeRh2As2 has a unique superconducting phase diagram in which a magnetic field drives a transition between superconducting states, believed to be of even and odd parity. Our understanding of this phenomenon is based on the crystal structure with locally broken inversion symmetry in the Ce layers and two Ce layers related by global inversion symmetry. Even in the case of pure singlet pairing within the layers, an odd-parity superconducting gap function can be reached by a sign change of the gap on the two Ce layers. This way of creating odd-parity superconductivity is different from the traditional one - where odd parity comes from the pairing function itself - and might be a direction of finding more odd-parity superconductors. In order to guide the search for new odd-parity superconductors, we need to understand, which material parameters favor its appearance. Here, I will give an overview on the current knowledge on CeRh2As2 including phase diagrams covering the normal state and angle dependence. I will also show results where we use pressure tuning to induce changes of the normal state and observe the effects on the superconducting states. We find that superconductivity is fostered by correlations in proximity to a quantum critical point. Furthermore, pressure effectively shifts the parity transition to lower fields.

Time-Reversal Symmetry-Breaking in Charge-Ordered Kagome-Lattice Systems Probed with Muon Spin Rotation

Zurab Guguchia

Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland

Kagome lattices stand at the forefront of research due to their fascinating interplay of topology, correlations, and magnetism [1-3]. In my talk, I aim to shed light on the latest experimental developments concerning superconductivity and the magnetic aspects of charge order in various kagome-lattice systems, studied from the perspective of local magnetic probe. This involves the use of muon-spin rotation (μ SR) as a function of depth from the crystal surface and under extreme conditions like hydrostatic pressure, uniaxial strain, ultra-low temperatures, and high magnetic fields. μ SR is complemented by magnetoresistance and X-ray diffraction techniques. Key systems under discussion will include: (1) The AV₃Sb₅ (A = K, Rb, Cs) compound series with V kagome lattice, notable for displaying a range of symmetry-breaking electronic orders, such as charge order and superconductivity. Here, we have identified a depth-tunable time-reversal symmetry-breaking state associated with charge order [4-7]. (2) The bilayer kagome material ScV₆Sn₆, where hidden magnetism within the charge-ordered state was observed [8]. (3) The LaRu₃Si₂ system with Ru kagome layers, in which we identified two distinct types of charge order (bond order), with one manifesting above room temperature [9,10]. This finding marks the first instance of observing a charge-ordered state at room temperature in a kagome lattice.

- [1] I. Syozi, Prog. Theor. Phys. 6, 306 (1951).
- [2] J.-X. Yin et. al., Nature Physics 15, 443 (2019).

[3] Z. Guguchia et. al., Nature Communications 11, 559 (2020).

[4] C. Mielke III, et. al., and Z. Guguchia, Nature 602, 245 (2022).

[5] Z. Guguchia et. al., Nature Communications 14, 153 (2023).

[6] Z. Guguchia et. al., NPJ Quantum Materials 8, 41 (2023).

[7] J.N. Graham et. al., and Z. Guguchia, arXiv:240211130 (2024).

[8] Z. Guguchia et. al., Nature Communications 14, 7796 (2023).

[9] I. Plokhikh et. al., and Z. Guguchia, arXiv:2309.09255 (2023).

[10] C. Mielke III, V. Sazgari, et. al., and Z. Guguchia, arXiv:2402.16219 (2024).

Spectroscopic evidence for a first-order transition to the orbital Fulde-Ferrell-Larkin-Ovchinnikov state

Menghan Liao,¹ Zongzheng Cao,² Hongyi Yan,³ Haiwen Liu,³ Ding Zhang,² and Alberto Morpurgo¹

¹ Department of Quantum Matter Physics, University of Geneva
² State Key Laboratory of Low Dimensional Quantum Physics and Department of Physics, Tsinghua University
³ Center for Advanced Quantum Studies, Department of Physics, Beijing Normal University

A Cooper pair in a superconductor may be driven into a distinct state with non-zero total momentum when the time reversal symmetry is broken. Recently, a new type of finite momentum superconducting pairing, namely the orbital Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state, has been proposed in superconductors with strong spin-orbit coupling materials such as multilayer NbSe2. Experimental demonstration for this state is limited to resistance measurements, which is not enough to establish the full physical picture. In this talk, I will show the first thermodynamic evidence for the orbital FFLO state. A first-order phase transition from the Ising pairing to the orbital FFLO state in NbSe2 is directly observed. By carrying out tunneling spectroscopy measurements with atomically flat Van der Waals tunneling junctions, we discover a discontinuity in the superconducting gap value as a function of the in-plane magnetic field. The phase transition shows clear hysteresis behaviors when sweeping the magnetic field back and forth. The observation matches our theoretic calculation by taking into account the melting of the Josephson vortex lattice.

Improper orders in nonsymmorphic systems

Aline Ramires¹ and Andras Szabo²

¹ Paul Scherrer Institute, 5232 Villigen PSI, Switzerland
² Institute for Theoretical Physics, ETH Zurich, 8093 Zurich, Switzerland

The study of improper phases in the context of multiferroic materials has a long history. In this talk, I highlight an overlooked mechanism that couples order parameter bilinears to odd-parity order parameters such that the latter emerge as improper orders. For that, we explore a novel perspective of nonsymmorphic symmetries based on extended symmetry groups in real space. We highlight how nonsymmorphic symmetries can generate rather nonintuitive couplings between order parameters. We are inspired by the phenomenology of the recently discovered superconductor CeRhAs, but our results also have implications for other primary orders. In particular, we find that a bilinear in the superconducting order parameter can couple linearly to odd-parity orders in centrosymmetric systems. Our findings open the door for exploring nonsymmorphic symmetries in the broader context of improper orders with potential applications to topological functional materials.

[1] https://arxiv.org/abs/2309.05664.

Nonunitariy superconductivity from competing electronic orders in multiorbital systems

Simon Hille,¹ Ilaria Maccari,³ Aline Ramires,² and Manfred Sigrist³

¹ Physikalisches Institut and Bethe Center for Theoretical Physics, Universität Bonn, Nussallee 12, 53115 Bonn, Germany
² Condensed Matter Theory Group, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland
³ Institute for Theoretical Physics, ETH Zurich, CH-8093 Zurich, Switzerland

Nonunitary superconducting states are among the most fascinating examples of unconventional Cooper pairing. Their condensate wave function breaks multiple symmetries and features a flavour polarisation, often with exotic topological properties. In multiorbital systems, non-unitary superconducting states [1] may involve other degrees of freedom and exhibit novel features compared to the single orbital case. How to stabilise these states is, however, still poorly understood. Here, we will discuss how the interplay between superconductivity and other electronic orders can stabilise nonunitary superconductivity in a two-orbital system. Starting from the case in which nonunitary superconductivity emerges from the competition with a charge-density wave [2], we will extend the study to the case where the competing electronic order is a spin-density wave.

A. Ramires, J. Phys.: Condens. Matter 34 304001 (2022).
T. M. R. Wolf, M. F. Holst, M. Sigrist, and J. Lado, Phys. Rev. Research 4, L012036 (2022).

Altermagnetism and spin symmetries

Libor Šmejkal^{1,2,3}

¹ Institut für Physik, Johannes Gutenberg Universität Mainz, D-55099 Mainz, Germany
² Institute of Physics, Czech Academy of Sciences, Cukrovarnická 10, 162 00, Praha 6, Czech Republic
³ Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany

In the last 90 years, magnetically ordered materials have been divided into two basic classes - ferromagnets and antiferromagnets. They are characterized by s-wave and no spin ordering in momentum space, respectively. In this talk, we will review our recent predictions of unconventional magnetic classes beyond ferromagnets and antiferromagnets[1,2]. Unconventional magnets are characterized by parameters of even (e.g. d-wave altermagnets) or odd (p-wave) wave ordering, which are not found in conventional ferromagnets and antiferromagnets. We show how the unconventional magnets can be identified using spin group theory, which considers - in contrast to conventional magnetic symmetries pairs of symmetry operations in spin and lattice space. We will discuss the implications of unconventional magnetism in unconventional spin and anomalous Hall phenomena as well as recent experimental observations of d-wave altermagnetism in MnTe[3].

[1] Beyond Conventional Ferromagnetism and Antiferromagnetism: A Phase with Nonrelativistic Spin and Crystal Rotation Symmetry, L. Šmejkal, Jairo Sinova, T. Jungwirth, Phys. Rev. X 12, 031042 (2022).

[2] Exchange spin-orbit coupling and unconventional p-wave magnetism, Anna Birk Hellenes, Tomáš Jungwirth, Jairo Sinova, Libor Šmejkal, arXiv:2310.17280v2.

[3] Altermagnetic lifting of Kramers spin degeneracy, J. Krempaský*, L. Šmejkal*, et al., Nature 626, 517 (2024).

Hidden order in the kagome magnet Co3Sn2S2 probed by RIXS

<u>Tianlun Yu</u>,¹ Wenliang Zhang,¹ Yuan Wei,¹ Dariusz Gawryluk,¹ Loïc Roduit,¹ Valdimir Strocov,¹ Gabriel Aeppli,^{1,2,3} Thorsten Schmitt,¹ and Yona Soh¹

Paul Scherrer Institut
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Kagome motifs can host flat bands as well as quantum spin liquids due to geometric frustration from the triangular lattice. $Co_3Sn_2S_2$ is a kagome lattice based on magnetic Co atoms. It is ferromagnetically ordered below Tc ~177 K with a small moment of 0.3 μ_B per Co. It has a large anomalous Hall effect regarding both Hall resistivity and Hall angle [1], with surface Fermi Arcs and Weyl points reported by ARPES, suggesting it is a time-reversal symmetry breaking magnetic Weyl semimetal [2]. Despite the large interest in the material, its magnetic structure and magnetic Hamiltonian are still not unravelled due to the small magnetic moment limiting the effectiveness of traditional neutron scattering methods [3]. Using magnetic circular dichroism RIXS, we discover time reversal symmetry breaking excitations of 0.3 eV, whose temperature dependence follows the static magnetic order, showing that the system has a hidden dynamic order in addition to the static order. With further RIXS cross-section analysis based on the polarization factors, we find that not only the spin degree of freedom, but the orbital degree of freedom also contributes to such excitations, and discover a possible explanation of the small moment in the FM order.

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Investigating Phase Transitions in Van Der Waals Magnets using a Quantum Sensor

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The advent of two-dimensional magnetic van der Waals(vdW) heterostructures has expanded the boundaries of nano-magnetism and led to novel ideas for information transfer in the field of spintronics[1]. By probing the intrinsic layer-dependent magnetic phases, it is possible to gain fundamental understanding of spin structure and dynamics[2]. We study these exotic magnetic phase transitions using a local, non-invasive scanning magnetometry technique. Our sensor consists of a single nitrogen-vacancy (NV) center in diamond that is attached to an AFM cantilever to enable scanning measurements at cryogenic temperatures[3].

In particular, we are studying the magnetic phases of CrSBr, a layered 2D vdW anti-ferromagnet with intralayer ferromagnetic (FM) and interlayer anti-ferromagnetic (AFM) coupling[4]. We quantitatively characterize the FM to AFM phase transition in bilayer CrSBr by directly imaging the FM-AFM phase boundary as it propagates through the sample[5]. Strikingly, we observe the formation of characteristic cusp-like features in the FM-AFM phase wall which leads to the creation and propagation of AFM-AFM domain walls. Furthermore, we correlate the interplay between the phase walls and neighboring connected CrSBr multilayers to ultimately decipher the spin configuration of the underlying layers.

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Spin liquid and deconfined criticality in maple-leaf quantum magnet

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We investigate the possibility of exotic phenomena, viz. quantum spin liquid (QSL) or deconfined quantum critical point (DQCP), in the spin- $\frac{1}{2}$ Heisenberg model on the maple-leaf lattice, a geometrically frustrated system formed by hexagons (coupling J_h), triangles (coupling J_t), and dimers (coupling J_d). We identify one promising region, given by $J_h > 0$ and J_t , $J_d < 0$, for hosting enticing physics. In this region, the system exhibits an interplay between Néel order and a gapped dimerized singlet phase, holding the possibility of harboring a QSL and a DQCP. Using bond-operator mean-field theory and density matrix renormalization group calculations, we delve into this uncharted territory, revealing tantalizing evidence of the existence of a QSL phase and highlighting its potential as a platform for DQCP.

EuCd2As2: a magnetic semiconductor

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EuCd2As2 exhibits antiferromagnetic order along the c direction with a Neel temperature TN 9.5 K [1]. Recent ab-initio calculations suggest that EuCd2As2 hosts a single pair of Dirac points at the Fermi level in its AFM configuration [2]. Interestingly, these calculations also predict that a single pair of Weyl points may be generated in a ferromagnetic state by applying an external magnetic field [3,4]. Moreover, the Fermi surface of EuCd2As2 appears to be strongly sensitive to the sample growth procedure [5], with a delicate interplay between magnetism and the Fermi surface. In this context, we investigate the electronic, optical, and magneto-optical properties of EuCd2As2, expecting to observe characteristic Landau-level transitions of Weyl fermions. This poster will present a comparative study of samples grown under different conditions. On high-quality crystals, we were able to reduce the number of carriers, leading to a strong increase in resistivity, which is in agreement with optical conductivity measurements. We will present magneto-reflection and transmission measurements on high-purity EuCd2As2. Interestingly, we found that this system is actually a semiconductor with a large gap of 0.77 eV, rather than a Dirac or Weyl semimetal. We will also show that an externally applied magnetic field has a profound impact on the band structure of the system, resulting in a significant decrease in the band gap, as large as 125 meV at 2 T.

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Resolving the polar interface in superconducting nickelate thin films

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Superconducting infinite-layer nickelates [1] were first predicated as a potential analogue to the high-Tc cuprates, though some key distinctions have emerged [2]. Notably, nickelates are the most polar layered oxide superconductor yet discovered, with +/-3 formally charged atomic planes. Thus far, superconductivity has only been stabilized in epitaxial thin films, further compounding this inherent polarity with a large polar discontinuity at the atomic interface. This interface presents important questions for understanding the phenomena observed in these films: for example, it was been predicted that an ideal interface between NdNiO2 and SrTiO3 may host a high-mobility two-dimensional electron gas (2DEG) [3]. Providing access to buried interfaces with high spatial and energy resolution, scanning transmission electron microscopy (STEM) and electron energy loss spectroscopy (EELS) can probe such effects with structural and chemical sensitivity. Elemental mapping reveals a single intermediate Nd(Ti,Ni)O3 atomic layer between the substrate and film. To more completely resolve the full interface structure, we combine precise experimental analysis and density functional theory with Hubbard U term (DFT+U) calculations. Together, the combination of atomic-resolution STEM-EELS and DFT+U calculations disentangle the contributions of various structural effects at this unique, strongly polar interface for alleviating the polar discontinuity [4].

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Discovery of high-Tc superconductivity in a nickelate under pressure

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High-transition-temperature (high-Tc) superconductivity in cuprates has been discovered for more than three decades, but the underlying mechanism remains a mystery. Cuprates are the only unconventional superconducting family that hosts bulk superconductivity with Tcs above the liquid nitrogen boiling temperature at 77 Kelvin. We found superconductivity in single crystals of La3Ni2O7 grown by the highpressure floating zone method with a maximum Tc of 80 K at pressures between 14.0-43.5 gigapascals [1,2]. Our collaborators have confirmed the high Tc superconductivity on our samples independently [3-5]. The superconducting phase under high pressure exhibits an orthorhombic structure of Fmmm space group with the 3dx2-y2 and 3dz2 orbitals of Ni cations strongly mixing with oxygen 2p orbitals [2,6]. Density functional theory calculations suggest the superconductivity emerges coincidently with the metallization of the IC-bonding bands under the Fermi level, consisting of the 3dz2 orbitals with the apical oxygens connecting Ni-O bilayers. ARPES and infrared measurements are consistent with our theoretical expectations [7,8]. Thus, the discoveries not only reveal important clues for the high-Tc superconductivity in this Ruddlesden-Popper double-layered perovskite nickelates but also provide a new family of compounds to investigate the high-Tc superconductivity mechanism. Indeed, La4Ni3O10 has also been found superconductivity below 20 K under pressure. The new progresses in the studies of nickelate high Tc superconductors will be introduced.

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The role of oxygen octahedra connectivity in orthorhombic perovskite heterostructures

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Controlling the atomic structure in epitaxial transition metal perovskite thin films is an effective way to tune their properties or to achieve new functionalities. This is linked to the intimate coupling of the electronic and structural degrees of freedom in this family of materials. For instance, the rotation angle of the oxygen octahedra is directly linked to the electronic bandwidth in nickelates or to the orbital ordering temperature in vanadates. Another example is a predicted novel ferroelectric state due to a tailored coupling of rotations in epitaxial heterostructures of different symmetries [1]. Achieving such a control requires an understanding of the mechanisms that determine the atomic structure - and may compete - in an epitaxially strained structure. In this work, we investigate orthorhombic perovskite films grown by pulsed laser deposition on orthorhombic substrates [2]. We show that there is a competition between oxygen octahedra connectivity and macroscopic strain leading to an "intermediate layer" and a "switching plane" that allow a re-orientation of the orthorhombic unit cell [3]. The detailed atomic structure of these oxide material combinations is probed using X-ray diffraction and scanning transmission electron microscopy.

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Altermagnetic property at a cuprate/manganite interface

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Using Resonant inelastic x-ray spectroscopy (RIXS) in conjunction with x-ray linear and magnetic dichroism (XLD/XMCD), we demonstrate an altermagnetic order at the interface of epitaxially grown heterostructure of Nd0.65(Ca0.7Sr0.3)0.35 MnO3 / YBa2Cu3O7. Cu-RIXS spectra and its polarization analysis indicate the presence of an usual [1,2] antiferromagnetic Cu-magnon mode corresponding to the bulk and a weakly dispersing lower-energy interfacial magnon mode, which exhibits a decreasing weight with increasing momentum transfer. This atypical magnon-behavior can be explained by a linear spin wave theory that takes into account a 2-D checkerboard-type orbital pattern made of dz2 and dx2-y2, coupled with a spin-order leading to 2-D altermagnetic property at the interface [3].

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Quantum metric and nonlinear magnetotransport from spin-momentum locking

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Quantum materials are characterized by electromagnetic responses that are directly related to the geometry and topology of electronic wavefunctions. These properties are encoded in the Berry curvature and quantum metric, which constitute the real and imaginary parts of the quantum geometric tensor, respectively. Berry curvature-mediated transport effects, including the anomalous Hall [1] and nonlinear Hall effect with time-reversal symmetry [2], have been observed in various magnetic and nonmagnetic materials. However, transport effects governed by the quantum metric remain limited to topological antiferromagnets [3-4]. Here [5], we show that spin-momentum locked electronic bands, which are commonly found at the surfaces and interfaces of materials with substantial spin-orbit coupling, are characterized by a nontrivial quantum metric that activates a nonlinear and nonreciprocal magnetoresistance. We observe the occurrence of this phenomenon and its gate-tunability in 111-oriented LaAlO₃/SrTiO₃ interfaces. The additional presence of the Berry curvature-mediated anomalous planar Hall effect further allows us to sense, for the first time and in a single nonmagnetic material, both components of the quantum geometric tensor. Our findings extend the application of quantum geometry to a vast class of materials and provide new strategies for designing electronic functionalities based on the geometric properties of electronic wavefunctions.

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An X-ray view of light-driven quantum materials

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Intense ultrashort lasers are an extremely effective tool for controlling the properties of quantum materials and inducing emergent states with novel functionalities. Some of the most spectacular light-induced phenomena, such as superconducting-like phases, transient charge density wave ordering, and excitonic condensation, are found to occur in materials dominated by strong electronic correlations with a large susceptibility to external stimuli. Microscopically understanding these states of matter requires a direct measurement of their transient electronic dynamics and effective interactions. In this talk, I will show how ultrafast x-ray spectroscopy enables interrogating the microscopic physics of photoexcited quantum materials with unprecedented detail. I will discuss the generation of prethermal and metastable electronic states in light-driven Mott insulators, such as quasi-1D copper oxides, which are key to the emergence η -pairing condensation and light-driven superconductivity. Further, I will illustrate how femtosecond x-rays can systematically determine the charge and spin dynamics of these nonequilibrium phases.

Long-lived non-thermal phases of strongly correlated electrons

Eckstein Martin

University of Hamburg

Ultrafast laser excitation offers a pathway to explore complex materials, and unveil states which are inaccessible through conventional equilibrium routes. Mott insulators, and more generally correlated electron systems at the verge of Mott localisation are a promising class of materials for this endeavour, since they exhibit exotic phenomena and complex phase diagrams already in equilibrium. Non-equilibrium superconductors, exciton condensates, or magnetic phases have been reported [1]. Key question are (i), how one can stabilize such non-thermal phases, extending their lifetimes or even inducing metastability, and (ii), whether one can find a simple universal description of such states, akin to a non-thermal free energy which depends only on few relevant slow variables. In my talk, we will examine possible mechanisms for long time stability, as well as theoretical ideas to unravel the long-time dynamics of such quantum systems.

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Direct detection of nonthermal phase switching in a 1T-TaS2 memory device

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Transition metal dichalcogenide (TMDC) compounds attract great interest because of their strong electron-electron and electron-phonon interactions, resulting in a multitude of emerging states. Of particular interest for applications is the ability to rapidly switch between different states via charge injection. Uniquely, in the layered TMDC 1T-TaS2 a nonvolatile, reversible metallic hidden (H) state can be induced from the insulating equilibrium charge density wave (CDW) state by applying an optical or electrical pulse. As a step towards the development of a new type of ultrafast, nonvolatile cryomemory cells, we have investigated 1T-TaS2 by combining spatially-resolved micro-beam X-ray diffraction and fluorescence, as well as in-situ transport measurements at the Swiss Light Source synchrotron. This unique combination of techniques allowed us to spatially resolve the insultating equilibrium CDW order, and after electrical switching the induced, nonthermal H state. Our experiment reveals that the electrically and optically switched H states are not only electronically but also structurally equivalent. Furthermore, we find a bulk material switch in a narrow channel in-between the electrodes of the devices. This input regarding device design and operation paves the way for the application of 1T-TaS2 in memory technology.

Unveiling the Electronic Properties of α -SnTe: From Ferroelectric Distortion to Unexpected Topological Surface State

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 α -SnTe offers a combination of semiconducting and ferroelectric properties, further enriched by a non-trivial topological behavior. At room temperature, SnTe has a rocksalt atomic structure with a mirror symmetry that protects a metallic topological surface state. However, when the temperature drops below a critical point, a spontaneous structural distortion occurs that not only suppresses the topological surface state but also leads to a macroscopic electric polarization, resulting in a significant Rashba splitting in the valence band.

In the first part of my presentation, I will discuss how we gain insights into the nature of the ferroelectric distortion by observing the temperature evolution of the Rashba splitting in the bulk valence band of SnTe. Our findings suggest an order-disorder phase transition with substantial deviations from a mean-field-like behavior [1].

Although ferroelectric SnTe(111) should be a trivial insulator, I will demonstrate in the second part how we can photoinduce a topological transition. Ultrashort and tailored light pulses allow us to transiently and electronically restore an unexpected topological state, even while the atomic structure remains distorted.

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Unlocking the Promise and Simplicity of Atomically Precise Synthesis for 4dand 5d Metal Oxides through Hybrid MBE

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The ability to achieve atomically precise material synthesis has marked a profound advancement in the field of materials science. Yet, it is often the degree of ease and precision in the synthesis process that paves the way for groundbreaking application and discovery. Consider an element of periodic table that is hard to oxidize and also difficult to evaporate, how do we create an atomically precise thin films of such metals, metal oxides or their heterostructures? This has been a central question in the synthesis science for many decades. In this talk, I will present my group's effort to address this question. We have recently shown that both the low vapor pressure and difficulty in oxidizing a "stubborn" element can be addressed by using a solid metal-organic compound with significantly higher vapor pressure, and with the added benefits of being in a pre-oxidized oxidation state along with excellent thermal and air stability. Using this approach, we show, for the first time, the synthesis of Pt, RuO₂, SrRuO₃ and superconducting Sr₂RuO₄ films with the same ease and control as afforded by III-V MBE. Finally, I will present a detailed MBE growth study of SrRuO₃ films combined with structural and transport characterizations emphasizing the role of structural inhomogeneity on anomalous hump-like magnetotransport, which has long been interpreted as a signature of Skyrmions formation.

Synthesis of Electronic-Grade Quantum Heterostructures by Hybrid PLD

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Modern quantum materials are inherently sensitive to point defects, and require a new synthesis route to produce epitaxial oxide thin films and interfaces clean enough to probe fundamental quantum phenomena. The recent discovery of robust superconductivity at KTaO₃ (111) and KTaO₃ (110) heterointerfaces on KaTaO₃ bulk single crystals offers new insights into the role of incipient ferroelectricity and strong spin-orbit coupling. Electronic grade epitaxial thin film platforms will facilitate investigation and control of the interfacial superconductivity and understanding the fundamental mechanisms of the superconductivity in KTaO₃. The major challenge of research on KTaO₃ system is that it is difficult to grow high-quality KTaO₃ epitaxial thin films due to potassium volatility. Recently, we have developed the hybrid PLD method for electronic grade KTaO₃ thin film growth, which successfully achieves this by taking advantage of the unique capabilities of PLD to instantly evaporate Ta_2O_5 in a controlled manner and evaporation of K₂O to maintain sufficient overpressure of volatile species. We successfully synthesized heteroepitaxial KTaO₃ thin films on 111-oriented KTaO₃ bulk single crystal substrates with a SmScO₃ template by hybrid PLD, followed by a LaAlO₃ overlayer. Electrical transport data show a superconducting transition temperature of \sim 1.35K. We anticipate that the ability to synthesize high-quality epitaxial complex oxides such as KTaO₃ that contain volatile elements will provide a new platform for exploring new physics and technological applications arising from unique characteristics such as large spin-orbit coupling.

This works has been done in collaboration with Jieun Kim, Jungwoo Lee, Muqing Yu, Neil Campbell, Shun-Li Shang, Jinsol Seo, Zhipeng Wang, Sangho Oh, Zi-Kui Liu, Mark S. Rzchowski, Jeremy Levy.

This work is supported by the Gordon and Betty Moore Foundation's EPiQS Initiative, Grant GBMF9065 to C.B.E., and a Vannevar Bush Faculty Fellowship (N00014-20-1-2844).

Controlling the Magnetic Properties of the van der Waals Multiferroic Crystals $Co_{1-x}Ni_xI_2$

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In the growing family of magnetic van der Waals materials multiferroic compounds CoI_2 and NiI_2 have drawn significant attention lately due to the multiferroicity down to the monolayer and frustrated cycloid ground state caused by Kitaev interactions, respectively [1-2]. Despite prior investigations of these materials, the evolution of magnetic ground states within the solid solution between them remains unresolved.

We have successfully grown crystals of the whole solid solution $Co_{1-x}Ni_xI_2$ by employing the selfselecting vapor growth (SSVG) technique and carefully tuning the synthesis conditions according to the composition. Both the lattice parameters and magnetic properties evolve continuously and smoothly from one end member to the other, showing that they can be finely chemically tuned. We also observe that the Ni substitution for Co affects the metamagnetic transition typical for CoI_2 . In particular, we find the existence of this metamagnetic transition of CoI_2 in the NiI₂ structure. Based on magnetic measurements we construct the phase diagram of the $Co_{1-x}Ni_xI_2$ system.

Controlling the magnetic properties by the chemical composition opens new pathways for fabricating electronic devices made of two-dimensional (2D) flakes of multiferroic van der Waals materials.

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Turning a metal into an insulator

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Rare-earth nickelates (RENiO₃) belong to the wider family of perovskite oxides and are well known for their temperature dependent metal-to-insulator transition (MIT), which occurs together with a lowering of the crystal symmetry, i.e. a breathing distortion of the NiO₆ octahedra units [1,2]. By means of RF off-axis magnetron sputtering, the growth of high quality epitaxial RENiO₃ solid solutions thin films and superlattices can be achieved. In a previous study involving nickelate superlattices, the characteristic length scale over which a metallic or an insulating phase can be established and the physics that sets it was investigated [3,4]. In this work, we design a system that exploits the phase boundary cost of maintaining an interface between a metal and an insulator to control the electronic properties of a nickelate based solid solution, specifically the orthorhombic and metallic La_{0.3}Nd_{0.7}NiO₃. We show that a single thin layer of this solid solution turns insulating when sandwiched in a superlattice with SmNiO₃ layers, whereas in the form of a bare thin film, it remains metallic down to low temperatures.

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The Chemistry of Quantum Materials

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Quantum materials are hoped to change technology in various aspects. However, most of the desired applications are hindered by the lack of suitable materials. In my group we are using concepts from chemistry to understand, predict and synthesize new quantum materials. In this talk, I will show how simple concepts, such as measuring bond distances, allow us to make predictions about electronic structures of materials, which we can then use to find new topological materials. We then can combine this with structural building blocks containing magnetic elements to design materials with non-colinear or even non-coplanar magnetism. Thinking about the degree of delocalization in a chemical bond can be helpful to find kagome or linear-chain materials with band structures that better resemble simple tight binding models. I will give a general overview how powerful chemical concepts are in materials discovery and highlight a flute of materials that were discovered in this light.
« Back to program

Phonons with magnetic character

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A phonon is a collective elementary excitation in a crystal and describes an excited state in quantum mechanics with the modes of atomic vibrations. This quasi-particle can interact with another type of excitation, leading to its mixed character. Such an interaction dominates a coupling among correlated degrees of freedom in ultrafast timescales. Here, I focus on two cases where a phonon possesses a magnetic character or angular momentum. (1) A chiral phonon involves rotational atomic vibrations, inducing an orbital angular momentum. Our study on a chiral crystal, quartz, by means of resonant inelastic X-ray scattering with circularly polarized X rays demonstrated the presence of chiral phonons [1]. We disclosed that circularly polarized X rays couple to chiral phonons at general momentum points, which allows us to measure chiral phonon dispersion. (2) An electromagnon is a polar phonon whose wave function hybridizes with that of a magnon and is a characteristic excitation in magnetoelectric multiferroics. We revealed its real-time dynamics by performing two time-resolved X-ray diffraction experiments [2]. Following a coherent excitation of an electromagnon mode, time-resolved resonant X-ray diffraction clarified its magnetic response while time-resolved non-resonant X-ray diffraction observed its phononic response. Combined dynamics disclosed how the electromagnon is excited.

[1] H. Ueda et al., Nature 618 946-950 (2023).

[2] H. Ueda et al., Nat. Commun. 14, 7778 (2023).

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Interplay of electronic orders in kagome metals

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The family of Kagome metals AV3Sb5 with A = K, Rb, Cs has attracted a lot of attention recently for the wealth of exotic phases its members exhibit. In particular, all three members enter a charge-density-wave phase at 100 K and below a critical temperature of 2 K, they become superconducting. While experimental results agree on an in-plane 2x2 reconstruction due to the charge density wave, the out-of-plane wave vector and exact nature of the ordered phase, specifically whether it breaks additional point-group or time-reversal symmetries in the form of loop-currents, has yet to be determined unambiguously. In addition, very little is known about the superconducting state. With multiple conflicting experiments and no clear microscopic understanding, a phenomenological description in the form of a Ginzburg-Landau analysis offers valuable insights. Studying charge-density waves and their interplay, and given recent transport experiments in the normal state, we arrive at a picture in this material class of correlated orders at a tipping point. Finally, the interplay of charge-density-wave order and superconductivity naturally leads to pair-density waves, a phenomenon recently uncovered in experiments.

New approach for nonlinear optical tensor determination. Application to Rare earth nickelates microcrystals

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We developed a novel experimental approach and data analysis technique for the reconstruction of nonlinear optical susceptibility tensors with microscopic resolution. This method is inspired by the rotational-anisotropy second harmonic generation (RA-SHG) [1] that is widely used for the readout of tensor elements of nonlinear susceptibilities of bulk materials. The standard RA-SHG mostly consists of measurements of the polarization-resolved nonlinear signal of bulk crystals and is not applicable in optical microscopes due to weak control of polarization. Our optical geometry combining a Bessel-Gaussian laser beam and a patented optical module [2] to preserve the polarization state allows us to overcome these restrictions and realize "static" RA-SHG analysis with microscopic precision and multiple polarization configurations in the same experiment. For the reconstruction of second-order nonlinear optical susceptibility tensor, we developed a fitting procedure based on evolutional algorithms that demonstrate high efficiency even for lowest-symmetry materials. This new approach is used to investigate the symmetry of the ground state in rare earth nickelates RNiO₃. It was predicted that this family of compounds may exhibit multiferroicity [3] and we will show that the nonlinear optical properties potentially provide experimental evidence for such behaviors.

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[2] V. Multian and J. Teyssier, "A beam splitting/mixing module for an optical system and an associated optical system," 23178209.5, Jun. 08, 2023.

[3] G. Giovannetti, S. Kumar, D. Khomskii, S. Picozzi, and J. van den Brink, "Multiferroicity in Rare-Earth Nickelates RNiO3," Phys. Rev. Lett., vol. 103, no. 15, p. 156401, Oct. 2009, doi: 10.1103/PhysRevLett.103.156401.

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Discovery of Giant Unit-Cell Super-Structure in PrNiO2

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A longstanding challenge regarding spectacular quantum phenomena such as high-temperature superconductivity in the cuprates is to – by design – realize similar physics in other materials. The discovery of superconductivity in infinite layer nickelates [1-3] has therefore sparked immediate excitement. A crucial characteristic of cuprates is the presence of two-dimensional charge order in the superconducting phase. Recently, a similar broken symmetry state – associated with charge order – has been revealed by resonant x-ray scattering in nickelates [4-6]. However, the interpretation of these results is surrounded by controversy and new studies propose that oxygen diffusion could lead to the observed superstructure [7].

To gain new insights into the nature of the observed superstructure, we performed high-energy grazingincidence x-ray diffraction on thin films of PrNiO2. We demonstrate, for the first time, how in-situ high temperature annealing of the thin films induces a giant unit-cell superlattice structure with a rare period-six in-plane and a period-four out-of-plane symmetry [8]. The stability of this superstructure suggests a connection to an energetically favorable electronic state of matter, possibly providing a new pathway – different from Moiré structures – to ultra small Brillouin zone electronics.

[1] D. Li et al., Nature 572, 624–627 (2019).

[2] D. Li et al., Phys. Rev. Lett. 125, 027001 (2020).

[3] S. Zeng et al., Phys. Rev. Lett. 125, 147003 (2020).

[4] G. Krieger et al., Phys. Rev. Lett. 129, 027002 (2022).

[5] M. Rossi et al., Nature Physics 18, 869-873 (2022).

[6] C. C. Tam et al., Nature Materials 21, 1116–1120 (2022).

[7] C. T. Parzyck et al., Nature Materials 23, 486–491 (2024).

[8] J. Oppliger et al., Manuscript in preparation (2024).

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Anomalous electrons in a metallic kagome ferromagnet

Sandy Adhitia Ekahana,¹ Y. Soh,¹ Anna Tamai,² Daniel Gosálbez-Martínez,^{3,4,5,6} Mengyu Yao,^{1,7} Andrew Hunter,² Wenhui Fan,^{8,9} Yihao Wang,¹⁰ Junbo Li,¹⁰ Armin Kleibert,¹ C.A.F. Vaz,¹ Junzhang Ma,^{1,11} Hyungjun Lee,³ Yimin Xiong,^{10,12,13} Oleg Yazyev,^{3,4} Felix Baumberger,^{1,2} Ming Shi,¹ and G. Aeppli^{1,3,14,15}

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We present our work on ferromagnet kagome Fe3Sn2 using micro-focused laser-based angle-resolved photoemission spectroscopy (ARPES). Our experiment reveals several results: First, we can observe the twinned domain of this breathing kagome lattice spatially which has not been reported before. Second, upon a closer investigation, we found a quasiparticle that lives near the Fermi level behaving in a marginal Fermi liquid way, usually found in the cuprates system. Lastly, this interesting quasiparticle is also found to share spectral functions with the nearby and similar band, before its disappearance after a subtle energy and temperature change, demonstrating a conservation of quasiparticles between these two bands. We propose a possible mechanism for how this anomalous electron can be formed by involving a nearby flat band located slightly above the Fermi level which leads to a logical conclusion that the electrons are fractionalized between these two bands.

[1] https://www.nature.com/articles/s41586-024-07085-w.

Exotic superconducting states in 2D materials and moiré engineering at oxide interfaces

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Inspired by surprising recent experiments on the superconducting state in twisted van der Waals moiré systems, we discuss, in the first part of the talk, two possible natural theoretical explanations. In one explanation [1], the 2D nature of these systems and thermal fluctuations are taken into account which naturally leads to interesting vestigial pairing states, yielding spectral functions that are consistent with experiment. In a second explanation [2], we ask the question whether similar spectral functions can also be obtained in a pure mean-field picture. The second part of the talk is motivated by another set of recent experiments demonstrating atomically sharp interfaces between twisted oxides with different Bravais lattices. We will discuss the general band theory for these types of moiré interfaces, uncovering novel forms of geometric magic angles, and explore the unprecedented possibilities of moiré band engineering provided by these systems.

[1] Poduval and Scheurer, Nature Communications 15, 1713 (2024).

[2] Christos, Sachdev, and Scheurer, Nature Communications 14, 7134 (2023).

[3] Putzer, Pupim, and Scheurer, arXiv:2404.12420.

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Observation of fractional quantum anomalous hall effect

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The interplay between spontaneous symmetry breaking and topology can result in exotic quantum states of matter. A celebrated example is the quantum anomalous Hall (QAH) effect, which exhibits an integer quantum Hall effect at zero magnetic field due to topologically nontrivial bands and intrinsic magnetism. In the presence of strong electron-electron interactions, fractional-QAH (FQAH) effect at zero magnetic field can emerge, which is a lattice analog of fractional quantum Hall effect without Landau level formation. In this talk, I will present experimental observation of FQAH effect in twisted $MoTe_2$ bilayer, using combined magneto-optical and -transport measurements. In addition, we find an anomalous Hall state near the filling factor -1/2, whose behavior resembles that of the composite Fermi liquid phase in the half-filled lowest Landau level of a two-dimensional electron gas at high magnetic field. Direct observation of the FQAH and associated effects paves the way for researching charge fractionalization and anyonic statistics at zero magnetic field.

[1] Observation of Fractionally Quantized Anomalous Hall Effect, Heonjoon Park et al., Nature,

https://www.nature.com/articles/s41586-023-06536-0 (2023).

[2] Signatures of Fractional Quantum Anomalous Hall States in Twisted MoTe2 Bilayer, Jiaqi Cai et al., Nature,

https://www.nature.com/articles/s41586-023-06289-w (2023).

[3] Programming Correlated Magnetic States via Gate Controlled Moiré Geometry, Eric Anderson et al., Science, https://www.science.org/doi/full/10.1126/science.adg4268 (2023).

Moiré is Different: Metal-Insulator Transitions, Kondo Lattice Physics and Chiral Spin Liquids in TMD Bilayers

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The greatest open questions in quantum matter physics revolve around strongly correlated electronic phases, traditionally observed in heavy fermions, cuprates and organics. In recent years, a new class of materials emerged where the strength of correlations can be engineered: "moiré materials". I will briefly introduce moiré materials such as twisted bilayer graphene and transition-metal dichalcogenide (TMD) bilayers. I will then focus on three recent results: a universal theory for continuous metal-insulator transitions [1], valley-charge-transfer and Kondo lattice physics under pressure in TMD homobilayers [2] and our prediction of a chiral spin liquid phase in TMD [3,4]. These results show that the wealth of phenomena observed in moiré materials allow for new insights in old correlated problems.

[1] Simone Fratini, Sergio Ciuchi, Vladimir Dobrosavljevic, Louk Rademaker, Universal scaling near band-tuned metal-insulator phase transitions, Phys. Rev. Lett 131, 196303 (2023); arXiv:2307.09292.

[2] Marta Brzezinska, Sergii Grytsiuk, Malte Rösner, Marco Gibertini, and Louk Rademaker, Tuning interactions using pressureinduced Γ-K valleytronics in moire bilayer WSe2, arXiv: 2404.07165.

[3] Dario Rossi, Johannes Motruk, Louk Rademaker, Dmitry A. Abanin, Schwinger boson study of the J1- J2-J3 kagome Heisenberg antiferromagnet with Dzyaloshinskii-Moriya interactions, Phys. Rev. B 108, 144406 (2023); arXiv:2305.15824.

[4] Johannes Motruk, Dario Rossi, Dmitry A. Abanin, Louk Rademaker, Kagome Chiral Spin Liquid in Transition Metal Dichalcogenide Moire Bilayers, Phys. Rev. Research 5, L022049 (2023); arXiv:2211.15696.

Electronic structure of encapsulated mono-, bi- and trilayer T_d -MoTe₂

Julia Issing, Ignacio Gutiérrez-Lezama, Fabian von Rohr, Alberto Morpurgo, Anna Tamai, and Felix Baumberger

Department of Quantum Matter Physics, University of Geneva

Bulk orthorhombic T_d -MoTe₂ is a type-II Weyl semimetal with topological Fermi arc surface states and becomes superconducting at a critical temperature of $T_c = 0.1$ K. Remarkably, superconductivity becomes far more robust in the 2D limit, contrary to generic models and the established trend in ultrathin metal films. Recent transport measurements reported a gradual increase in T_c as the thickness is reduced with T_c reaching 7.6 K in the monolayer [1]. The reasons for the strong increase in T_c as well as the nature of the superconducting state remain unknown. Here, we present the electronic structure of exfoliated mono-, bi- and trilayer T_d -MoTe₂ probed by micro-focused angle resolved photoemission. Our thickness-dependent measurements reveal that mono-, bi- and trilayer MoTe₂ are compensated metals. The electron pocket of monolayer MoTe₂ shows signatures of strong coupling to optical phonons with a mass enhancement $\lambda \approx 1.5$. In bi- and trilayer MoTe₂ electron-phonon coupling is weaker consistent with thickness dependence of T_c .

[1] D. A. Rhodes et al., Nano Lett. 2021, 21, 6, 2505-2511.

Tuning electronic characteristics of MoS₂-Au heterostructures via twist angle manipulation: STM insights

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Transition metal dichalcogenides, exemplified by molybdenum disulfide (MoS_2), have undergone extensive examination on metal surfaces. However, scant attention has been paid to these fundamental heterostructures' twist angle-dependent electronic characteristics. This aspect presents considerable potential for the creation of functional quantum materials. Within this discourse, we will delve into a comprehensive investigation utilizing scanning tunneling microscopy and spectroscopy to scrutinize the electronic traits of monolayer MoS_2 interfacing with gold, focusing on twist angle variations.

Our findings reveal a noteworthy modulation of the semiconductor band edges and consequent band gap in correspondence with the moiré wavelength, which arises from the interaction between MoS_2 and gold. Notably, this modulation diminishes progressively as the twist angle increases. We attribute these observations to the hybridization between the nearest gold and sulfur atoms, which exhibits greater spatial uniformity as the twist angle enlarges [1].

[1] I. Pushkarna, A. Pásztor, and C. Renner, "Twist-angle-dependent electronic properties of exfoliated single layer MoS₂ on Au(111)," Nano Letters, vol. 23, no. 20, pp. 9406-9412, 2023.

Low-density Hall response of two-dimensional electrons with a local and energy-dependent self-energy

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In recent years, various techniques have been developed to control the density of carriers in twodimensional systems, which led to unexpected results for the Hall effect [1]. On the theoretical side, the Hall effect is not well understood at very low density of carriers, where the Boltzmann description looses validity. We study the Hall constant R_H for systems of 2D correlated electrons in the low-density regime, using a Kubo-formula approach where correlations are described by a local self-energy. Even if the energy-dependence of the self-energy is neglected, we find that the Hall constant deviates from the standard $R_H^0 = -1/(|e|n)$ behavior [2]. Beyond such behavior, several microscopic systems yield a scattering rate that is not independent of energy but vanishes as a power law at low energy. For these models, we compute the Hall effect and find non-universal behaviors in the relation between R_H and n, in particular power laws that reflect the power-law in the self-energy.

F. Wu, I. Gutiérrez-Lezama, S. A. López-Paz, M. Gibertini, K. Watanabe, T. Taniguchi, F. O. von Rohr, N. Ubrig, and A. F. Morpurgo, Quasi-1D electronic transport in a 2D magnetic semiconductor, Adv. Mater. 34, 2109759 (2022).
 G. Morpurgo, L. Rademaker, C. Berthod and T. Giamarchi, Hall response of locally correlated two-dimensional electrons at low density, Phys. Rev. Research 6, 013112 (2024).

New superconducting radiofrequency materials serving the future FCC collider

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After the luminosity upgrade of the LHC proton collider, it is recognized that the next research machine in particle physics will be a high-energy lepton collider. Among the projects under study such as the ILC, the CLIC and the muon collider, the FCC-ee (Future Circular Collider - electron positrons) appears to be the most attractive option to cover a broad energy spectrum at a high intensity.

The FCC-ee RF system currently includes more than 1,400 cavities, 25% of which are constructed using niobium thin film technology on a copper substrate, a "CERN specialty" since the 1990s which has demonstrated very high reliability in operation with the LEP and the LHC accelerators. The need to push the accelerating gradient and the quality factor of this cavity type to a level never reached before led to new ideas of superconducting materials optimized in the radiofrequency regime. These new approaches include enhanced chemical surface treatments, improved techniques of thin layer deposition and up-to-date assembly methods in ultra-clean environments.

This presentation will present in details all these aspects and will show the recent progress achieved on prototype cavities specially built for the FCC-ee study.

Towards the development of superconducting joints between REBCO coated conductors: a thermomechanical study

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High-Temperature Superconductors (HTS), particularly Rare Earth Barium Copper Oxides (REBCO), are pivotal in high field applications due to their exceptional properties, notably surpassing conventional superconductors in the upper critical magnetic field (Bc2). REBCO Coated Conductors (CCs) enable the creation of superconducting solenoids generating magnetic fields exceeding 30T. This technological advancement is crucial for Nuclear Magnetic Resonance (NMR), where resolution scales with magnetic field intensity. NMR magnets must operate in persistent mode, with current flowing in a continuous superconducting loop, to ensure necessary field stability. Achieving this requires superconducting joints to address limitations stemming from the available unit lengths of CCs, which are challenging to produce beyond 100-200 meters. However, the complex process of producing superconducting joints in REBCO entails simultaneous temperature and pressure application. The fragility of CCs and the need for controlled oxygen doping in REBCO diminish CCs performance post-thermomechanical cycles. Understanding the effects of temperature and pressure combinations on the critical current (Ic) achievable after joint procedures is crucial. We investigated the effects of temperature and pressure combinations ranging between 600-850°C and 50-80 MPa, respectively, on commercial CCs' Ic at 77K. Complementary TEM and EDX studies were conducted to correlate changes in the REBCO microstructure with Ic alterations.

Controlling and investigating domain and domain walls in PbTiO₃ ferroelectric thin films and heterostructures

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PbTiO₃ is a material that exhibits a bulk paraelectric-ferroelectric phase transition at a critical temperature T_c of 765 K, with a polarisation that develops along the c-axis mostly due to ionic displacements. Theoretical studies of domain structures in PbTiO₃ thin films have revealed complex phase diagrams with regions of distinct domain configurations as a function of different parameters [1].

We study the domain configuration in PbTiO₃ heterostructures, epitaxially grown on $(110)_{o}$ -oriented DyScO₃ substrates, with bottom and top SrRuO₃ electrodes using a combination of atomic force microscopy, laboratory and synchrotron x-ray diffraction, and high resolution scanning transmission electron microscopy. We observe a large asymmetry in the domain configuration due to the anisotropic strain imposed by the orthorhombic substrate, and we find that the periodicity of the domain wall deviates from the Kittel law. As the ferroelectric film thickness increases, the domain configuration evolves from flux-closure to an a/c-phase, with a larger scale arrangement of domains into superdomains [2].

Moreover, above a critical value of $PbTiO_3$ thickness, we observe a modulation in the structure of the top SrRuO₃ electrode, demonstrating the possibility of domain nano-engineering via structural coupling to ferroelastic domains [3].

[1] Schlom et al., Annu. Rev. Mater. Res., 37, 589-626 (2007).

[2] Lichtensteiger, ..., L.T. et al., APL Mater. 11, 061126 (2023).

[3] Lichtensteiger, ..., L.T. et al., APL Mater. 11, 101110 (2023).

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ABSTRACTS

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Signatures of skyrmion stripes in nematic superconductors

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In a type-II superconductor below T_c , the magnetic field penetrates in the form of flux lines (vortices) which, due to their reciprocal repulsion, arrange into a regular (Abrikosov) lattice. Unlike the standard case, in nematic superconductors, electron pairs are polarized in one, spontaneously chosen direction, thus breaking the rotational symmetry of the normal state. In either case, the overlapping field profiles of the superconducting vortices create a well-defined magnetic field distribution, which can be detected experimentally via local probes such as muons through the degree of their spin depolarization. Intriguingly, nematic superconductors can host coreless vortices (skyrmions) consisting in a bound state of two spatially separated half-quantum vortices. Such topological excitations are thought to be good candidates for low-power data-storage technologies. Recently, the skyrmion configurations that may arise in nematic superconductors were calculated and predicted to form striped patterns [1]. Remarkably, their μ SR signature was shown to correspond to a peculiar two-peak distribution, notably different from that of standard type-II superconductors. By investigating selected nematic superconductors, such as CaSn₃ or LiFeAs, we bring compelling evidence of their unusual magnetic response, thus corroborating the skyrmion-stripe scenario [2].

[1] M. Speight, T. Winyard, and E. Babaev, Phys. Rev. Lett. 130, 226002 (2023).

^[2] H. Siddiquee et al., Phys. Rev. B 105, 094508 (2022).

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STEM-EELS studies of interfaces between perovskite oxide membranes and single-crystal carrier substrates

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Perovskite-structure transition metal oxide epitaxial thin films exhibit a variety of functionalities that make them highly promising for the development of novel electronic devices. In recent years, interest has arisen in transforming these thin films into perovskite membranes because of their potential benefits of, for instance, no structural mismatch strain effects, possibilities to create texture (wrinkles), and versatile stacking [1]. In our work, SrTiO₃ (STO) membranes are grown on Sr₃Al₂O₆ (SAO) sacrificial layers on STO(001) substrates using pulsed laser deposition. After dissolving the SAO layer in deionized water, the resulting STO membrane is transferred onto a Nb-doped STO(001) carrier substrate. This membrane heterostructure is either left "as is", or is subjected to a thermal annealing at one of a series of temperatures. We focus on cross-section studies of these membranes using Cs-corrected scanning transmission electron microscopy, where atomic structure quality and flatness/roughness can be precisely assessed. By combining with electron energy-loss spectroscopy, we further apply this approach with a goal of probing the bonding of membranes transferred to single crystal substrates, and how this evolves with thermal annealing.

[1] A. J. Yang et al., ACS Nano. 17, 9748-9762 (2023).

Charge order above room temperature in kagome superconductor LaRu3Si2

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Paul Scherrer Institute

The present work focuses on LaRu3Si2, which has one of the highest critical temperatures (Tc = 7 K) among kagome superconductors. The structural motif of this material represents Ru-based kagome layers placed between LaSi2 hexagonal nets. Our current single-crystal X-ray diffraction study of the pristine and Fe-doped LaRu3Si2 reveals a cascade of structural phase transitions with temperature, consistent with the previously predicted charge order instabilities. Above 600K, the material crystallizes in an undistorted P6/mmm structure (HT-hex), which doubles along the c-direction upon cooling (LT-hex). Below 400K, additional charge order (CO-I) reflections with q1 = (1/4 0 0) evolve, followed by the second charge order transition into CO-II with q2 = (1/6 0 0) below 180K. Apart from detailing the transition in reciprocal space, I will also describe the corresponding structural transformations observed in real space and discuss their potential implications on superconductivity.

ets August 14-16, 2024 SWM 2024 - Swiss Workshop on Materials with Novel Electronic Properties

Poster-1-4

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Rashba coupling to polar modes in superconducting KTaO₃

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The discovery of superconductivity in KTaO₃ (KTO) heterostructures and uncapped surfaces has recently triggered significant interest. Remarkably, the T_c shows high sensitivity on the crystallographic orientation, reaching values an order of magnitude larger than that of SrTiO₃ (STO) heterostructures [1]. As such, insights into the pairing mechanism are of great interest. We study a pairing mechanism based on spin-orbit assisted coupling between the t_{2g} conduction electrons and the soft ferroelectric (FE) modes present in the material. The theoretical approach was developed for bulk STO and generalized to any incipient FE [2]. By combining ab initio calculations and a microscopic model, we find a strongly anisotropic Rashba-like interaction as well as a strong electron-phonon coupling to the soft transverse FE mode [3,4].

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« Back to program

Interplay of charge density wave order and superconductivity

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In many superconductors, the superconducting state emerges on top of a charge density wave (CDW). An intriguing example is the AV₃Sb₅ (A=K,Rb,Cs) family of superconductors, where a 2 × 2 in-plane CDW ordered phase, potentially breaking time-reversal symmetry, appears at $T \approx 100$ K. To determine the microscopic origin and structure of the ordered phases, one often studies the CDW and superconductivity on the kagome lattice independently. However, it remains an outstanding question to understand the mutual influence of the different orders.

In our work, we present a phenomenological theory of CDW and superconducting orders based solely on symmetry arguments for the kagome lattice. For this purpose, we derive a Ginzburg-Landau free energy of possible 2×2 CDW order and superconductivity and explore the impact of the dominant coupling terms. In particular, we study the consequences of additional spatial or time-reversal-symmetry breaking of the CDW order, coupling to a pair density wave, and we discuss possible experimental consequences. Our study uncovers a rich phenomenology with interesting differences to the results of earlier studies in tetragonal systems.

« Back to program

Anomalous magnetic domain patterns in Kagome semimetal Co3Sn2S2

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Investigating magnetism in topological materials reveals intriguing correlations between magnetic and electronic states, notably in the magnetic Weyl semimetal Co3Sn2S2, which features a cobalt ion kagome lattice [1-4]. This work employs Lorentz mirror electron microscopy (L-MEM) and X-ray magnetic circular dichroism photoemission electron microscopy (XMCD-PEEM) to explore the temperature- and field-dependent dynamics of magnetic domains in Co3Sn2S2. We observe spontaneous magnetic bubbles of tens of micrometers under zero-field and minimal-field cooling conditions, illustrating an intrinsic exchange bias effect as seen in M-H curves via SQUID. The asymmetric domain evolution during field-cooling and warming processes offers a microscopic view into the thermomagnetic hysteresis observed in M-T curves. Furthermore, the field-dependent behaviors of these magnetic bubbles suggest the potential existence of hybrid domain walls. This research contributes to our understanding of the complex magnetic phenomena in Co3Sn2S2.

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Quantum sensing of correlated electrons in moiré hétérostructures

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Quantum sensing is a fast developing area, where properties specific to the quantum realm are exploited to get more accurate data on a much sensitive scale. We present a new sensing scheme aimed at in-depth studies of the highly tunable moiré Transition Metal Dichalcogenides (TMDs). The technique aims to probe local phenomena as well as large-scale electronic correlations, which are prominent in these systems. We obtain this precision by studying dipolar intraleyers excitons through the degree of circular polarisation obtained by photoluminescence (PL), which allows to not average over domains or disorder. As a case study, we will present our PL results on a dual moiré hétérostructure of WSe2/MoSe2/WSe2 and compare them to reflectance results and simulations. We could observe spectral jumps of IX with blue- and red-shifts, occuring at what we identified to be certain rational fillings of the electronic moiré lattice. These results introduce moiré confined IX excitons as a powerful tool to refine our understanding of light-matter interactions in systems with complex electronic structures.

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Poster-1-8

The Josephson effect in long, clean SNS junctions

Silvan Aepli

ETH Zürich

If we have a Josephson junction where the weak link is a long, pure metal, Andreev bound states form. I will show what Andreev bound states are and what happens when spin-singlet and spin-triplet superconductors are coupled. I will also show the current phase relation at zero temperature for couplings between conventional and unconventional superconductors (s-wave, d-wave and p-wave).

Superconducting and normal state properties of the kagome system $Ta_2V_{3.1}Si_{0.9}$ probed by muon spin rotation

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Recently, the Kagome lattice has been extensively explored as a model system to host several diverse quantum phases, from frustrated magnetism to unconventional superconductivity [1-3]. Ta₂V_{3.1}Si_{0.9} is a newly identified Kagome superconductor with a T_c of 7.5 K, a record high for Kagome metals at ambient pressure [4]. Here we conducted comprehensive μ SR measurements on the superconducting and normal state properties of Ta₂V_{3.1}Si_{0.9} [5], to reveal bulk superconductivity with an extremely low superfluid density, which is comparable to cuprates and currently the lowest T_C/ λ ⁻² ratio of all the Kagome superconductors [3]. In addition, below T_c, μ SR reveals two nodeless gaps, which are robust against hydrostatic pressure up to 1.8 GPa, and an anomalous paramagnetic shift in response to an external magnetic field. In the normal state, we find a sizeable increase in the zero-field muon spin depolarization rate below 170 K. This shows similarities with other Kagome-lattice superconductors, suggesting a potential state of time-reversal symmetry breaking [6,7], and requires further study to determine its origin. This combination of results classifies Ta₂V_{3.1}Si_{0.9} as possessing both an unconventional superconducting and normal state.

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Superconductivity in Atomically Thin Films: Diodes and 2D Critical State Model

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A superconducting diode carries dissipationless supercurrents in one direction, but resistive normal currents at finite voltages in the opposite direction, a phenomenon that occurs when the critical current is different in magnitude depending on the polarity. They offer perfect voltage rectification if an alternating current of magnitude between these values is applied. Despite the similar names coined, diodes and superconducting diodes have key symmetry differences due to their vastly different microscopic physics [1]. The comprehensive understanding of superconductivity is a multi-scale task that involves several levels, starting from the electronic scale determining the microscopic mechanism, going to the phenomenological scale describing vortices and the continuum-elastic scale describing vortex matter, to the macroscopic scale relevant in technological applications. The prime example for such a macro- phenomenological description is the Bean model that is hugely successful in describing the magnetic and transport properties of bulk superconducting devices. Motivated by the development of novel devices based on superconductivity in atomically thin films, such as twisted-layer graphene, here, we present a simple macro-phenomenological description of the critical state in such two-dimensional (2D) thin films. While transverse screening and demagnetization can be neglected in these systems, thereby simplifying the task in comparison with usual film- and platelet shaped samples, surface- and bulk pinning are important elements to be included. We use our 2D critical state model to describe the transport and magnetic properties of 2D thin-film devices, including the phenomenon of non-reciprocal transport in devices with asymmetric boundaries and the superconducting diode effect.

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Poster-1-12

« Back to program

Schwinger boson study of the J1-J2-J3 kagome Heisenberg antiferromagnet with Dzyaloshinskii-Moriya interactions

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Schwinger boson mean-field theory is a powerful approach to study frustrated magnetic systems, which allows to distinguish long-range magnetic orders from quantum spin liquid phases, where quantum fluctuations remain strong up to zero temperature. In this paper, we use this framework to study the Heisenberg model on the kagome lattice with up to third-nearest-neighbor interaction and Dzyaloshinskii-Moriya (DM) antisymmetric exchange. This model has been argued to be relevant for the description of transition metal dichalcogenide bilayers in certain parameter regimes [1], where spin liquids could be realized. By means of the projective symmetry group classification of possible ansätze, we study the effect of the DM interaction at first-nearest neighbor and then compute the J2-J3 phase diagram at different DM angles. We find a phase displaying chiral spin liquid characteristics up to spin S=0.5, indicating an exceptional stability of the state.

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« Back to program

Studies of the artificial flux pinning in ternary Nb₃Sn multifilamentary wires with internally oxidized nanoparticles

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Nb₃Sn is still defending its place against high temperature superconductors in high-field applications, like high-resolution NMR spectrometers, fusion magnets and laboratory magnets, and has even regained interest pulled by the projected Future Circular Collider of CERN. To meet the expectations of applications requiring ever increasing performance, we are implementing the internal oxidation process to increase the defect density in Nb₃Sn (grain boundaries and nanoprecipitates) and thus improve pinning force and consequently critical current density. Internal oxidation involves Nb-alloys containing high oxygen-affinity elements like Zr or Hf and an oxygen source (SnO₂). Using the X-ray Absorbing Near-Edge Structure (XANES), we demonstrated that the oxide nanoparticles (HfO₂ or ZrO₂) are formed during the synthesis of Nb₃Sn[1], which limits the growth of Nb₃Sn grains and increases the grain boundary density[2]. Based on Transmission Electron Microscopy images we determined the precipitate size to be in the 4-10 nm range, approximately twice the coherence length of Nb₃Sn (3nm), which makes them effective pinning centers. The pinning enhancement is set by size and number concentration of nanoparticles, which are strongly influenced by Nb₃Sn formation temperature[3]. A deep understanding of the nanoparticle growth mechanism is required to bring the internal oxidation process to industrial, kilometer-long wires.

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Unusual magnetoresistance response in van der Waals antiferromagnetic semiconductor CrPS₄ vertical transport

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Vertical transport through antiferromagnetic multilayer devices has been intensively investigated, and negative magnetoresistance due to injection-limited tunneling processes has been found in all cases. Here, antiferromagnetic semiconductor CrPS_4 , in which transport is not injection-limited but space charge-limited, is investigated. The I-V characteristics of our devices exhibit a trap-limited regime -with a small current that increases rapidly with increasing bias and a trap-free regime, with a current that depends quadratically on the applied bias (and transport mediated by states in the conduction band). In the trap-limited regime, we observe a very large and positive magnetoresistance when the magnetic field B is well below the spin-flip transition. We attribute the phenomenon to the response of the wavefunction of localized states to the applied magnetic field. Specifically, the wavefunction is squeezed as B is increased, resulting in an exponential decrease of the overlap of the wavefunction of impurity states in layers with the same spin (the next-next layers, at small B). Finally, in the trap-dominated regime, we observe large magnetoresistance oscillations, whose origin remains to be explained in detail. Our experiments reveal a transport regime that had not so far been observed in 2-dimensional magnetic semiconductors.

Moiré magnetism in CrBr3 multilayers emerging from differential strain

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Interfaces between twisted 2D materials host a wealth of physical phenomena originating from the long-scale periodicity associated with the resulting moiré structure. Besides twisting, an alternative route to create structures with comparably long -or even longer- periodicities is inducing a differential strain gradient between adjacent layers in a van der Waals (vdW) material. Despite recent theoretical efforts analyzing its benefits, this route has not yet been implemented experimentally. Here we report evidence for the simultaneous presence of ferromagnetic and antiferromagnetic regions in CrBr3 - a hallmark of moiré magnetism- from the observation of an unexpected, low-temperature magnetoconductance in CrBr3 tunnel barriers with ferromagnetic Fe3GeTe2 and graphene electrodes. We attribute the phenomenon to the presence of a strain gradient in the CrBr3 multilayer, which locally modifies the stacking and the interlayer exchange between adjacent CrBr3 layers, resulting in spatially modulated spin textures. Our conclusions indicate that inducing differential strain in vdW multilayers is a viable strategy to create moiré-like superlattices, which may offer in-situ continuous tunability in the future.

Long Ranged Proximity Effect in $YBa_2Cu_3O_{7-\delta}$ - Sr_2IrO_4 Thin Film Multilayers Revealed by X-ray Absorption Spectroscopy

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Thin film heterostructures consisting of the high- T_C superconductor YBa₂Cu₃O₇ (YBCO) and the iridate Sr₂IrO₄ (SIO) have been predicted to host induced superconducting spin-triplet [1] or Majorana bound states [2] and to find applications in devices such as superconducting diodes. These possibilities emerge because of the strong spin-orbit coupling [3] and the peculiar magnetic properties [4] of SIO.

Using X-ray Absorption Spectroscopy at both the Cu L_3 and the Ir L_3 edge, we observe a large charge transfer in multilayers of these materials with holes being transferred from YBCO to SIO. This leads to insulating behavior for thin YBCO layers. We also study the influence of the interface on the magnetism of both materials with X-ray circular dichroism. We find that the Ir⁴⁺ ions in sufficiently thick SIO carry a magnetic moment as previously seen in [4]. Further, we also observe an induced magnetic moment in the YBCO layer within the superconducting phase.

The interplay between superconductivity and magnetism in the YBCO layer raises hopes to induce spin-triplet superconductivity and further emerging exotic properties. This work provides important insights on interface interactions in these heterostructures which is a crucial step towards real life applications and devices.

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Electrical transport study near a zero-Kelvin metal-insulator transition of bulk nickelates Pr1-xLaxNiO3

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The discovery of superconducting phases in different types of nickelates, including infinite-layer nickelates [1], quintuple-layer nickelates [2], and pressure-induced bulk nickelates [3], has sparked significant interest and motivated further exploration for new nickelate superconductors. Superconductivity in cuprates, Cu-based analogue of nickelates, is strongly influenced by magnetic fluctuations associated with an antiferromagnetic quantum phase transition [4]. Understanding the mechanism of Cooper pairing in cuprates, which cannot be fully explained by the conventional BCS theory, requires investigating anomalous phenomena connected to magnetic quantum phase transition, which could also play a crucial role in nickelate superconductors. The compound RNiO3 (where R represents rare earth elements) exhibits diverse ground states, such as metallic paramagnet and insulating antiferromagnet, depending on the specific rare earth element [5]. By applying pressure to PrNiO3, a compound located near a zero-Kelvin metal-insulator transition (MIT), it is possible to tune the insulating antiferromagnetic (I-AF) ground state into a metallic paramagnetic (M-PM) state at a critical pressure of Pc \sim 1 GPa [6]. Near Pc, temperature-dependent electrical resistivity, measured above 5 K, was fitted with a temperature exponent of 4/3, which may be related to the antiferromagnetic fluctuation associated with the critical point. The phase transition from I-AF to M-PM of PrNiO3 can also be achieved by La-doping, which leads to a structural transition from a monoclinic structure (P21/n) to an orthorhombic structure (Pbmn) [5]. In this presentation, we will revisit the zero-Kelvin MIT of PrNiO3 via La-doping. We have successfully synthesized a series of Pr1-xLaxNiO3 polycrystals using high-pressure synthesis and measured the electrical resistivity of the samples down to T = 0.5 K in order to investigate the anomalous phenomena associated with quantum fluctuations near the zero-Kelvin MIT.

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Poster-1-18

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Noncollinear textures in moiré magnets

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University of Geneva

Two-dimensional magnetism and moiré physics are two very rapidly growing fields due to recent experimental advances. In this work, we demonstrate how noncollinear magnetic textures may arise in a bilayer of two-dimensional ferromagnets when the interlayer Heisenberg coupling is stacking-dependent. In particular, we focus on the chromium halides (CrX_3) and study theoretically how the magnetic textures can be controlled through a twist, strain, or an external magnetic field. We find that ferromagnetic and antiferromagnetic regions can coexist by forming noncollinear textures in two dimensions. These can be controlled and forced to undergo spin-flip or spin-flop transitions through external parameters. ets August 14-16, 2024 SWM 2024 - Swiss Workshop on Materials with Novel Electronic Properties

Poster-1-19

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Doping and temperature evolution of the pseudogap state of bulk electron-doped Sr₂IrO₄

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 Sr_2IrO_4 is a layered perovskite isostructural to the high Tc cuprate superconductor La_2CuO_4 . The strong spin-orbit coupling of the 5d Ir⁴⁺ ions lifts the degeneracy of the t_{2g} orbitals resulting in a single narrow half-filled band described by pseudospin $J_{eff}=1/2$ degrees of freedom. This promotes a Mott insultating ground state with antiferromagnetic order below 240 K despite the modest Coulomb interaction in the Ir 5d shell. These similarities with cuprates extend to the unusual metallic state of lightly electron doped Sr_2IrO_4 characterized by Fermi arcs and a pseudogap [1]. Based on this analogy, d-wave superconductivity was predicted [2] but to date no superconductivity was observed down to 100 mK.

In this presentation, I will show Angle Resolved Photoemission (ARPES) results on electron doped bulk crystals up to 10% doping, nearly two times higher than previously achieved. Our results show that nodal states become more coherent with increased doping while the antinodal pseudogap persists up to the highest doping. Following the temperature evolution of these features, we show that the pseudogap closes around 200 K for 10% doping. Concomitantly, we find a redistribution of spectral weight along the Fermi surface, reminiscent of the doping induced spectral weight redistribution in cuprates [3].

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« Back to program

The puzzle of metallic and insulating phases in the CDW system 1T-TaSe₂

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In the layered transition-metal dichalcogenide 1T-TaSe2 the formation of a star-of-David charge density wave results in a half-filled band at the Fermi surface that is sensitive to electron correlations. Interestingly, while the bulk material remains a metal, the surface displays a mix of different phases, ranging from insulating to metallic, all with the same in-plane charge ordering. We used microfocus ARPES to investigate the quasiparticle dispersion in these different spatial domains. Insulating areas show characteristics of a band insulator, while metallic regions exhibit a chiral Fermi surface. Additionally, within the metallic phase, we found a series of bands varying in number and energy position. A direct comparison to DMFT calculations considering slabs of different thickness allows us to reconcile this puzzle as the combined effect of stacking faults between the layers and quantum confinement.

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Poster-1-21

Light Matters: HHG Spectroscopy of Solids

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Intense laser pulses, with energies comparable to electron binding in solids, unlock a new regime: extreme nonlinear optics. This phenomenon produces high-order harmonic light from within the material, a breakthrough that birthed the field of attosecond science. It offers access to previously unseen spectral ranges, enabling attosecond-scale exploration and novel spectroscopy techniques. These techniques allow detailed probing of a material's electronic structure. This section focuses on our research utilizing high harmonic spectroscopy to investigate various solid-state systems. We explore properties like topology, superconductivity, disorder, and strong correlations in condensed matter. By correlating different optical excitations with high harmonic generation, we reveal the ultrafast dynamics of both single-particle and collective electronic excitations in these materials. We show how HHG spectroscopy can probe exotic Majorana fermions [1], reveal various strongly correlated phases in a cuprate superconductor [2], probe multifractality of wavefunctions in quasiperiodic materials [3], and track phase transitions from the Mott to a charge density wave phase in strongly correlated systems [4]. Our research emphasizes the significant potential of extreme nonlinear optics in understanding various solid state quantum phenomena.

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« Back to program

Surface symmetry characterization of SrTiO3(111) via optical second harmonic generation

Changjae Roh and Andrea Caviglia

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In this presentation, we report experimental findings regarding the structural symmetry evolution of SrTiO3(111) single crystal using optical second harmonic generation (SHG). We monitor finite and clear anisotropy of azimuth-angle dependent SHG response that is allowed by the structural discontinuity at surface. In particular, we observe three different types of SHG responses depending on the temperature. Above 105 K, in triangular lattice of cubic phase along (111) direction, azimuth-angle dependent SHG pattern displays six-fold anisotropy reflecting the trigonal symmetry at the surface. Below 105 K, SHG pattern manifests two-fold symmetry with six lobes, which reflects symmetry lowering. Below 40 K, SHG response acquires a different two-fold pattern with four lobes associated with the quantum paraelectric phase. We analyze the monitored SHG patterns by considering electric dipole contributions and discuss surface symmetry evolutions resulting from the two structural phase transitions: triclinic-monoclinic phase transition and monoclinic-quantum paraelectric phase transition at 105 K and 40 K, respectively.
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Poster-1-23

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Tunneling conductance and spectroscopy at step edges in chiral triplet superconductors

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Surface Andreev bound states and the spectra of single-particle excitations provide valuable insights into the electronic structures of unconventional superconductors, offering clues to the determination of pairing symmetry [1]. Recently, an STM study of heavy-fermion superconductor UTe_2 has observe electron-hole asymmetric tunneling differential conductance inside the superconducting gap at step edges [2]. Supported by crystallographic symmetry arguments and further experimental indications of triplet pairing, this observation suggests a realization of chiral triplet topological superconductivity. However, the cause of asymmetric tunneling signals remains elusive and awaits theoretical explanation.

In this study, we explore possible causes and models of the asymmetric tunneling signature in UTe_2 using Bogoliubov-de Gennes equations and the tunneling Hamiltonian formalism [3] to simulate STM experiments of chiral triplet superconductors. We discuss the relationship between chiral edge states and their contribution to tunneling signals. In addition, we carry out quantum transport analysis in normal-superconductor (NS) junctions based on BTK Formalism [4], which allows us to attribute the asymmetric tunneling signals to momentum selective tunneling at sample edges at a phenomenological level.

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Poster-1-24

Scanning Nitrogen-Vacancy Magnetometry to Study the Origin of Exchange Bias in 2D van der Waals Heterostructures

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2D van der Waals magnets are an interesting platform to explore new magnetic phenomena at a reduced dimensionality. Their atomically sharp and clean surfaces offer unique opportunities to investigate interface effects and utilize them in novel heterostructures, such as the exchange bias between a 2D ferromagnet (FM) and antiferromagnet (AFM). However, the origin of exchange bias is often poorly understood due to a lack of experimental tools that are sensitive to the exact magnetic state at the interface. Scanning nitrogen-vacancy magnetometry (S-NVM) can directly probe the magnetic order with high sensitivity and nanoscale spatial resolution of such an interface, providing unique insights into these heterostructures [1].

Here, we study a heterostructure between the 2D FM Fe_3GeTe_2 and AFM $MnPS_3$. Although $MnPS_3$ exhibits a perfectly compensated magnetic surface, anomalous Hall measurements reveal a strong exchange bias on Fe_3GeTe_2 . Using S-NVM, we reveal that at temperatures well below its Néel temperature, $MnPS_3$ deviates from its ideal bulk magnetic structure and shows a non-zero remanent magnetic moment with easy-plane anisotropy. The correlation of the temperature dependence indicates that this anomalous moment is the underlying mechanism of the exchange bias in the heterostructure [2].

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Poster-1-25

« Back to program

Probing the electronic structure of cuprate vortex cores by STM

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The magnetic vortices in cuprates have been intensely studied over the years. It has been known for a long that vortex halos of HTS cuprates host exotic electronic orders modulating the local density of states (LDOS) at atomic length scales [1]. Earlier scanning tunneling microscopy (STM) investigations revealed charge modulations oriented along the Cu-O bond directions (period \approx four Bi-Bi lattice spacing) inside the vortex halo region [2], which were later understood in terms of dispersive vortex-enhanced quasiparticle interference patterns [3]. However, the vortex cores were still lacking conventional signatures such as the zero-bias conductance peak (ZBCP) at the core center originally predicted [4] for d-wave superconductors. Only recently, a study performed at a low field in heavily overdoped Bi-2212 reported the observation of d-wave core signatures [5]. Here, we present a thorough STM study of the charge order and vortex cores in Bi-2212 as a function of a very broad range of hole doping, magnetic field, and temperature. They provide novel insight into the checkerboard-like charge order, the subgap states and ZBCP in the vortex core, the pseudogap, and the superconducting gap.

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Poster-1-26

« Back to program

Soft phonons in strained multiferroic TbMmO3 films

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We use far-infrared ellipsometry to determine the anisotropic optical response of the TbMnO3 film in the spectral range of 100-700 cm-1 and temperature range of 10-300 K. The 44 nm thick sample was grown by Pulsed Laser Deposition on an orthorhombic YAlO3 (010) substrate.

We were able to extract phonons properties, and observe softening due to the multiferroic phase transition. The analysis of the TbMnO3 thin film is complicated by the anisotropic response of the YAlO3 substrate, which we have precisely determined a priori on a series of YAlO3 crystals with various surface cuts.

Poster-1-27

« Back to program

Weak ergodicity breaking in multi-band fermionic systems

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Many-body scars are excited states that violate the Eigenstate Thermalization Hypothesis and are therefore responsible for weak ergodicity breaking. We extend the Group-Invariant formalism for constructing Hamiltonians with many-body scars to the multi-band electron systems. We derive the generalizations of the scar families known in the single-band case including the eta-pairing states. We demonstrate that most of the interactions that are usually considered in the context of unconventional superconductivity in materials do support many-body scars. Poster-1-28

« Back to program

Tuning a CDW Phase Through Intrinsic Doping in Bulk ZrSe₂

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Using low-temperature scanning tunnelling microscopy and spectroscopy (STM/STS), we investigated bulk $ZrSe_2$, a layered transition metal dichalcogenide (TMD). We show that intrinsic impurities dope the system and shift the Fermi level into the conduction band, causing a semiconductor-to-metal transition accompanied by the appearance of charge density wave (CDW) phases. The CDW phase is a collective phenomenon in which the electrons in a material arrange themselves in a periodic pattern, leading to a modulation in the charge density. Due to the local nature of the doping impurities, we successfully correlate the presence of impurities with shifts in the Fermi level and finite CDW modulation amplitudes, highlighting the tunability of correlated electronic phases through doping in TMDs. Furthermore, due to the nature of the electronic bands and their crossing with the Fermi level, our investigation also highlights the k-dependence of STM, inciting increased attention to systems with similar electronic structures.

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Poster-1-29

« Back to program

Frustration-induced diffuse magnetic scattering in metallic HoInCu4

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Materials with magnetically frustrated interaction often host unconventional phases of matter, such as multiferroics, (quantum) spin liquid and exotic magnetic phases. However, most research on frustrated materials have been performed on insulating spin systems, but only little work has been done on metallic systems.

In metallic HoInCu4, frustration stems from the cubic face-centered arrangement of the rare-earth ions, likely leading to a magnetic ground state with partial magnetic order where only half of the Holmium moments exhibit long-range magnetic order, the other half remaining short-range correlated [1]. Here, we use neutron scattering to elucidate the microscopic mechanism leading to this intriguing ground state. Notably, we will show diffuse magnetic scattering results of HoInCu4 as function of temperature and external magnetic field. We will discuss how the diffuse signal can be attributed to magnetic nearest and next-nearest neighbor interactions, and compare the measured magnetic excitations to the predicted model calculations.

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Poster-1-30

Applying Coherent Two-Dimensional Spectroscopy to a Pulsed Magnetophononic System

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Coherent two-dimensional spectroscopy is a powerful tool to distinguish non-linear contributions to the non-equilibrium physics of quantum systems. The technique has no frequency-range limitation and thus has recently been used in the terahertz regime to observe the high-order response of magnon excitations [1]. In linear magnetophononics, the modulation of magnetic interactions by laser-driven phonons, the coupled phononic and magnetic excitations both have frequencies similar to that of the driving pulse. In this work we use the new frequency axis offered by coherent two-dimensional spectroscopy to isolate the non-linear response of such a system by applying the methodology to a straightforward model of a gapped quantum spin chain with strong magnetophononic coupling [2]. Pulsed driving in this model reveals non-linear contributions of hybrid phononic and magnetic nature, including the sum and difference frequencies of composite phonon-bitriplon excitations [3]. We demonstrate that coherent two-dimensional spectroscopy offers both qualitative and quantitative separation of the different non-linear contributions emerging at strong coupling in pulsed magnetophononics.

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Poster-1-31

Calculating the complete spectral functions of quantum magnetic models and materials

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We report on the development of systematic cylinder matrix-product-state (MPS) methods to perform unbiased calculations of the full spectral function, $S(\mathbf{q}, \omega)$, of any spin model with local interactions. By applying these methods to different systems in all applied magnetic fields up to saturation, we show how spectral fingerprints reveal novel phenomena. In unfrustrated Heisenberg antiferromagnets, we examine the presence of field-induced shadow modes, which are found experimentally in the squarelattice material $(CuF_2(H_2O)_2)2pyz$ [1] and the honeycomb-lattice compound YbBr₃ [2]. In the ideally frustrated "Shastry-Sutherland material," SrCu₂(BO₃)₂, we reveal the presence of the spin-nematic phase, which is a low-field S = 2 condensate [3]. In the triangular-lattice Heisenberg system CsYbSe₂, we benchmark and offer an explanation for the extensive scattering continua [4]. While a quantitative calculation of excitation spectra constitutes an evolution in the understanding of unfrustrated models, it is a veritable revolution for frustrated ones. The provision of unbiased MPS spectral functions allows the problem of understanding to be factorised into the two separate stages of expression and interpretation, thereby sharpening the focus on the latter step. We conclude that there is still plenty of new physics to be found in the spectral response.

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SWM 2024 - Swiss Workshop on Materials with Novel Electronic Properties

Poster-1-32

« Back to program

Probing electronic excitations in the Shastry-Sutherland compound SrCu2(BO3)2 with resonant inelastic x-ray scattering

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When multiple spins interact, they can give rise to complex collective behaviour and exotic quantum phases. This is particularly true when competing effects, including magnetic frustration, prevent the formation of simple ordered magnetic states. An important test case to investigate these phases is the Shastry-Sutherland model, a 2-dimensional network of orthogonal interacting spin dimers, together with its experimental material realization $SrCu_2(BO_3)_2$ [1]. To gain a comprehensive understanding of exotic quantum effects in this system, it is necessary to account not only for the role of spin interactions and geometric frustration but also for their coupling to the lattice and high-energy electronic states. Although spin-lattice coupling has been quantified in this system [2], neither the nature of electronic excitations nor their coupling with the magnetic interactions have ever precisely been determined. Here we have conducted a Cu L-edge and O K-edge resonant inelastic X-ray scattering (RIXS) experiment to gain deep insight into the electronic excitations of the Shastry-Sutherland compound $SrCu_2(BO_3)_2$. RIXS was able to unambiguously reveal the charge-transfer (CT) or intra-orbital character of the excitations and provides a more comprehensive understanding of the coupling between spin and orbital degrees of freedom in quantum spin systems.

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[2] F. Giorgianni et al. (2023) Ultrafast Frustration-Breaking and Magnetophononic Driving of Singlet Excitations in a Quantum Magnet.

« Back to program

Breaking new ground in quantum detection with SNSPDs: the search for light-mass dark matter and high-critical-temperature superconductors

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Initially developed for deep-space communication and quantum information science, SNSPDs possess specific characteristics that make them particularly suited for detecting light dark matter (DM). Although these detectors have already shown promising results [1], they require further development before being used in the final designs for a DM experiment. In first part of my talk, I will discuss the remaining technological challenges, design, and characterization of the devices.

The operation of SNSPDs based on conventional superconductors, which have a low critical temperature (Tc), requires costly and bulky cryocoolers. This motivated exploration of other superconducting materials with higher Tc that would enable single-photon detection at elevated temperatures, yet this task has proven exceedingly difficult. Here I show that with proper processing, high-Tc superconductors can meet this challenge [2][3]. We fabricated superconducting nano- and microwires out of thin flakes of BSCCO, thin MgB2 films and LSCO-LCO bilayer films and demonstrated their single-photon response up to 25, 20 and 8 K, respectively. High-Tc based SNSPDs exhibited single-photon sensitivity at the technologically important 1.55 um telecommunications wavelength. This demonstration expands the family of superconducting materials for SNSPD technique, opens the prospects of raising the temperature ceiling, and raises important questions about the underlying mechanisms of single-photon detection by unconventional superconductors.

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[2] I. Charaev et al., Single-photon detection using high-temperature superconductors, Nat Nanotechnol, vol. 18, no. 4, 2023, doi: 10.1038/s41565-023-01325-2.

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Poster-2-2

« Back to program

Probing mono- and few-layer 1T-TaSe₂ with ARPES

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Physical properties can change significantly when bulk materials are thinned down to a few atomic layers. Here, we study the intriguing example of the metallic charge density wave system $1\text{T-}TaSe_2$. Previous transport experiments on $1\text{T-}TaSe_2$ found a metal to insulator transition at a thickness of 5 layers [1]. Monolayer $1\text{T-}TaSe_2$ was proposed to be a Mott insulator and is a candidate quantum spin liquid [2]. We perform Angle resolved photoelectron spectroscopy (ARPES) measurements on ultra clean exfoliated few layer $1\text{T-}TaSe_2$ to study this intriguing phase of matter.

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[2] Chen, Y., et al., Nat. Phys. 16, 218-224 (2020).

Poster-2-3

Uncovering novel properties in RECo5 permanent magnets

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Rare-earth (RE) permanent magnets gain the excellent magnetic properties from the interaction between localized f-electrons and itinerant conduction electrons. However, the search for the underlying mechanisms that account for the interactions between electrons in this class of materials continues to challenge the community of magnetism.

In this work, we will present new trends that advance on the understanding of low-lying energy scales in the family of compounds RECo5 (RE= Nd, Sm and Y). In a first case study, the role that crystal electric field (CEF) plays in both magnetic anisotropy and spin reorientation of the single crystal NdCo5 is investigated by inelastic neutron scattering (INS) and theoretical calculations [1]. In a second case study, we discuss a systematic study of Sm substitution in YCo5, namely, the polycrystal SmxY1-xCo5 (x = 0 to 1) [2]. Combining bulk physical properties (electrical transport, magnetization and specific heat) and x-ray spectroscopies (XRD, XPS and XAS) we uncover how the tuning of f-electrons influences on different magnetic, electronic and valence states leading to a rich variety of phase transitions, electronic correlations and energy excitations which create new routes for the realization of hard magnets.

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Probing the superconducting gap symmetry of infinite-layer nickelates through electron irradiation induced disorder

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Superconducting infinite-layer nickelates saw their experimental realisation two decades after their theoretical prediction [1], generating significant interest for being isoelectronic to $3d^9$ superconducting cuprates. This feat was achieved by combining epitaxial thin film synthesis with topochemical reduction to stabilise the required nickel electronic configuration [2]. While sharing similarities in phase diagrams [3], nickel- and copper-based systems exhibit notable disparities in band structure and hybridisation [4-6].

Determining the superconducting nickelate's pairing symmetry has posed a significant challenge [7], partly due to limitations of thin-film sample geometry and surface degradation during chemical reduction processes [8]. Various techniques to investigate the superconducting order parameter symmetry, including studies of London penetration depth through mutual inductance [9] or tunnel diode oscillator method [10], single-particle tunnelling [11], photoemission spectroscopy [12-14], and thermal transport are challenging to perform or interpret on these chemically reduced thin films.

In addressing this challenge, we employ high-energy electron irradiation to introduce disorder into superconducting nickelate thin films in a controlled manner. By examining the impact of pair-breaking defects on superconductivity, we aim to shed light on the nature of the gap symmetry. Our initial findings show the suppression of superconducting transition temperature and increase of normal state resistivity with induced disorder.

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Poster-2-6

« Back to program

Magnetic and magnetoelectric properties of LiFePO₄

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The ability to control magnetic and electric properties is attractive for tailoring materials for devices, data storage and sensor technology. In magnetoelectric materials, these two degrees of freedom are closely linked and this makes them particularly interesting [1]. Here we re-visit one such system, LiFePO₄, which has been known since the 60s and is now a well-known battery material [2]. Early on, it turned out that LiFePO₄ is also a complex antiferromagnetic and magnetoelectric system [3,4]. By combining electric polarization measurements and neutron diffraction under pulsed magnetic fields as well as mean-field calculations we identify the spin-flop phase above 31 T and observe the corresponding change in the magnetoelectric tensor symmetry [5,6]. However, the persistence of off-diagonal magnetoelectric tensor elements above the critical field suggests a lowering of the magnetic point group symmetry and hence a more complex magnetic structure in the high-field phase. Moreover, our mean-field calculations show that the system is less frustrated than first anticipated. The results demonstrate the effectiveness of combining pulsed-field neutron diffraction and electric polarization measurements to elucidate the magnetic structures and symmetries at the highest attainable field strengths.

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Progress in the study of rare-earth silicate systems

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Rare-earth silicates are an interesting class of materials owing their potential for optical (laser diodes, scintillators) and environmental barrier coating (EBC) applications. One of the major difficulties encountered in the synthesis and study of these systems is due to the existence of a relatively large number of chemical phases and polymorphism possible at ambient pressure. Moreover, there is an overlap of the thermodynamic stability ranges of the different polymorphs and/or chemical phases, thus hindering the synthesis of pure phase ceramic materials by conventional solid-state reaction. To overcome these drawbacks and study the intrinsic properties of these systems, one can attempt to prepare these materials in crystal form. We successfully prepared large, high quality, crack-free and pure phase single crystals of R_2SiO_5 (R = Dy, Ho and Er) using a laser-diode-heated floating zone furnace. Here, we present the results of our investigations to optimize the synthesis and crystal growth conditions of R_2SiO_5 , and discuss the properties of these materials [1]. The progress in preparing single crystals of these study of the intrinsic structural, chemical and physical properties of rare-earth silicate systems which will open the route for improving the properties of these materials for applications.

[1] V.C. Ciomaga Hatnean et al., Crystal Growth of the R2SiO5 Compounds (R = Dy, Ho, and Er) by the Floating Zone Method Using a Laser-Diode-Heated Furnace, Crystals 2023, 13, 1687.

« Back to program

Simulating 2D-1D dimensional crossover with ultracold atoms

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As a function of dimensionality, in quantum physics we have access to a broad range of phenomena. In this presentation, we describe the dimensional crossover along two integer dimensionalities, namely 2D to 1D, in strongly interacting ultracold atomic gases as a function of the transverse confining potential V_y . We showcase the analytical tools that can be used to describe the large V_y case where the system is well described by weakly-coupled chains, such as *bosonization* [1]. In this regime, we use a mean-field approach to decouple the chains and study the temperature at which we expect the crossover to occur and its scaling as a function of V_y . We extend the analysis to a broader range of V_y by meaning of QMC simulations [2] and study the superfluid fraction and the evolution of the one-body density matrix $g_1(x)$ by comparing with experiment [3]. These results allow us to define in the $V_y - k_b T$ plane a phase diagram which ranges from BKT physics to 1D Luttinger liquid going through a distinct intermediate phase.

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[2] H. Yao, L. Pizzino, T. Giamarchi, "Strongly-interacting bosons at 2D-1D dimensional crossover". SciPost Phys. 15, 050 (2023).[3] Y. Guo et al. "Observation of the 2D-1D crossover in strongly interacting ultracold bosons". Nat. Phys. (2024).

Poster-2-9

« Back to program

Investigation of charge order fluctuations in La_{1.675}Eu_{0.2}Sr_{0.125}CuO₄

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This study reports direct observation of charge order fluctuations (CF) in the unconventional cuprate superconductor $La_{1.675}Eu_{0.2}Sr_{0.125}CuO_4$ (LESCO) through resonant inelastic x-ray scattering (RIXS). Charge order (CO) is closely related to and even competes with superconductivity in cuprates [1], making the excitations stemming from this order, CF, critical for understanding the low-energy physics in this system. Although intensive studies have focused on CO in cuprates [2,3], CF has not been fully investigated due to experimental challenges in isolating the CF signal. "Thanks to the advent of high-resolution RIXS technique [4], we can now resolve the low-energy excitations, including CF and phonons. Indirect studies of CF on several compounds based on phonon anomalies have been carried out in the past few years [5-7], while direct observation of CF is yet to be explored.

This study focusses on lanthanum-based cuprate deep inside the charge order phase. We managed to separate out the CF signal from the low-lying phonons by numerical simulations, which allows for a direct extraction of the information of CF. Our work not only advances the understanding of CF in superconductivity but also introduces a useful numerical technique for isolating CF from low-energy excitations, facilitating future quantum material studies.

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[3] R. Arpaia, et al., Journal of the Physical Society of Japan 90.11 (2021): 111005.

- [4] K-J. Zhou., et al., Journal of Synchrotron Radiation 29.2 (2022): 563-580.
- [5] J. Li, et al., Proceedings of the National Academy of Sciences 117.28 (2020): 16219-16225.
- [6] W. Lee, et al., Nature Physics 17.1 (2021): 53-57.
- [7] L. Chaix, et al., Nature Physics 13.10 (2017): 952-956.

Spin-orbital excitations encoding the magnetic phase transition in the van der Waals antiferromagnet FePS₃

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Magnetic van der Waals (vdW) materials offer new avenues for exploring exotic magnetic phases and collective behavior. [1] Recent research, mainly using optical spectroscopy, reveals the sensitivity of the acoustic phonon response to magnetic states even in few-layer structures. [2] FePS₃, whose interlayer exchange interaction is very small, is an S = 2 zig-zag quasi-two-dimensional antiferromagnetic insulator with a honeycomb lattice. [3] Here we performed resonant inelastic X-ray scattering (RIXS) at Fe L₃-edge as a function of temperature across the magnetic transition to elaborate the spin-orbital excitations of FePS₃ and their relation to magnetism. The multiplets probed by Fe L3 RIXS have a large sensitivity to the spin state. By comparing with ligand-field-theory calculations, we identified the essential role of the trigonal lattice distortion and negative metal-ligand charge transfer to account for the low-energy spin-orbital excitations. We reveal the robustness of these elementary excitations adown to the few atomic layer limits, in accordance with the persistent magneto-optical excitations and phonon modes in monolayers measured by Raman scattering. [4] This provides crucial insight into how the spontaneous magnetic symmetry-breaking stabilizes in the quasi-two-dimensional limit of the vdW magnet FePS₃. Our work highlights RIXS as an ideal generalized approach for studying 2D magnetic materials, featuring sensitivities to all degrees of freedom.

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Poster-2-11

« Back to program

Geometrically, electrostatically and thermally tunable phonon polaritons in SrTiO₃-based interfaces

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Surface phonon-polaritons (SPhPs) - strongly coupled light-phonon modes bound to interfaces between two media, one of which is a polar material with negative permittivity - hold high promise in nanophotonics due to their capacity to squeeze the electromagnetic energy on ultra-subwavelength scales. While the SPhPs are extensively studied in conventional semiconductors (SiC, AlN) and van der Waals materials (hBN, MoS₂), little is done in the vast family of complex perovskite oxides ABO₃. Using scattering-type near-field optical microscopy (s-SNOM) we explored SPhP modes in LaAlO₃(LAO)/SrTiO₃(STO) heterostructures [1] and 100 nm-thick transferable STO membranes [2]. The presence of conducting 2D electron gas (2DEG) at the LAO/STO interfaces strongly increases the temperature dependence of the PhP frequency, due to a coupling between the SPhPs in STO and the plasmon-polaritons in the 2DEG and also allows for electrostatic tuning by applying voltage to a back gate [1]. In ultrathin membranes, we observe an even-odd SPhP mode splitting, where the low energy mode shows a propagating behavior with a strongly confined wavelength, while the high-energy mode (Berreman mode) shows the epsilon-near-zero (ENZ) behaviour with a huge enhancement of the electric field inside the sample. Our work shows great potential of oxides for infrared nano-photonics.

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Poster-2-12

« Back to program

Structural studies on new, layered K-Cu-Te oxides

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The family of layered alkali (A) transition metal (M) oxidotellurates(VI) with a composition of $A_2M_2TeO_6$ can exhibit promising electrochemical properties (e.g. Li₂Ni₂TeO₆ [1]) as well as frustrated 2D antiferromagnetism (e.g. $Na_2Co_2TeO_6$ [2] and $Na_2Ni_2TeO_6$ [3]) due to the honeycomb sublattice of the transition metal atoms.

The new phase $K_2Cu_2TeO_6$ was synthesized using the hydroflux method [4]. Its crystal structure consists of $[CuTe_2O_6]$ layers separated by K⁺ cations. The honeycomb sublattice of the Cu atoms is distorted due to the pronounced Jahn–Teller effect of Cu(II).

The structural evolution of $K_2Cu_2TeO_6$ at increased temperatures and pressures was investigated by high-temperature synchrotron powder diffraction and high-pressure Raman spectroscopy. During the latter, hints of a second-order phase transition at pressures of 5–7 GPa were observed.

 $K_2Cu_2TeO_6$ is prone to incorporate water molecules besides the K⁺ cations between the layers; this process can be tracked by the shifting of reflections to smaller angles in X-ray powder diffraction measurements. Furthermore, there exist two stoichiometric hydrates (mono-, and tetrahydrate) of $K_2Cu_2TeO_6$, which can be obtained under hydroflux conditions as well.

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Investigating Strain-Dependent Magnetoresistance and Metal-Insulator Transition in LCMO Films at Cryogenic Temperatures Using Near-Field Techniques

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Metal-insulator transitions (MITs) in complex oxides like manganites present intriguing phenomena with significant implications for fundamental physics and potential applications [1]. In this study, we investigate the MIT in manganites, focusing on the perovskite lanthanum calcium manganese oxide (LCMO). Scattering scanning near-field optical microscopy (s-SNOM) emerges as a powerful tool, offering high spatial resolution and sensitivity to local conductivity [2]. By Using s-SNOM, we explore the MIT in LCMO and its modulation under strain. Building upon successful applications in other materials like vanadium dioxide (VO_2) [3] and neodymium nickel oxide ($NdNiO_3$) [4], we present preliminary findings on the impact of strain on the MIT transition in LCMO. We will present preliminary results on colossal magneto resistance on LCMO where different strain translates to different transition temperatures. [5]

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« Back to program

Quantum oscillations in focused ion beam prepared microstructures of ZrSiS

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Nodal-line semimetals are a topological phase of matter whose unique physics has only begun to be explored. The intersection of adjacent two-dimensional electronic bands creates closed nodal loops in reciprocal space with various potential configurations, providing a rich playground to explore correlation effects and different topological phases. Bulk ZrSiS has already proven to be an excellent probe into nodal-line semimetal physics, as quantum oscillation measurements have allowed for complete Fermi surface mapping in good agreement with density-functional-theory calculations [1] and it has shown a topological quantum phase transition under pressure [2]. Focused ion beam microstructuring techniques unlock new experimental capabilities, as sample sizes can be of order with their electronic mean free path leading to novel quantum coherent orbits [3]. Microstructures of ZrSiS allow for the exploration of these finite size effects. Here we present a size dependent study of magneto-quantum oscillations in microstructured ZrSiS, with particular emphasis on low strain in the sample. The appearance of new oscillation frequencies requires interpretation beyond the conventional Lifshitz-Kosevich formalism.

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Les	Diablerets										14-16,	2024
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Electron-phonon coupling across a WS₂/hBN van der Waals interface

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Electronic states in a two-dimensional system and bosonic excitations in an adjacent substrate may be strongly coupled. These interfacial interactions are still poorly characterized in van der Waals heterostructures, where one would expect that they play a marginal role. However, recent optics experiments report remarkably large coupling between excitons in a monolayer transition metal dichalcogenide and the underlying hexagonal Boron Nitride (hBN) substrate [1]. Here, we investigate the nature and magnitude of such interactions in the electronic states of a WS₂/hBN heterostructure via angle-resolved photoelectron spectroscopy. We resolve dispersing satellites separated from the intense quasiparticle WS₂ valence band by energies comparable to Γ phonon modes in hBN. We derive a spectral function model to describe the interfacial coupling between charges in the WS₂ layer and the lattice vibrations of the polar hBN substrate, which we employ to provide a qualitative estimation of the interaction strength. Finally, we evaluate the entity of this coupling at large out-of-plane WS₂-to-hBN distance in a WS₂/graphite/hBN heterostructure. Our findings will define the impact of many-body interfacial correlations in the transport properties of a two-dimensional semiconductor across a van der Waals gap.

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Poster-2-16

« Back to program

Imaging ultrafast electronic order fluctuations of Fe₃O₄

Nelson Hua,¹ Yanwen Sun,² Pooja Rao,³ Nanna Z. Hagström,³ Bojan Stoychev,⁴ Eric Lamb,⁴ Meera Madhavi,³ Surya T. Botu,³ Spencer Jeppson,³ Maël Clémence,^{1,5} Aidan G. McConnell,^{1,5} Shih-Wen Huang,¹ Serhane Zerdane,¹ Roman Mankowsky,¹ Henrik T. Lemke,¹ Mathias Sanders,¹ Vincent Esposito,² Patrick Kramer,² Diling Zhu,² Takahiro Sato,² Sanghoon Song,² Eric E. Fullerton,⁴ Oleg G. Shpyrko,⁴ Roopali Kukreja,³ and <u>Simon Gerber</u>¹

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Speckle patterns manifesting from the interaction of coherent light with matter offer a glimpse into the dynamics of nanoscale domains that underpin many emergent phenomena in quantum materials. While the dynamics of the average structure can be followed with time-resolved X-ray diffraction, the ultrafast evolution of local structures and nonequilibrium conditions have thus far eluded detection due to experimental limitations, such as insufficient coherent flux. Here we demonstrate the experimental realization of a nonequilibrium X-ray speckle visibility experiment using a so-called split-and-delay setup. Photoinduced electronic domain fluctuations of the magnetic model material Fe₃O₄ reveal changes of the trimeron network configuration due to charge dynamics, offering a unique perspective on the ultrafast dynamics of the lattice structure and electronic heterogeneities.

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Highly anisotropic in-plane ferroelectricity in CaTiO₃ thin films

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While $CaTiO_3$ is non-polar in its bulk form, ferroelectricity has been demonstrated in epitaxial thin films [1,2,3]. We have discovered two unusual, highly anisotropic in-plane ferroelectric states in $CaTiO_3$ films caused by the interaction between polarization, oxygen octahedral rotations, and epitaxial strain. Films deposited on (110)-oriented NdGaO₃ substrates show uniaxial in-plane ferroelectricity with a regular dielectric response in the orthogonal in-plane direction. In films on (001)-oriented NdGaO₃, the polarization lies near the *a* axis in the ground state — however, electric fields along the *b* axis cause a discontinuous rotation of the polarization, resulting in antiferroelectric-like double-hysteresis loops.

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 Haislmaier et al., Adv. Funct. Mater. 26, 7271 (2016).

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« Back to program

Optical detection of a chiral spin liquid in transition metal dichalcogenide moiré bilayers

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The first valence or conduction band of many moiré bilayers consisting of transition metal dichalcogenide (TMD) sheets can be effectively described by an extended Hubbard model on the triangular lattice. Since the standard Hubbard model on this lattice at half filling has been theoretically predicted to host a chiral spin liquid (CSL) ground state at intermediate interaction strength, TMD moiré bilayers, given their remarkable tunability, represent a promising candidate to experimentally realize this elusive state of matter. However, the identification of such a state in an experiment remains challenging. Based on the possibility of optical manipulation and readout of the spin in TMDs, we propose a pump-probe protocol to detect the characteristic spin Hall conductivity of the CSL. We calculate the spin dynamics within a parton picture benchmarked by matrix product state simulations for small system sizes and discuss under which circumstances the quantization of the spin Hall conductivity can be detected.

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Poster-2-19

« Back to program

Quantum sensor cryogenic search for dark matter in light mass range (QROCODILE)

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Dark matter remains one of the big unsolved mysteries of modern physics. After decades of research at the electroweak scale, the research efforts have been shifted towards sub-GeV mass ranges. Among various approaches, superconductors offer unprecedented combination of performance [1]. Superconducting Nanowire Single Photon detectors (SNSPDs) are sensitive to the deposition of energies in the sub-eV range [2]. The SNSPD can be used both as the target and the sensor. By coupling with the advanced fabrication techniques, this device becomes a promising approach for exploration of new territories in the detection of low energy dark matter.

In this work we demonstrate the high quantum efficiency of detectors for energies lower than 0.8 eV. We report on a measurement performed with a SNSPD to set new constraints on dark matter which scatters on an electron as a function of the dark matter mass. Further we provide bounds on DM absorption in SNSPD for a relic dark photon with an exposure of 415 hours for an energy threshold of 112 meV.

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Synthesis of Novel Materials Using Cubic Multi-Anvil High-Pressure Systems at the University of Geneva

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High-pressure synthesis has become an indispensable tool for the synthesis and discovery of various quantum materials. The synergy of high pressure and temperature can be crucial, as it surpasses the limitations imposed by enthalpy-driven compound formation in traditional solid-state synthesis. We will outline the methods available at the Laboratory for Quantum Materials Discovery at the University of Geneva. We are currently using two systems: (i) A multi-anvil press equipped with a walker module configuration in a cubic arrangement. Operating at temperatures up to 1200 °C and pressures up to 3-4 GPa. (ii) A multi-anvil press equipped with a home-made configuration in a cubic arrangement, capable of reaching pressures up to 10 GPa and a maximal temperature of 1600 °C. Furthermore, we will present some of the results from our synthesis and crystal growth attempts using these systems.

Poster-2-21

« Back to program

Bismuth-Rich Intermetallic Rods with Strong Spin-Orbit Coupling

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During the search for novel topologically non-trivial materials, materials containing heavy elements, with large spin-orbit coupling were investigated. A particular focus lay on materials containing the heaviest non-radioactive element bismuth, as its large spin-orbit coupling has proven highly advantageous in finding compounds that exhibit the desired properties. In the course of these investigations, the novel bismuth-rich mixed halide $Bi_{21}Rh_4Cl_6I_7$ was found.^[1] The black needle-shaped crystals of this material showcase an orthorhombic structure that consists of infinite intermetallic rods $\frac{1}{\infty}[Bi_9Rh_2]^{3+}$ and discrete anionic groups $[Bi_2^{II}Cl_5I_2]^3$ and $[Bi^{III}Cl_4I_2]^3$. The rods consist of Rh-centered [RhBi₈] polyhedra that alternately share triangular and rectangular faces. Using traditional electron counting rules, the intermetallic rod can be interpreted as a covalent polymer with Rh₂ dumbbells bonded to molecular Bi₂ and Bi₅ units, while a quantum-chemical bonding analysis shows that the bonds involving Rh atoms are largely diffuse, while two-center bonds dominate in the bismuth units. Resistivity measurements indicate two temperature regimes, of which one showcases a temperature-independent resistance and this, along with the strong spin-orbit coupling inherent to this bismuth-rich compound, makes it a candidate for a topological insulator.

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Poster-2-22

« Back to program

Growth of YVO₃ thin films by pulsed laser deposition

Matthieu Fanetti, Clémentine Thibault, Jean-Marc Triscone, and Stefano Gariglio

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The perovskite structure adapts its unit cell symmetry, volume and internal distortions to the ionic radii of its different elements. For the ReVO₃ family, the ionic radius of the rare-earth (Re) determines the degree of orthorhombicity (orthorhombic strain s = 2(a - b)/(a + b)) and the angle of rotation of the oxygen octahedra: Re=La (ionic radius $r(La^{3+}) = 1.16$ Å) leads to an almost in-plane square lattice (s = -0.0011), while for Re=Y ($r(Y^{3+}) = 1.019$ Å) the in-plane lattice is strongly orthorhombic (s = 0.0571). Such asymmetry poses a challenge for the epitaxial growth on square-lattice substrates, potentially resulting in a large shear strain for the layer. We present results on the growth of YVO₃ thin films by pulsed laser deposition on (110)_o NdGaO₃ substrates. The structural characterization by X-ray diffraction and atomic force microscopy reveals the substrate temperature - oxygen pressure growth window to obtain layers with high crystalline perfection. Analysis of the diffraction data shows that the rotations of the oxygen octahedra of the layer are coupled to the ones of the substrate.

« Back to program

Entanglement spectrum across the semimetal-diffusive metal transition in a disordered Weyl system

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Disordered Weyl semimetals exhibit an intriguing phase diagram featuring three distinct phases. While the system is stable for weak disorder, it undergoes a quantum phase transition into a diffusive metal at a critical disorder strength, with Anderson localization deferred to even stronger disorder. Here I focus on the Weyl semimetal (WSM)-diffusive metal transition. Specifically, I introduce a real-space partitioning of the system into two subsystems, and showcase the evolution of entanglement spectrum with disorder, which is reconstructed in the two-dimensional momentum space perpendicular to the cut direction. A key observation is that the Fermi arc sruface states, which are a hallmark of the topology of WSMs, leave their imprint on the entanglement spectrum, showing a clear distinction between states that are connected to the atomic limit, and those that represent an obstruction to it. I show that, as the diffusive metal is topologically trivial, this signature gradually fades from the entanglement spectrum, which becomes featureless at the critical disorder strength. I also comment on the scaling of entanglement entropy on either side of the phase transition.

Poster-2-24

« Back to program

Strontium Vanadate thin films growth for optical applications

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Light-matter interaction can be strongly enhanced by confining the electric field in optical cavities. These require a well-suited stacking of reflecting and transparent materials selected for the frequency range of interest. In our study, we target the Terahertz spectrum and have chosen the SrVO3 compound for its high reflectivity in this frequency range.[1] We report results on the growth of SrVO3 thin films by pulsed laser deposition unraveling the complex dependence of resistivity and crystalline quality on the Ar/O2 growth atmosphere as well as laser fluence and target-substrate distance. The investigation of electric transport reveals the role of electron-phonon coupling in the conduction of this material, in line with recent literature.[2] Optical measurements performed by Fourier Time-domain InfraRed spectroscopy show that the films reflectivity window is within the scope of our applications.

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Thermodynamical Signatures in the Superconducting Haldane Model

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Inspired by experimental results of the Kagome materials AV3Sb5, we want to gain a better understanding of the behavior of thermodynamical quantities, especially the thermal conductivity, in C6v-symmertric systems when transitioning into the superconducting state. Particularly, we look at the evolution of the thermal hall conductivity for different superconducting order parameters when its normal state value is non-zero. To this end we examine the spinful Haldane model without inversion symmetry breaking (M=0). Even though in this case the Chern number is zero for each band, we can get a non-vanishing Hall conductivity by placing the chemical potential inside a band. Introducing attractive onsite, nearest-neighbor and next-nearest-neighbor couplings we map out the leading instabilities and examine the behavior of the thermodynamical quantities across the different gap openings.

Superconductivity and magnetotransport in non-Fermi lquids: exact results from Yukawa-SYK lattice models

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Strange-metal phases, found in, e.g., heavy fermions, pnictides, and cuprates, host partially coherent superconducting states, born out of incoherent, non-Fermi liquid (NFL) normal-state spectra [1-4]. Such properties can be reproduced in Sachdev-Ye-Kitaev (SYK) approach [5-7], based on all-to-all interactions among N fermion species ("flavors"), where superconductivity emerges by coupling fermions to M bosonic flavors (the Yukawa-SYK model), responsible for Cooper pairing and for normal-state incoherence [8,9]. In this work, we generalize the Yukawa-SYK model to a lattice with random hopping parameters. We exactly solve the model in the spin-singlet large-N limit, at N=M and at particle-hole symmetry, we construct the phase diagram, and we characterize the FL to NFL crossovers in the normal and superconducting states [10,11]. Hopping exponentially decreases the critical temperature in FL regime, which is maximal in the single-dot NFL limit at given coupling. The phase stiffness and the condensation energy are maximal precisely at the NFL/FL crossover, analogously to experimental evidence found in superconducting cuprates [11]. We then generalize the theory to 2D dispersive fermions and bosons, and apply this model to DC and AC strange-metal magnetotransport [12]; we study interaction-driven renormalization of the cyclotron resonance, and nonlinear T dependence of the Hall angle.

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Temperature dependence of the energy band gap in ZrTe5: Implications for the topological phase

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Zirconium pentatelluride (ZrTe5) is a widely studied material, with a single band with an aproximately conical dispersion in the centre of a Brillouin zone and a narrow energy band gap. ZrTe5 is predicted to be a topological insulator [1], however, to this day there is no consensus on whether it is a strong [2] or weak [3] topological insulator as different studies (both experimental and theoretical) show contradicting results.

Using Landau-level spectroscopy, we determine the temperature dependence of the energy band gap in ZrTe5. We find that the band gap reaches $Eg = (5\pm1)$ meV at low temperatures and increases monotonically when the temperature is raised. This implies that ZrTe5 is a weak topological insulator, with noninverted ordering of electronic bands in the center of the Brillouin zone [4]. Our magnetotransport experiments performed in parallel show that the resistivity anomaly in ZrTe5 is not connected with the temperature dependence of the band gap.

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Poster-2-29

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A New Look on an Old Problem: Mass Enhancement in Fermi Liquids

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We show that the mass enhancement in Fermi liquids due to quasiparticle weight reduction leads to results for the specific heat that are different than Landau's phenomonelogical theory predicts. Our analytical results are benchmarked numerically, by applying Dynamical Mean Field Theory (DMFT) to a triangular lattice Hubbard model.

Poster-2-30

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Determining the nature and strength of proximity induced spin-orbit coupling in graphene by quasiparticle interference imaging

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Inducing and controlling spin-orbit coupling (SOC) in graphene is key to create topological states of matter, and for the realization of spintronic devices. The most successful strategy to achieve this goal so far is to place graphene onto a transition metal dichalcogenide. However, there is no consensus as to the nature and the magnitude of the induced SOC. In this talk, we show that the presence of backscattering in graphene-on-WSe₂ heterostructures can be used to probe SOC and to determine its strength quantitatively, by quasiparticle interference (QPI) imaging using a scanning tunneling microscope [1]. Analyzing QPI images of heterostructures with selected twist angles between 0° and 30°, we find that the induced SOC consists of a valley-Zeeman ($\lambda_{vZ} \approx 2$ meV) and a Rashba ($\lambda_R \approx 15$ meV) term. These results are in excellent agreement with transport experiments, both finding that the Rashba term is an order of magnitude larger than current theoretical predictions. QPI further gives unambiguous evidence that the measured SOC is the result of a modified band structure and demonstrate a viable strategy to determine SOC quantitatively by imaging quasiparticle interference.

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Poster-2-31

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An Ab Initio Study of Superconductivity in Mono- and bilayer Molybdenum disulfide

Wouter Bos

MSc student

The two-dimensional electron doped form of molybdenumdisulfide (MoS2) exhibits superconducting properties around liquid-helium temperatures. Ion-liquid gating experiments have shown a layer dependent increase in critical temperature from 1-2 Kelvin (K) to around 7 K in the transition from monolayer to bilayer MoS2 converging to 10 K in bulk MoS2 [1, 2, 3]. In this thesis an attempt has been made to increase the understanding of conventional superconductivity in doped monolayer and bilayer MoS2 by using state of the art ab initio techniques such as, DFT, DFPT, Wannier interpolation and Eliashberg theory. These techniques were ultimately used to predict trends in critical temperatures differentiating by layer thickness, spin polarization and charge distribution. The valley and band resolved electron-phonon coupling strengths were calculated using a self-written Python script, which showed electron occupation of the Q-region to be crucial to superconductivity in bilayer MoS2.

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Poster-2-32

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Superconductivity in metallic hydrogen

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Superconductivity, the amazing phenomenon of lossless transmission of electric current through metallic wires, requires cooling of the wire to low temperatures. Metallic hydrogen is considered as the most likely candidate for superconductivity at very high temperatures, possibly even room temperature. However, as a result of various approximations used, conflicting theoretical predictions exist for the range of temperatures where superconductivity is expected to occur. Here we avoid those approximations and confirm that metallic hydrogen is indeed a superconductor, but this is limited to temperatures far below previous estimates. We exploit the "jellium" model proposed in 1966 by De Gennes, where superconductivity is caused by the combination of Coulomb repulsion between the electrons and Coulomb attraction between the protons and the electrons. We find that the superconducting order develops over an energy range far exceeding the characteristic phonon energy, and that the phase of the order parameter flips 180 degrees at the characteristic phonon energy above and below the Fermi energy.

