Electronic Order in Kagome Metals

824. WE-Heraeus-Seminar

8 Dec - 12 Dec 2024
at the Digital Hub Logistics Event Location, Hamburg/Germany

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Introduction

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Aims and scope of the 824. WE-Heraeus-Seminar:

Kagome metals have emerged as a platform for correlated and topological physics in itinerant electron systems due to their high degree of orbital frustration. The Dirac cone and flat-band physics of toy models is modified in material realizations that give rise to strongly interacting ground states, such as charge order and superconductivity. Tied to the lattice, these systems promise to realize the long-sought dream of controlling intertwined electronic orders, which both advances our understanding of these materials as well as promises novel applications of quantum materials. With a focus on the AV3Sb5 (A = K, Rb, Cs) class of materials, we address the mounting experimental evidence for a thus-far unexplained state that bears characteristics of a chiral state with delocalized orbital anti-ferromagnetism. The contradictory state of experimental evidence points to extreme sensitivity of this state to external perturbations, a point of focus at the workshop. With this highly interactive workshop, we aim for a convergence of a minimal model for the interacting state in such Kagome metals, and to derive a roadmap addressing the current open questions on microscopics, proposing complementary materials platforms and solidifying ideas towards interacting topological electronics.

Scientific Organizers:

Prof. Dr. Philip Moll	MPI for the Structure and Dynamics of Matter, Hamburg, Germany E-mail: philip.moll@mpsd.mpg.de
Prof. Dr. Titus Neupert	University of Zurich, Switzerland E-mail: neupert@physik.uzh.ch
Prof. Dr. Eun-Ah Kim	Cornell University, Ithaca, NY, USA E-mail: eun-ah.kim@cornell.edu

Introduction

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Registration:

Martina Albert (WE-Heraeus Foundation)
at the PierDrei Hotel, next to reception
Sunday (14:00 h – 17:00 h)
and
Monday (08:30 – 12:30 h) at the Digital Hub Logistics Event Location

Program

Electronic Order in Kagome Metals
824th WE. Heraeus Seminar

December 8 - 12, 2024
Hamburg, Germany

Sunday, December 8th							
14:00	**15:45**	**16:00**	**16:30**	**17:10**	**17:30**	**19:10**	**22:00**
Registration in PierDREI Hotel Lobby	Meet in PierDREI Hotel Lobby	Walk to "Flusi," Hamburg's "floating church"	Opening Talk by Stephen Wilson (40 minutes)	Heraeus Talk by Stefan Jorda (10 minutes)	Pickup by Meyer Barge **17:45** Departure	Arrive to Övelgönne Wharf & Hoppe's Restaurant	End of dinner, return to PierDREI via public transportation

Time	Monday, December 9th	Tuesday, December 10th	Wednesday, December 11th	Thursday, December 12th
08:00	Breakfast in PierDREI Hotel			
09:00	Talk – Liang Wu	Talk – Mark H. Fischer	Talk – Riccardo Comin	Talk – Srinivas Raghu
10:00	Talk – Brian Møller Andersen	Talk – Roser Valentí	Talk – Berthold Jäck	Talk – Aharon Kapitulnik
11:00	Benedikt Mehmel (to 11:10) Poster Session	Poster Session	Poster Session	Talk – Andrei Bernevig
12:30	Lunch Served in Krähennest Event Space			Short Break
13:00				Closing Remarks
14:00	Talk – Maia G. Vergniory	Talk – Ion Errea		Departure
15:00	Talk – Chunyu Guo	Talk – Raquel Queiroz	Poster Flash	
16:00	Discussion and Coffee Hour	Open Podium Discussion: Future Directions	Poster Session	
17:00	Talk – Zurab Guguchia	Talk – Andreas P. Schnyder		
18:30	Dinner (free for you to plan)	Dinner (free for you to plan)	Heraeus Conference Dinner on Rickmer Rickmer's ship	

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December 8 - 12, 2024
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List of Talk Titles

Monday, December 9th

Liang Wu: Scanning Time-Resolved Optical Studies on Kagome Superconductors
Brian Møller Andersen: Kagome Superconductivity: Conventional or Unconventional?
Benedikt Mehmel: Quantum Technologies Made in Hamburg: An overview about the Ecosystem
Maia G.Vergniory: New Electronic Properties with a Shake
Chunyu Guo: FIB-Fabricated Microstructures Reveal Intrinsic Electronic Symmetry in AV3Sb5 Kagome Superconductors
Zurab Guguchia: Muon Spin Rotation Insights into Superconductivity and Charge Order in Kagome Metals

Tuesday, December 10th

Mark H. Fischer: Interplay of Electronic Orders in Kagome Metals
Roser Valentí: Electron-Phonon Versus Electron-Electron Interactions in Kagome Systems
Ion Errea: Phonon Collapse and the CDW Phase Transition in Kagome Metals
Raquel Queiroz: Flat Bands, Bound States, and Linear Response of 2D Metal Pd5Al2I
Andreas P. Schnyder: Topological Superconductivity Near van Hove Fillings

Wednesday, December 11th

Riccardo Comin: Connection Between Charge Order and Fermiology in AV3Sb5 Kagome Metals
Berthold Jäck: Visualizing Loop Current Excitations

Thursday, December 12th

Srinivas Raghu: Density Wave Order on the Kagome Lattice: Theory and Experimental Implications
Aharon Kapitulnik: Optical Search for Time-Reversal Symmetry Breaking Effects in Kagome Metals
Andrei Bernevig: No Title

Important Addresses in Hamburg

PierDREI Hotel: Am Sandtorkai 46, 20457 Hamburg
Flussschifferkirche: Hohe Brücke 2, 20459 Hamburg
Hoppe's Restaurant: Övelgönne 6, 22605 Hamburg
Digital Hub / Event Space: Workshop Rooms in 4th Floor & Krähennest Event Location in 5th Floor Am Sandtorkai 32, 20457 Hamburg
Rickmer Rickmer's Historic Sailing Ship: Bei den St. Pauli-Landungsbrücken 1a, 20459 Hamburg

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Posters

Posters

Manex Alkorta	**Analysis of the competition between the possible emerging Charge-Density-Wave phases of CsV3Sb5**
Giuseppe Allodi	**Grain-boundary driven electronic phase separation in AV3Sb5 compounds**
Wei Bao	**Kagome Metals with Noncollinear Antiferromagnetic Order**
Pietro Bonfa'	**Unveiling the nature of electronic transitions in RbV3Sb5 with Avoided Level Crossing μSR**
Ginevra Corsale	**Study of local charge and structural configurations of Kagome superconductor**
Pengcheng Dai	**Recent Progress on Understanding the interplay between charge density wave and magnetism in kagome lattice magnet FeGe**
Matthew Day	**Toward controlling the chirality of charge order in the Kagome Metal CsV3Sb5**
Francesco Grandi	**Theories for charge-driven nematicity in kagome metals**
Robin Guehne	**Orbital selective commensurate modulation of the local density of states in the Kagome metal ScV6Sn6 probed by nuclear spins**
Amir-Abbas Haghighirad	**Pressure-dependent Electronic Instabilities in CsV3Sb5 Probed by High-Resolution X-Ray Diffraction**
Moshe Haim	**Pomeranchuk Instability Induced by an Emergent Higher-Order van Hove Singularity on the Distorted Kagome Surface of Co3Sn2S2**
Kenichiro Hashimoto	**Superconducting gap structure in the new family of kagome lattice superconductors AV3Sb5**

Posters

Sofie Castro Holbæk	**Interplay of superconductivity and charge-density-wave order in kagome materials**
Haoyu Hu	**Kagome superconductors LaRu3Si2**
Yi Jiang	**FeGe as a LEGO Building Block for the 1:1, 1:6:6, and 1:3:5 families, and Catalogue of Phonon Instabilities in 1:6:6 family**
Arunava Kar	**Frustrated charge density wave and quasi-long-range bond-orientational order in the magnetic kagome FeGe**
Sun-Woo Kim	**Competing charge density waves and their manipulation in kagome metals**
Itamar Kimchi	**Frustration, Chirality, and Disorder**
Heqiu Li	**Mechanism for Loop Current Order in Kagome Metals from Intertwined van-Hove Singularities**
Ben-Chuan Lin + Shuo Wang	**Spin-polarized p-wave superconductivity in the kagome material RbV3Sb5**
Hubertus Luetkens	**Unconventional superconductivity in kagome lattice compounds AV3Sb5 (A = K, Rb, Cs) as seen by muon spin rotation and relaxation**
Bernhard Lüscher	**Unconventional gapping behavior in a kagome superconductor**
Charles Mielke III	**Time-reversal symmetry-breaking charge order in kagome metals**
Vesna Mitrović	**Microscopic nature of the charge density wave in Kagome metals**
Youcef Mouffok	**Magnetoelectronic and thermodynamic properties of new heusler alloys as superconductors**

Posters

Ilija Nikolov	**Emergent charge order seen by local magnetic probes in highly doped CsV3Sb5-xSnx**
Hanqi Pi	**A New Moiré Platform Based on M-Point Twisting**
Michael Rübhausen	**Higgs spectroscopy as a novel tool to characterize unconventional forms of superconductivity**
Jiwoo Seo	**Emergent Phase Transitions in RbV3Sb5 measured by nuclear magnetic resonance**
Avdhesh Kumar Sharma	**Domain wall engineering in distorted Kagome magnet**
Jean Souza	**Visualizing the kagome origin of the heavy-Fermion-like phenomenology in Ni3In**
Alexander Tsirlin	**Tailoring electronic structure of the AV3Sb5 kagome metals by pressure**
Ece Uykur	**Pressure-induced Lifshitz transitions in magnetic kagome metal Fe3Sn2 traced via structural and electronic changes**
Glenn Wagner	**Phenomenology of bond and flux orders in kagome metals**
Hao Wang	**The Complex Magnetic Structure and Giant Topological Hall Conductivity in Kagome Metal YnMn6Sn6**
Maxim Wenzel	**Optical study of ATi3Bi5 (A = Rb, Cs) compounds**
Xianxin Wu	**Emergent Loop Current Order in the Kagome Lattice**
Jiangchang Zheng	**Microscopic insights into the chiral flux phase of CsV3Sb5**

Abstracts of Lectures

(in alphabetical order)

Kagome superconductivity: conventional or unconventional?

Brian M. Andersen

Niels Bohr Institute, University of Copenhagen, 2100 Copenhagen, Denmark

I will discuss recent theoretical investigations of disorder response and the spin susceptibility of unconventional superconductivity on the kagome lattice. Despite the existence of a sign-changing gap structure [1], which sums to zero over the Fermi surface, such unconventional pairing states remain robust to disorder and exhibit a Hebel-Schlichter peak in the temperature-dependent spin-relaxation rate [2]. It originates from destructive interference effects peculiar to the kagome lattice. For the same reason, unconventional pairing states on the kagome lattice do not exhibit a neutron resonance peak. These results build on previous theoretical studies of the surprising robustness of unconventional pairing states to disorder on the kagome lattice [3]. Taken together these results imply that unconventional superconductivity on the kagome lattice is deceptive in the sense that its properties may appear similar to conventional non-sign-changing superconductivity. These results may be of relevance to the superconducting state of the kagome superconductors AV_3Sb_5 (*A*: K, Rb, Cs) and $CsTi_3Bi_5$.

References

[1] A. Rømer, S. Bhattacharyya, M. H. Christensen, R. Valenti, and B. M. Andersen, Phys. Rev. B 106, 174514 (2022).

[2] Y. Dai, A. Kreisel, B. M. Andersen, ArXiv:2404.10835.

[3] S. C. Holbæk, M. H. Christensen, A. Kreisel, B. M. Andersen, Phys. Rev. B 108, 144508 (2023).

Andrei Bernevig

Princton University, Princton, NJ, USA

I will present two aspects of Kagome materials: A CDW state in ScSn6V6 that appears at a different wave vector than the phonon condensation, and which we analytically attribute to flat band phonon fluctuations and a theory of superconductivity in LaRuSi where weashow that, contrary to prior belief, flat bands in 3D might be suitable for superconductivity only upon fine tuning. For ScV_6Sn_6 (space group 191), we explore a ~95K charge density wave (CDW) at K^{-} = (1/3, 1/3, 1/3) and its connection to phonon behavior. Despite no nesting in the electron susceptibility at K^{-}, ScV_6Sn_6 shows a collapsed phonon mode at H = (1/3, 1/3, 1/2) and an imaginary flat phonon band near H, linked to SnT mirror-even vibrations along z. A force constant model and Gaussian hopping approximation describe the phonon collapse. We propose a two-order-parameter model to explain the CDW at K^{-}, with the H order parameter (OP) undergoing a second-order phase transition and inducing the first-order K^{-} transition. We then investigate the Kagome superconductor $LaRu_3Si_2$ through first-principles calculations. The stable structure above the charge-density wave (CDW) transition temperature (T_a) was determined via soft phonon condensation, consistent with recent X-ray diffraction data. The electron-phonon coupling (EPC) is mode-enhanced, driven by the interaction between the local x-phonon mode and Ru $d_{x^2-y^2}$ orbitals in the Kagome lattice. This enhancement is identified as a universal feature in transition-metal-based Kagome materials. Doping further amplifies EPC and significantly increases the superconducting transition temperature (T_c) due to the high density of states (DOS) from the Kagome flat band.

Connection between charge order and fermiology in AV_3Sb_5 kagome metals

R. Comin[1]

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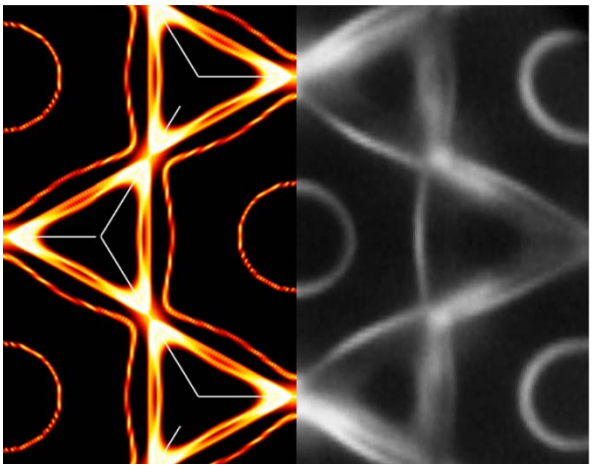

Ternary kagome metals that exhibit a remarkable range of emergent electronic phases, including superconductivity, charge-density-waves, nematicity, current-loop order, and pair-density-waves. A key focus of current research is to understand how the unique electronic structure of the kagome lattice gives rise to these diverse phenomena, which is crucial for a complete picture of symmetry breaking in kagome metals. This talk will present our recent angle-resolved photoemission spectroscopy (ARPES) studies of van Hove singularities (vHs) in AV_3Sb_5 compounds, and their connection to the emergence of charge-density-waves. These vHs exhibit two sublattice types (*p* and *m*), both near the Fermi level. The *m*-type vHs, originating from V 3dxz/3dyz orbitals, show prominent Fermi surface nesting, while the *p*-type vHs, derived from V 3dxy/3dx2–y2 orbitals, display the largest gap, suggesting a strong-coupling origin of charge order, likely driven by electron-lattice interaction [1]. I will further discuss recent work on ARPES signatures of band folding and resulting electron pockets in AV_3Sb_5, linking them to the microscopic charge-density-wave texture and the emergence of stripe and pair-density-wave orders [2,3].

References

[1] M. Kang et al., Charge order landscape and competition with superconductivity in kagome metals, Nat. Mater. **22**, 186 (2023).
[2] M. Kang et al., Twofold van Hove singularity and origin of charge order in topological kagome superconductor CsV3Sb5, Nat. Phys. **18**, 301 (2022).
[3] H. Li et al., Small Fermi Pockets Intertwined with Charge Stripes and Pair Density Wave Order in a Kagome Superconductor, Phys. Rev. X **13**, 031030 (2023).

Phonon collapse and the CDW phase transition in Kagome metals

Manex Alkorta[1,2], Martin Gutierrez-Amigo[3], Maia G. Vergniory[4,5] and Ion Errea[1,2,5]

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The charge-density wave (CDW) mechanism and resulting structure of the AV_3Sb_5 family of kagome metals has posed a puzzling challenge since their discovery. In fact, the lack of consensus on the origin and structure of the CDW hinders the understanding of the emerging phenomena. Here, by employing a non-perturbative treatment of anharmonicity from first-principles calculations [1], we reveal that the charge-density transition in CsV_3Sb_5 is driven by the large electron-phonon coupling of the material and that the melting of the CDW state is attributed to ionic entropy and lattice anharmonicity [2]. The calculated transition temperature is in very good agreement with experiments, implying that soft mode physics are at the core of the CDW transition. Contrary to the standard assumption associated with a pure kagome lattice, the CDW is essentially three-dimensional as it is triggered by an unstable phonon at the L point. The unusually large linewidth of the soft mode explains why inelastic scattering experiments did not observe any softened phonon.

By further relaxing the crystal structure below the CDW considering in the free energy the lattice entropy and anharmonicity, our first-principles calculations unveil the low-symmetry CDW structure of CsV_3Sb_5 as well as the character of the CDW transition.

References

[1] Ion Errea, Matteo Calandra, Francesco Mauri, Phys. Rev B **89**, 064302 (2014)
[2] Martin Gutierrez-Amigo, Đorđe Dangić, Chunyu Guo, Claudia Felser, Philip J. W. Moll, Maia G. Vergniory, and Ion Errea, Communications Materials **5**, 234 (2024)

Interplay of electronic orders in kagome metals

M.H. Fischer[1], G. Wagner[1,2], S. Castro Holbæk[1], T. Neupert[1], P.J.W. Moll[3], C. Guo[3]

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[2]Institute for Theoretical Physics, ETH Zurich, Zurich, Switzerland
[3]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

The family of Kagome metals AV_3Sb_5 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 ~1-3 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, rather 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, we show how a superconducting state emerging on top of a charge density wave mimics the broken symmetries of the charge order, as recently observed in scanning tunneling microscopy experiments.

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

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Kagome lattices stand at the forefront of research due to their fascinating interplay of topology, correlations, and magnetism [1-3]. Their special geometry enables various quantum phenomena, such as frustration and correlated orders, and features an electronic structure with flat bands, van Hove singularities, and Dirac cones. This makes them a prime subject for both experimental and theoretical research, offering insights into complex physical properties and potential technological applications.

In my poster, I aim to summarize the latest experimental developments concerning 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 (μSR) as a function of depth from the sample surface and under extreme conditions like hydrostatic pressure, uniaxial strain, ultra-low temperatures, and high magnetic fields. μSR is complemented by magnetoresistance and X-ray diffraction techniques. Key systems under discussion will include: **(1)** The AV_3Sb_5 (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, as well as unconventional superconductivity [4-7]. **(2)** The bilayer kagome material ScV_6Sn_6, where hidden magnetism within the charge-ordered state was observed [8]. **(3)** The $LaRu_3Si_2$ 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 or above room temperature in a correlated 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, D. Das, et. al., and Z. Guguchia, Nature **602**, 245 (2022).
[5] Z. Guguchia et. al., Nature Communications **14**, 153 (2023).
[6] Z. Guguchia, Khasanov, Luetkens, NPJ Quantum Materials **8**, 41 (2023).
[7] J.N. Graham et. al., and Z. Guguchia, Nature Comm. **15**, 8978 (2024).
[8] Z. Guguchia et. al., Nature Communications **14**, 7796 (2023).
[9] I. Plokhikh et. al., and Z. Guguchia, Comm. Physics **7**, 182 (2024).
[10] Mielke III, V. Sazgari, et. al., and Z. Guguchia, arXiv:2402.16219 (2024).

FIB-fabricated microstructures reveal intrinsic electronic symmetry in AV_3Sb_5 Kagome superconductors

C. Guo[1]*, G. Wagner[2], C. Putzke[1], D. Chen[3,4], K. Wang[1], L. Zhang[1], D. Chen[3], M. Gutierrez-Amigo[5, 6], I. Errea[5, 7, 8], M. G. Vergniory[7,3], C. Felser[3], M. Fischer[2]*, T. Neupert[2]* and P. J. W. Moll[1]*

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[8]*Fisika Aplikatua Saila, Gipuzkoako Ingeniaritza Eskola, University of the Basque Country (UPV/EHU), Donostia-San Sebastian, Spain*

Spontaneously broken symmetries are at the heart of many phenomena of quantum matter. However, determining the exact symmetries broken can be challenging due to experimental imperfections. Focused-ion-beam is an ideal micro-fabrication tool with high precision, which allows us to minimize these extrinsic imperfections, rendering the exploration of intrinsic electronic symmetries possible. The particular material under the spotlight is the Kagome superconductor CsV_3Sb_5, where electronic correlations result in a cascade of charge-ordered phases [1], leading to possible spontaneous symmetry breaking with chiral electronic states [2,3]. Using the FIB technique, we successfully fabricated hexagon-shaped devices with high precision [4]. Great care was taken to minimize shape deviations to avoid any symmetry lowering due to the structure's shape itself. The directional in-plane electric transport unambiguously reveals that the in-plane C_6 rotational symmetry remains intact down to cryogenic temperatures. Moreover, spontaneous symmetry breaking occurs only when external perturbations, such as magnetic field and uniaxial strain, are included. Our results provide a unifying picture of the controversial charge order in Kagome metals and highlight the need for microscopic materials control in the identification of broken symmetries.

References

[1] H. Zhao et al., Cascade of correlated electron states in the kagome superconductor CsV3Sb5; Nature 599, 216(2021).

[2] C. Guo et al., Switchable chiral transport in charge-ordered kagome metal CsV3Sb5; Nature 611, 461(2022)

[3] Y. Xu et al., Three-state nematicity and magneto-optical Kerr effect in the charge density waves in kagome superconductors; Nature Physics 18, 1470 (2022).

[4] C. Guo et al., Correlated order at the tipping point in the kagome metal CsV3Sb5; Nature Physics 20, 579(2024).

Visualizing Loop Current Excitations

Berthold Jäck
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Microscopic loop currents are a sought-after route to creating topological quantum states. Their detection remains an open question due to the challenging nature of detecting orbital-only magnetic order in measurements of the macroscopic material properties. Recent findings propose loop current order could exist in the kagome metals AV_3Sb_5 (A=K, Rb or Cs). We employed individual magnetic atoms as quantum sensors to directly detect microscopic loop currents in CsV_3Sb_5 by visualizing its quasiparticle excitations with the scanning tunneling microscope (STM) [1]. We observe a spatially localized low-energy state whose distinct spectral signatures establish it as the quasiparticle excitation of a loop current order parameter. Our work demonstrates the topological character of this loop current phase and introduces a novel method to examine other topological states, such as the fractional Chern insulator, with the STM.

We gratefully acknowledge funding by the Hong Kong RGC (Grant Nos. 26304221, 16302422, and C6033-22G) and the Croucher Foundation (Grant No. CIA22SC02).

References

[1] J. Zheng, B. Jäck, *et al. submitted* (2024)

Optical Search for Time-Reversal Symmetry Breaking Effects in kagomé metals

D. Saykin[1,2], *C. Farhang*[3], *J. Xia*[3] *C. Shekhar*[4], *C. Felser*[4], *and A. Kapitulnik*[1,2]

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[4]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany.

Recently discovered class of kagomé metals exhibit an unusual charge–ordered phase, which is argued to host orbital current order and break time–reversal symmetry (TRSB). In this talk we report high resolution polar Kerr effect measurements on CsV_3Sb_5 and ScV_6Sn_6 metals. Our measurements are supplemented by simultaneous coherent reflection ratio measurements in the same optical volume as the Kerr measurements, which are sensitive to birefringence and optical activity. Measurements are performed using three different versions of zero-area loop Sagnac interferometers (ZALSI), two operating at 1550 nm wavelength [1] and one at 830 nm [2]. Our results introduce stringent bounds to the possible "ferromagnetic-like" TRSB effects. We further analyze the bulk of optical effects in these materials and show that they host a unique chiral structure below the CDW transition.

References

[1] David R. Saykin, Camron Farhang, Erik D. Kountz, Dong Chen, Brenden R. Ortiz, Chandra Shekhar, Claudia Felser, Stephen D. Wilson, Ronny Thomale, Jing Xia, Aharon Kapitulnik, Phys. Rev. Lett. 131, 016901 (2023).S. Author, Journal **100**, 101101 (2009)

[2] David R. Saykin, Camron Farhang, Jing Xia, Chandra Shekhar, Claudia Felser, Aharon Kapitulnik, Preprint (2024).

Flat bands, bound states, and linear response of 2D metal Pd5Al2I

Raquel Queiroz

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Materials hosting flat electronic bands are a central focus of condensed matter physics as promising venues for novel electronic ground states. Two-dimensional (2D) geometrically frustrated lattices such as the kagome, dice, and Lieb lattices are attractive targets in this direction, anticipated to realize perfectly flat bands. Synthesizing these special structures, however, poses a formidable challenge, exemplified by the absence of solid-state materials realizing the dice and Lieb lattices. An alternative route leverages atomic orbitals to create the characteristic electron hopping of geometrically frustrated lattices. We report the realization of frustrated hopping in the van der Waals (vdW) intermetallic Pd5AlI2, emerging from orbital decoration of a primitive square lattice. The band structure of PdAlI includes linear Dirac-like bands intersected at their crossing point by a flat band. Moreover, PdAlI is exceptionally stable, with the unusual bulk band structure and metallicity persisting in ambient conditions down to the monolayer limit. We also show that frustated lattices are a natural place to find bound states in the continuum, quantum states that remain localized despite existing within a continuum of extended, delocalized states. We observe two defect states that remain localized within the metallic continuum of Pd5AlI2, stabilized by hopping interference in the Pd5AlI2 lattice.

Density wave order on the Kagome lattice: theory and experimental implications

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In this talk, I will discuss recent results for charge density wave (CDW) and pair density wave (PDW) instabilities on the kagome lattice near a van Hove singularity. I then discuss the relevance of these results to experimental observations in kagome metals such as CsV_3Sb_5.

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Topological superconductivity near van Hove fillings

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Topological superconductors have become an important research topic, stimulated by their potential for quantum and superconducting applications. Since the topology only protects against perturbations smaller than the superconducting gap, it is of paramount importance to find topological superconductors with large gaps and high transition temperatures. One possible path to high-temperature topological superconductivity is to consider materials where the Fermi level lies close to van Hove singularities (VHSs), which enhance the density of states. Motivated by this, we theoretically analyze the conditions under which topological superconductivity emerges close to van Hove fillings on the square [1] and kagome lattices [2,3]. For the kagome lattice we investigate how the different sublattice textures of the m-type and p-type VHSs influence the propensity for topological superconductivity. We review recent ARPES experiments and DFT calculations showing that in AV_3Sb_5 both m-type and p-type VHSs are close to the Fermi level. Considering electron-electron and electron-phonon mediated pairing in the Holstein-Hubbard model, we investigate the preferred pairing symmetries for the AV_3Sb_5 family of kagome superconductors. Close to van Hove fillings, the sublattice profile plays a crucial role in determining the pairing symmetry: at the p-type van Hove filling, the E_{1u} (*p*-wave) and B_{2u} (*f*-wave) pairings become leading; at the m-type van Hove filling, the E_{1u} and A_{2g} (*i*-wave) pairings get promoted. We discuss the properties of this variety of topological superconducting states, including Majorana edge and corner modes.

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Electron-phonon versus electron-electron interactions in Kagome systems

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The rich low-temperature behavior of AV_3Sb_5 compounds (with A=K,Rb,Cs), including charge density waves, superconductivity, and possibly broken time-reversal symmetry has ignited a long debate regarding the origin of the various phases in these kagome metals. We present a microscopic analysis of the interplay of electron-electron interactions versus electron-phonon interactions based on interacting models and discuss the appearance of various correlated phases at different fillings, from itinerant to Mott insulating states [1-3]. We then make the link to the present experimental situation on Kagome-based materials.

This work has been done in collaboration with Francesco Ferrari, Federico Becca and Qimiao Si. We acknowledge the DFG for funding through TRR288.

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New Electronic Properties with a Shake

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Charge density waves (CDWs) in two-dimensional (2D) materials have been a major focus of research in condensed matter physics for several decades due to their potential for quantum-based technologies. In particular, CDWs can induce a metal-insulator transition by coupling two Dirac fermions, resulting in the emergence of a topological phase. Following this idea, here we explore the behaviour of multiple CDWs in a 1D and 2D materials and their electronic transitions.

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Scanning time-resolved optical studies on Kagome superconductors

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The kagome lattice provides a fascinating playground to study geometrical frustration, topology and strong correlations. The newly discovered kagome metals AV_3Sb_5 (A = K, Rb, Cs) exhibit exotic phases including charge density waves (CDWs) and superconductivity. In our study, we perform scanning birefringence and circular dichroism (CD) microscopy on CsV_3Sb_5. The scanning birefrigence demonsate six-fold rotational symmetry breaking in the CDW phase and three domains that are 120 degree to each other. The emergence of opposite CD domains within the same birefringence domain, along with field-induced CD switching, indicate broken time-reversal symmetry. Furthermore, ultrafast pump-probe reflectivity measurements reveal a splitting of charge density wave induced phonon modes in all three birefringence domains. Such a breaking in degeneracy corroborates the six-fold rotation symmetry breaking in the charge ordered phase.

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Abstracts of Posters

(in alphabetical order)

Analysis of the competition between the possible emerging Charge-Density-Wave phases of CsV_3Sb_5

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Since its recent discovery, many studies have tried to characterize the intriguing CDW phases of the family of kagome metals AV_3Sb_5 (A=K, Rb, Cs). Even though unveiling the crystal structure of the CDW phase is crucial to understand the exotic properties of these materials, there is still lack of consensus in the emerging topological phases below the CDW transition temperature (T_{CDW}). Previous theoretical studies showed that this kagome family has phonon instabilities at the M=(1/2, 0, 0) and L=(1/2, 0, 1/2) q-points in the Brillouin zone, what opens the door to a six dimensional CDW order. Later studies showed that the CDW melting is due to ionic entropy, finding the instability in L as triggering mechanism. Here we resolve for the first time the free-energy landscape of the low-symmetry topological phases emerging from the six-dimensional CDW, which leads to a competition of two CDW phases that correspond to the P6/mmm (No. 191) and Fmmm (No. 69) space-groups. By studying the temperature dependence of the free-energy of these phases considering fully the ionic kinetic energy and anharmonicity, we are able not only to get spot on results on the T_{CDW}, but also to understand all the stable topological phases below it.

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Grain-boundary driven electronic phase separation in AV_3Sb_5 compounds

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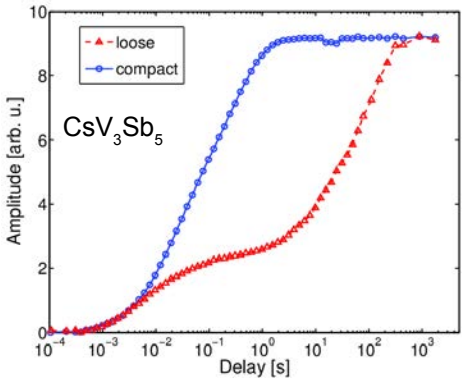
Vanadium-based kagome compounds AV_3Sb_5 (A = Rb, Cs, K) have gained vast research interest in recent years due to their rich physics, stemming from magnetic frustration and their marked quasi-2D character, which reflects in a complex band structure exhibiting van Hove singularities and topological features. Their properties encompass the onset of a commensurate chiral charge density wave (CDW) at T_{CDW} = 78-102 K and low-temperature superconductivity below T_C =1-3 K [1], while the breaking of time-reversal symmetry between T_C and T_{CDW} is still debated [2, 3].
Nuclear spin resonance is a fantastic tool to investigate these materials, as all atomic species except K are provided with good NMR nuclei locally probing the electronic spin susceptibility. Moreover, all of them exhibit large spins (I > ½), hence they are also sensitive to local lattice distortions through their quadrupolar coupling. [4].
In this workshop we present the results of a NMR/NQR investigation of CsV_3Sb_5 and RbV_3Sb_5 single crystals and powders. In loosely packed powders of all compositions NMR and NQR reveal, well above the superconducting T_C and up to 10-12 K, the spatial segregation of domains with enriched and depleted DOS at the Fermi level, witnessed by bimodal nuclear spin-lattice relaxations with enhanced and strongly depressed rates. Such a coexistence of volume fractions with marked metallic and virtually insulating properties (approximately 20% and 80% at 5K, respectively), however, is absent in single crystals and it is suppressed in compact powders. This indicates that electronic phase separation, though a bulk effect, is apparently controlled by the crystallite surface, as in the case of inter-grain tunneling, which is possibly a macroscopic sign of the topological character of these materials.



^{51}V NMR signal recovery from saturation vs. time (T_1 experiment) in loose (red) and in compact powders (blue), at T = 5K

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Kagome Metals with Noncollinear Antiferromagnetic Order

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Kagome metals are important for exploring emergent phenomena due to the interplay between band topology and electron correlation. Motivated by the recent discovery of charge density waves in the kagome lattice antiferromagnet FeGe, we investigate the impact of Sb doping on the structural, charge, and magnetic order of FeGe. The superlattice distortion induced by charge order disappears with only slight Sb doping (~1.5%) down to 80 K. The antiferromagnetic ordering temperature gradually shifts to 280 K for FeGe0.7Sb0.3. For FeGe1−*x*Sb*x* with *x* _ 0.1, crystal structures with a slightly distorted Fe kagome lattice are formed. A significant change in magnetic anisotropy from easy axis to easy plane with increasing *x* is identified from magnetization measurements. Interestingly, neutron diffraction reveals noncollinear antiferromagnetic structures widely exist below *TN* for all samples with *x* _ 0.1. These noncollinear magnetic orders could possibly be unconventional and result from on-site repulsion and filling conditions of the kagome flat band, as predicted by a recent theoretical work.

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Unveiling the nature of electronic transitions in RbV_3Sb_5 with Avoided Level Crossing μSR

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Kagome superconductors AV3Sb5 (A=Cs,K,Rb) provide a unique platform for studying the interplay between a variety of electronic orders, including superconductivity (SC), charge density waves (CDW), nematic phases and more. In addition, a spontaneous time reversal symmetry breaking (TRSB) transition taking place before superconductivity and therefore possibly creating exotic SC states, has been proposed. Previous zero-field (ZF) and high-field muon spin rotation studies [1-3] have indeed shown a two-step increase in the relaxation rate of the μSR signal, with characteristic temperatures of T1 □ TCDW □ 100 K and T2 □ 50 K. This increase was further enhanced by an applied magnetic field thus suggesting a magnetic contribution to the relaxation rate. In this study, we used the avoided level crossing μSR technique [4] to investigate charge order in near-zero applied field. By tracking the temperature dependence of quadrupolar level-crossing resonances, we examined the electric field gradient at the V nuclei in the kagome plane. Our results show that a second rearrangement of the charge density takes place at T2 and shares the same temperature trend of the μSR signal observed in ZF.

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Study of local charge and structural configurations of Kagome superconductor

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Kagome materials, thanks to their geometry made of hexagons and corner sharing triangles, offer a fertile ground to study several emergent quantum phenomena. These last are a direct consequence of the interplay between frustrated geometry, electronic correlation and a non-trivial band structure.
Among them, the newly discovered vanadium-based Kagome materials AV_3Sb_5 (A=K, Rb, Cs) have drawn attention thanks to their unique properties. Interestingly, these materials not only exhibit unconventional superconductivity (SC) but also a unique high temperature transition known as charge density wave (CDW) modulation and for this reason are nowadays used to further investigate these phenomena.

Following our previous experience with A=Rb [1], here we focused our attention on CsV_3Sb_5 and used both Nuclear Quadrupole Resonance (NQR) and Density Functional Theory (DFT) to study the evolution of the CDW transition and of the local charge and structural configurations.
More specifically, we followed the CDW modulation by analyzing ^{121}Sb NQR spectra and by studying the characteristics of the peaks obtained at different temperatures both above and below the transition [2]. Moreover, using DFT, we investigated different structures and found that the Tri-Hexagonal structure with a π-shift along the c axis is the most stable one.

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Recent Progress on Understanding the interplay between charge density wave and magnetism in kagome lattice magnet FeGe

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Two-dimensional (2D) kagome lattice metals are interesting because they display flat electronic bands, Dirac points, Van Hove singularities, and can have interplay between charge density wave (CDW), magnetic order, and superconductivity.In kagome lattice antiferromagnet FeGe, a short-range CDW order was found deep within an antiferromagnetically ordered state, interacting with the magnetic order. Surprisingly, post-growth annealing of FeGe at 560 C can suppress the CDW order while annealing at 320 C induces a long-range CDW order, with the ability to cycle between the states repeatedly by annealing. Here we perform transport, neutron scattering, scanning transmission electron microscopy (STEM), and muon spin rotation (μSR) experiments to unveil the microscopic mechanism of the annealing process and its impact on magneto-transport, CDW, and magnetic properties of FeGe. We find that 560 C annealing creates germanium vacancies uniformly distributed throughout the FeGe kagome lattice, which prevent the formation of Ge-Ge dimers necessary for the CDW order. Upon annealing at 320 C, the system segregates into stoichiometric FeGe regions with long-range CDW order and regions with stacking faults that act as nucleation sites for the CDW. The presence or absence of CDW order greatly affects the anomalous Hall effect, incommensurate magnetic order, and spin-lattice coupling in FeGe, thus placing FeGe as the only known kagome lattice material with a tunable CDW and magnetic order, potentially useful for sensing and information transmission.

Toward controlling the chirality of charge order in the Kagome Metal CsV_3Sb_5

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Tailored ultrafast laser fields are a powerful tool to selectively manipulate the macroscopic properties of quantum materials. By leveraging a range of light-quantum matter coupling mechanisms, experiments have demonstrated optical control of magnetism, ferroelectricity, topology, charge ordering, structural phases, femtosecond electronic motion, and superconducting-like metastable. In the Kagome metal CsV_3Sb_5, chiral charge ordering partially determines the ground-state transport properties in unstrained samples at temperatures above the superconducting transition temperature. Given that chiral electronic orders may couple strongly to chiral photons, the nonreciprocal transport response which originates from the chiral charge order in CsV_3Sb_5 is a candidate for optical manipulation. Here, we will utilize intense circularly polarized mid-infrared fields to bias the helicity of the low-temperature charge order. In this way, we aim to control the directionality of non-reciprocal c-axis magneto-transport which has been previously observed in unstrained a-c lamellas. By cooling the sample in the presence of a given polarization handedness and studying both the onset temperature and direction of nonreciprocal magneto-transport as a function of laser parameters and temperatures, we will develop an experimental protocol for deterministic control over charge order in CsV_3Sb_5. Experiments are ongoing, and we present our preliminary results.

Theories for charge-driven nematicity in kagome metals

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Kagome metals AV_3Sb_5 (A = K,Rb,Cs) form an intriguing class of compounds that show superconductivity at low temperatures (T_{sc}=1K) and an exotic 2x2 charge order (CO) at higher temperatures (T_{co}=100K). Besides this evidence, the experimental reports are quite in contradiction one with another regarding the presence of an additional transition within the 2x2 CO domain (especially for the caesium member of the family): some suggest the stabilization of a state that breaks the rotational symmetry of the lattice (nematicity), some others the transition to a one-dimensional 1x4 CO and others that no transition take place between T_{sc} and T_{co}.

In this poster presentation, I will focus on the nematic state, which might be described as an intra-unit cell (zero momentum) CO that occurs within the enlarged 2x2 unit cell of the system. A symmetry based Ginzburg-Landau analysis of the 2x2 CO allows to describe under which conditions the system develops a nematic charge order [1].

I will then describe two microscopic theories for nematicity in the kagome metals [2]: Starting from an effective low-energy model for the electronic bands at the Fermi level in the 2x2 phase, I will show that, for some values of the electronic interactions, the system might go through a d-wave charge Pomeranchuk instability and to a transition towards a 1x4 CO. While the Pomeranchuk instability might naturally explain the onset of nematicity in this class of compounds, there might be another mechanism related to the presence of strong fluctuations of the 1x4 CO near the phase boundary. Differently from the iron-based superconductors, where nematicity might be explained thanks to the presence of spin fluctuations, charge fluctuations might be the key to explaining nematicity in the kagome metals.

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Orbital selective commensurate modulation of the local density of states in the Kagome metal ScV_6Sn_6 probed by nuclear spins

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The two-dimensional Kagome network build from cornersharing triangles is a key structural motif in modern solid state physics as it hosts special electronic states related to Dirac cones, van-Hove singularities, and flat bands. Compounds based on stacked Kagome planes have repeatedly been shown to be rich platforms to study critical phenomena including electronic correlation, superconductivity, and charge order. The non-magnetic, Vanadium based Kagome metal ScV6Sn6 undergoes a charge density wave (CDW) transition below about 96 K. The unconventional nature of the CDW, its formation mechanism, and accompanying effects that imply some unidentified mechanism for time-reversal symmetry breaking have attracted further attention. Given the variety of interesting phenomena that demand for a microscopic picture of the structural and electronic properties of ScV_6Sn_6 we employ ^{51}V nuclear magnetic resonance (NMR) to investigate the CDW phase from a local point of view. Aided by density functional theory (DFT), we can relate the dynamics of the local magnetic field to the changes in the V density of states (DOS), we find the reported reconstruction of the unit cell reflected in a characteristic modulation of the charge symmetry at V nuclei, while the local magnetic field reveals a substructure of Fermi level states suggesting orbital selective modulation of the local DOS [1].

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Pressure-dependent Electronic Instabilities in CsV3Sb5 Probed by High-Resolution X-Ray Diffraction

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In this contribution I will present, crystal growth, characterisation and high-resolution single crystal x-ray diffraction study of Kagome superconductor CsV3Sb5, exploring its response to variations in pressure and temperature. We discover that at low temperatures, the structural modulations of the electronic superlattice, commonly associated with charge density wave order, undergo a transformation around p ~ 0.7 GPa from the familiar 2 × 2 pattern to a long-range ordered modulation at wavevector q = (0, 3/8, 1/2). Our observations align with inferred changes in the CDW pattern from prior transport and nuclear magnetic resonance studies, providing new insights into these transitions. Interestingly, the pressure-induced variations in the electronic superlattice correlate with two peaks in the superconducting transition temperature as pressure changes, hinting that fluctuations within the electronic superlattice could be key to stabilizing superconductivity. Details regarding the crystallographic structure, will be discussed.

Pomeranchuk Instability Induced by an Emergent Higher-Order van Hove Singularity on the Distorted Kagome Surface of Co3Sn2S2

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Kagome metals have drawn significant attention in condensed matter physics due to the geometrical arrangement of the lattice that gives rise to a flat band and two van Hove singularities (VHS) that flanks a Dirac node. This poster will focus on scanning tunneling microscopy (STM) data on the Co termination of the kagome compound $Co_3Sn_2S_2$ (a ferromagnetic Weyl semimetal). The distortion of the surface gives rise to a high order VHS. I will present real space spectroscopic data that is combined with a super sampling technique [1] this will allows us to observe the different phases of the electronic wave function. Finally, I will present the possibility of a Pomeranchuk instability of the fermi surface and how it is embedded in quasi-particle interference measurements [2].

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Superconducting gap structure in the new family of kagome lattice superconductors AV_3Sb_5

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The kagome superconductor AV_3Sb_5 (*A* = K, Rb, Cs) exhibits an unusual charge-density-wave order (CDW) with time reversal and rotational symmetry breaking, which is considered to be driven by a unique band structure characterized by van Hove singularities (vHSs). Recent theories suggest various unconventional superconducting (SC) symmetries, including a chiral order parameter. In addition, recent experiments have revealed distinct CDW orders in K/RbV_3Sb_5 compared to CsV_3Sb_5, which may lead to different SC gap structures. Experimentally, however, the SC gap structure in AV_3Sb_5 is still under debate.

Here, we report on the SC gap structure in AV_3Sb_5 revealed by magnetic penetration depth measurements. Our experiments on CsV_3Sb_5 [1] have revealed that an anisotropic fully-gapped state changes to an isotropic full-gap state without passing through a nodal state as impurities increase upon electron irradiation, indicating that CsV_3Sb_5 is a non-chiral, anisotropic *s*-wave SC with no sign change. Further studies on Rb/KV_3Sb_5 [2] have revealed that the SC gap structure becomes more isotropic in the order of Cs, Rb, and K. The evolution of the SC gap anisotropy can be explained by changes in the van Hove singularity near the Fermi level depending on the CDW ordering pattern, which reduce bond-order fluctuations. These findings suggest that in CsV_3Sb_5, an anisotropic *s*-wave SC state emerges due to bond-order fluctuations driven by vHSs, whereas in K/RbV_3Sb_5, isotropic *s*-wave SC states appear primarily through phonon-mediated fluctuations.

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Interplay of superconductivity and charge-density-wave order in kagome materials

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In several superconductors, the superconducting state emerges out of a charge-density-wave (CDW) order. To determine the microscopic origin and structure of the ordered phases, one often studies the CDW and superconductivity independently. However, the mutual influence of the individual orders can be crucial for understanding the phase diagram. An intriguing example is the AV_3Sb_5 (A = K, Rb, Cs) kagome metals, where a 2x2 in-plane CDW ordered phase, potentially breaking time-reversal symmetry, appears at a temperature of approximately 100K, followed by a transition into a superconducting phase at T_c ~ 1-3K.

In our work, we present a phenomenological theory of CDW and superconducting orders for the kagome lattice. Considering the CDW as a static background, we derive a Ginzburg-Landau free energy of possible superconducting and 2x2 CDW orders and explore the impact of their mutual coupling. Motivated by experiments, we consider additional spatial or time-reversal-symmetry breaking of the CDW order. Furthermore, given the unclear nature of the superconducting state in the AVS compounds, we discuss *s*-wave, *d*-wave, and pair-density-wave order parameters, investigating the consequences of which provides the leading instability. Our results shed light on how the superconducting state mimics the broken symmetries of the charge order and can guide future microscopic calculations and the experimental identification of the superconducting state in the AVS kagome materials.

Kagome superconductors LaRu3Si2

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Kagome materials manifest a rich variety of physical properties due to the emergence of abundant electronic phases. Here, we conduct a thorough investigation, using detailed numerical and analytical methods, of the flat-band kagome superconductor $LaRu_3Si_2$, which has recently been reported to host both charge density wave and superconductivity. We observe that superconductivity is predominantly driven by the coupling between kagome phonons and kagome flat bands. The impact of doping on the electron-phonon coupling (EPC) and superconductivity is also examined, revealing that, while heavy doping can introduce instability and magnetism, in cases of weak doping, the superconducting Tc is significantly enhanced—by approximately 50%—due to the high density of states provided by the kagome flat band.

FeGe as a LEGO Building Block for the 1:1, 1:6:6, and 1:3:5 families, and Catalogue of Phonon Instabilities in 1:6:6 family

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The electronic structure and interactions of kagome materials such as 1:1 (FeGe class),1:6:6 (MgFe6Ge6 class), and 1:3:5 (CsV3Sb5 class) are complicated and involve many orbitals and bands at the Fermi level. In this work, we show that the complicated electronic bands near the Fermi level can be decomposed into three groups of orbitals. Our three minimal Hamiltonians can reproduce the quasi-flat bands, van Hove singularities, topology, and Dirac points close to the Fermi level. We also obtain the interacting Hamiltonian of d orbitals in FeGe using the constraint random phase approximation method. We then use FeGe as a fundamental LEGO-like building block for the 1:6:6 kagome materials, which can be obtained by doubling and perturbing the FeGe Hamiltonian. We further extend the formalism developed for the 1:1 family to the 1:3:5 family AB3Z5 (A = K, Rb, Cs; B = Cr, V, Ti; Z = Sb, Bi), demonstrating the broad applicability of the LEGO building block approach.

We also carry out a high-throughput first-principles study of the 1:6:6 family MT6Z6 materials in SG 191, focusing on their phonon instability and electronic flat bands. We classify the phonon instabilities into three types. Type-I instabilities involve the in-plane distortion of kagome nets, while type-II and type-III present out-of-plane distortion of trigonal M and Z atoms. Our predictions suggest a vast kagome family with rich properties induced by the flat bands, possible CDW transitions, and their interplay with magnetism.

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Frustrated charge density wave and quasi-long-range bond-orientational order in the magnetic kagome FeGe

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Abstract:

The intrinsic frustrated nature of a kagome lattice is amenable to the realization of exotic phases of matter, such as quantum spin liquids or spin ices, and more recently the multiple-charge density waves (CDW) in the kagome metals. Despite intense efforts to understand the mechanism driving the electronic modulations, its origin is still unknown and hindered by competing interactions and intertwined orders. Here, we identify a dimerization-driven 2D hexagonal charge-diffuse precursor in the antiferromagnetic kagome metal FeGe and demonstrate that the fraction of dimerized/undimerized states is the relevant order parameter of the multiple-q CDW of a continuous phase transition. The pretransitional charge fluctuations with propagation vector $q=q_M$ at $T_{CDW}<T<T^*$(125 K) are anisotropic, hence holding a quasi-long-range bond-orientational order. The broken translational symmetry emerges from the anisotropic diffuse precursor, akin to the Ising scenario of antiferromagnetic triangular lattices. The temperature and momentum dependence of the critical scattering show parallels to the stacked hexatic B-phases reported in liquid crystals and transient states of CDWs and highlight the key role of the topological defect-mediated melting of the CDW in FeGe.

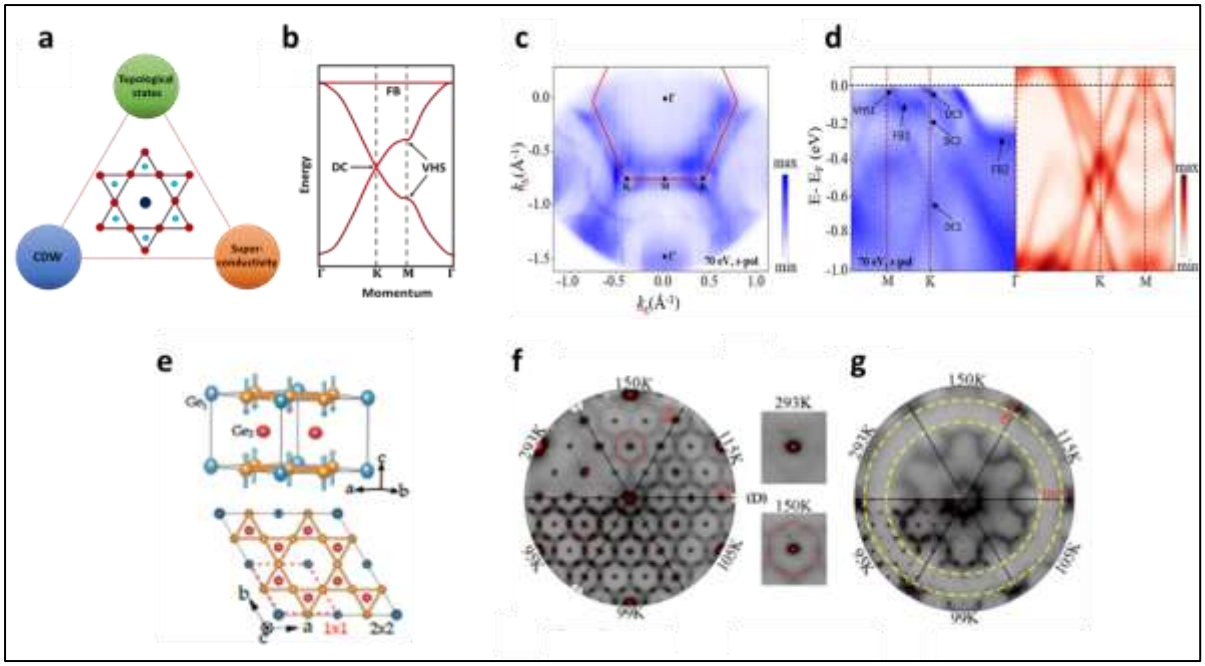

Figure: (a) Exotic Electronic orders in Kagome lattice including Superconductivity, charge density wave (CDW), and Topological state. (b) Schematic representation of the ideal band structure of Kagome lattice with Dirac cones (DC), Van Hove singularity (VHS), and flat band (FB) in momentum space. (c)-(d) Fermi surface and electronic band structure of FeGe. (blue bands from ARPES and orange bands from DFT). (e) Geometric structure of FeGe. (f)-(g) Temperature dependence diffuse scattering mapping of (h k 2) and (h k 3/2) planes, respectively.

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Competing charge density waves and their manipulation in kagome metals

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Charge density waves (CDWs), periodic modulations of charge density arising from electron-electron interaction and/or electron-phonon coupling, have been central themes of modern condensed matter physics. CDWs have been studied in various compounds, including transition metal dichalcogenides, cuprates, nickelates, and more recently, kagome metals. Among these, CDWs in kagome metals have attracted significant attention due to their intriguing characteristics, such as time-reversal symmetry breaking and their interplay with superconductivity and nematic phases.

In the first part of the presentation, I will introduce our recent theoretical proposal on monolayer AV_3Sb_5 as an exciting platform to study the intriguing interplay between van Hove singularities (VHSs) and exotic CDW orders [1]. Due to its reduced symmetry compared to the bulk, the monolayer reformulates the distribution of VHSs, enriching their characteristics. As a result, the monolayer hosts various competing orders, including novel CDW orders, such as the doublet formation of commensurate CDWs and incommensurate CDWs without bulk counterparts. We further show that the competition between CDW orders can be fine-tuned via strain and doping.

In the second part of the presentation, I will discuss our comprehensive first-principles study on the origin of competing CDWs in the kagome metal ScV_6Sn_6 [2]. We develop a theory of CDW order in ScV_6Sn_6 based on anharmonic phonon-phonon calculations combined with density functional theory. Our theory predicts a temperature-driven phase transition from the high-temperature $\times 2$ CDW to the low-temperature $\times 3$ CDW order, fully explaining experimental observations. Additionally, we construct a phase diagram of the competing CDWs in the lattice parameter space and demonstrate that the out-of-plane lattice parameter plays a pivotal role in manipulating the competing CDWs in ScV_6Sn_6. We propose compressive bi-axial strain as an experimental protocol to stabilize the $\times 2$ CDW order. Furthermore, we suggest Ge and Pb doping at the Sn site as another potential avenue to control CDW instabilities. Our work provides crucial insights into understanding CDWs in the kagome metal family.

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Frustration, Chirality, and Disorder

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We will discuss theoretical models showing possible emergent behavior, on the Kagome lattice as well as with Kagome-type frustration, involving chirality and arising via disorder. The relevant materials include the YCOB-Cl family of kagome magnets with two doping parameters that also introduce disorder [1]; trimer-honeycomb Mn3Si2Te6, which undergoes a metal-insulator crossover with 10-million drop in resistivity, potentially arising from chiral orbital “loop” current ferromagnetism [2]; and relation to Kitaev models and interactions on the honeycomb and kagome lattices [3].

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Mechanism for Loop Current Order in Kagome Metals from Intertwined van-Hove Singularities

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Recent experiments on kagome metals AV_3Sb_5 (A=Cs,Rb,K) indicated spontaneous time-reversal symmetry breaking in the charge density wave state in the absence of static magnetization. The loop current order (LCO) is proposed as its cause, but a microscopic model explaining the emergence of LCO through electronic correlations has not been firmly established. We show that the coupling between van-Hove singularities (vHS) with distinct mirror symmetries is a key ingredient to generate LCO ground state. By constructing an effective model, we find that when multiple vHS with opposite mirror eigenvalues are close in energy, the nearest-neighbor electron repulsion favors a ground state with coexisting LCO and charge bond order. It is then demonstrated that this mechanism applies to the kagome metals AV_3Sb_5. Our findings provide an intriguing mechanism of LCO and pave the way for a deeper understanding of complex quantum phenomena in kagome systems.

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Spin-polarized p-wave superconductivity in the kagome material RbV_3Sb_5

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The study of kagome materials has attracted much attention due to the presence of many electron-electron interaction-driven phases in a single material. In this work, we report the discovery of intrinsic spin-polarized p-wave superconductivity in the thin-flake kagome material RbV_3Sb_5. A hysteresis in resistance as a function of the applied in-plane magnetic field is observed, indicating the emergence of an intrinsic time-reversal symmetry-breaking superconducting phase. Interestingly, a finite resistance state can be quenched to a zero-resistance state by applying a large current within the hysteresis loop. Moreover, a magnetic field-driven re-entrance of superconductivity is also observed. We suggest that the pairing symmetry, which is consistent with the crystal symmetry and the observed novel properties, is a time-reversal symmetry-breaking, p-wave pairing state with net spin polarization.

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Unconventional superconductivity in kagome lattice compounds AV_3Sb_5 (A = K, Rb, Cs) as seen by muon spin rotation and relaxation

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Kagome lattice materials exhibit exiting properties due to the intertwining of topology, correlation, and magnetism. The electronic structure of these compounds features a van Hove singularity, a flat band and Dirac cones. Therefore, these materials have recently been subject to tremendous experimental and theoretical studies. Here, we will review our recent experimental progress on superconductivity in the kagome compounds AV_3Sb_5 (A = K, Rb, Cs) from a local magnetic probe point of view [1-5]. We employed muon spin rotation and relaxation under extreme conditions like hydrostatic pressure, low temperatures and high magnetic fields and observed tunable unconventional time-reversal symmetry-breaking superconductivity.

We observe superconductivity with a nodal energy gap in $(K,Rb)_3Sb_5$ and a nodeless energy gap in CsV_3Sb_5 at ambient pressure as well as a reduced superfluid density which can be attributed to the competition with the charge order. Upon applying pressure, the charge-order transition is suppressed, the superfluid density increases, and the superconducting state progressively evolves from nodal to nodeless in KV_3Sb_5 and RbV_3Sb_5. Once the charge order is eliminated, we find a superconducting pairing state that is not only fully gapped and also spontaneously breaks time-reversal symmetry in all three systems. These results demonstrate the tunability of unconventional kagome superconductivity that is competing with time-reversal symmetry-breaking charge order and provide unique insights into the nature of the pairing state.

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Unconventional gapping behavior in a kagome superconductor

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Determining the types of superconducting order in quantum materials is a challenge, especially when multiple degrees of freedom, such as bands or orbitals, contribute to the fermiology and when superconductivity competes, intertwines, or coexists with other symmetry-breaking orders. Here, we study the Kagome-lattice superconductor CsV3Sb5, in which multiband superconductivity coexists with a charge order that substantially reduces the compound's space group symmetries. We uncover two superconducting regimes with distinct transport and thermodynamic characteristics, while finding no evidence for a phase transition separating them. To unify these results we propose band-selective superconductivity on the V- and the Sb -derived fermi surface with remarkable decoupling of the two superconducting gaps.

Time-reversal symmetry-breaking charge order in kagome metals

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Kagome lattice metals have long been predicted to be the ideal platform for hosting unconventional phases, given the band structure arising from the geometric frustration featuring flat bands, van Hove singularities, and topological Dirac points. One of the most important recent findings in kagome materials is highlighted by the unconventional coupling of charge ordering and time-reversal symmetry-breaking (TRSB). This unconventional coupling was discovered in KV_3Sb_5 [1], enabled by the powerful combination of zero-field and high-field μSR, and later observed in RbV_3Sb_5 and CsV_3Sb_5 as well [2,3]. While this TRSB charge order is ubiquituous in the AV_3Sb_5 (where A = K, Rb, Cs) family, it has also been observed in other kagome metals, including the prototypical kagome superconductor $LaRu_3Si_2$. In the case of $LaRu_3Si_2$, however, an exceptionally high-temperature charge order has been observed from 400 K [4], which gives way to a second charge order which breaks time-reversal symmetry below 80 K [5]. Such unconventional charge order arising from the kagome lattice provides an exquisite and tantalizing step towards control and comprehension of the complex interplay between competing states in condensed matter physics.

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Microscopic nature of the charge density wave in Kagome metals

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The recently discovered vanadium-based Kagome metals AV_3Sb_5 (A = K, Rb, Cs) undergo a unique phase transition into charge-density wave (CDW) order which precedes both unconventional superconductivity and time-reversal symmetry breaking. Therefore, the essential first step in building a full understanding of the role of CDW in establishing these unconventional phases is to unveil the symmetries and the microscopic nature of the charge-ordered phase. In this talk, I will present ways in which microscopic measurements and theory can be coupled to determine the exact nature of the charge density wave state. Specifically, I will present determination of the exact structure of the 2 × 2 × 2 superlattice that develops below the charge-density wave ordering temperature (T_{CDW}) in RbV_3Sb_5. This is achieved by a comprehensive set of ^{51}V, ^{87}Rb, and ^{121}Sb nuclear magnetic resonance (NMR) measurements and density functional theory simulations of NMR observables to provide a unique site-selective view into the local nature of the charge-ordered phase. The combination of these experimental results with simulations provides compelling evidence that the CDW structure prevailing below 103 K in RbV_3Sb_5 is the so-called inverse Star of David pattern, π-shifted along the c axis. These findings put severe constraints on the topology of these Kagome compounds and thus provide essential guidance for the development of an appropriate theoretical framework for predicting properties of exotic electronic orders arising within the CDW phase. Furthermore, I will discuss the nature how the charge ordering evolves as a function of the hole doping in $CsV_3Sb_{5-x}Sn_x$, Kagome metals.

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Magnetoelectronic and thermodynamic properties of new heusler alloys as superconductors

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We show in this paper the prediction of stoichiometric Nb_2GdZ (Z= Si, In) ordered ternary intermettalic heusler alloys as superconductors. We report, based on density functional theory calculations and using the FPLAPW-(SO) calculations implemented in wien2k package, the electronic and magnetic proprerties within Spin orbite calculation which have crucial role and the effect of U hubbard can not be neglected, the calculations have been performed in order to understand structural and elastic properties and thermodynamic properties show important temperature which not have been predicted previously. This debye temperature makes this new compounds as potential candidates for next supercondutors applicatoins .

Emergent charge order seen by local magnetic probes in highly doped $CsV_3Sb_{5-x}Sn_x$

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The kagome superconductor CsV_3Sb_5 undergoes a high-T transition into a charge density wave (CDW) state that precedes superconductivity (SC). Both are believed to arise from nested van Hove singularities being proximal to the Fermi energy. By means of Sn partial substitution amounting to hole-doping in $CsV_3Sb_{5-x}Sn_x$, we can track the evolution of the charge correlations. Previous work saw the suppression of the CDW into the first SC dome [1, 2] and stabilization of incommensurate, quasi-1D charge stripes [3].

Here, two local probes at zero field (ZF), nuclear quadrupolar resonance (NQR) and muon spin resonance (ZF-μSR) demonstrate that the short-ranged (SR-CDW), in fact, persists up to at least x = 0.35 and mimics the SC double-dome structure, Fig 1. On cooling, we discovered further charge restructuring via an electronic inhomogeneity (EI) contribution to the nuclear spin relaxation time akin to previously seen stripes. Finally, before reaching the SC state, in the absence of local spins, μSR senses another charge rearrangement whose true microscopic nature lies in a few contestant theories, including orbital antiferromagnetism, orbital currents, and electronic nematicity.

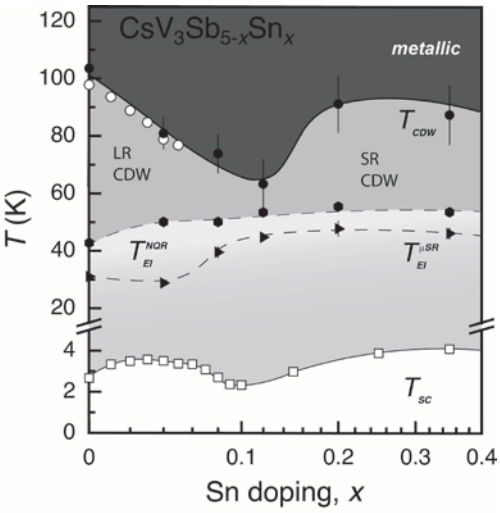

Fig1. Hole-doping $CsV_3Sb_{5-x}Sn_x$ phase diagram to compare magnetic susceptibility χ (white symbols) [1] with NQR and μSR (present work).

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A New Moiré Platform Based on M-Point Twisting

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We introduce a new class of moiré systems and materials based on monolayers with triangular lattices and low-energy states at the M points of the Brillouin zone. These M-point moiré materials are fundamentally distinct from those derived from Γ- or K-point monolayers, featuring three time-reversal-preserving valleys related by three-fold rotational symmetry. We propose twisted bilayers of experimentally exfoliable 1T-$SnSe_2$ and 1T-ZrS_2 as realizations of this new class. Using extensive *ab initio* simulations, we develop quantitative continuum models and analytically show that the corresponding M-point moiré Hamiltonians exhibit emergent momentum-space non-symmorphic symmetries and a kagome plane-wave lattice in momentum space. This represents the first experimentally viable realization of a projective representation of crystalline space groups in a non-magnetic system. With interactions, these materials represent six-flavor Hubbard simulators with Mott physics, as can be seen by their flat Wilson loops. Furthermore, the presence of a non-symmorphic momentum-space in-plane mirror symmetry makes some of the M-point moiré Hamiltonians quasi-one-dimensional in each valley, suggesting the possibility of realizing Luttinger liquid physics. We predict the twist angles at which a series of (conduction) flat bands appear, provide a faithful continuum Hamiltonian, analyze its topology and charge density and briefly discuss several aspects of the physics of this new platform.

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Higgs spectroscopy as a novel tool to characterize unconventional forms of superconductivity

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Recently it was shown that Kagome lattices of the type AV3Sb5 (A = K, Rb, Cs) can become superconducting. They also exhibit unconventional competing orders such as unconventional chiral charge order. This leads to a complex electronic excitation spectrum with multiple and competing gaps in the electronic excitation spectrum. In my presentation I will reflect on an alternative pathway to disentangle competing ordering phenomena by transient inelastic light scattering. In particular the Higgs mode of superconductors can be studied by NEARS (Non Equilibrium Antistokes Raman Scattering) and disentangled from e.g. competing charge order.[1-6] The Higgs mode is unique to the superconducting state and serves as a key indicator for the formation of the superconducting state going beyond gap opening or pair breaking.[3-5,7] I will discuss the state of the art in Higgs spectroscopy [7] in superconductors and its possible application to Kagome systems in order to disentangle different competing ordering phenomena.

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Emergent Phase Transitions in RbV3Sb5 measured by nuclear magnetic resonance

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Vanadium-based kagome superconductors AV3Sb5 (A = K, Rb, Cs) have received great attention as hosts for some of the most intriguing phenomena in condensed matter physics, including unconventional superconductivity, charge density wave (CDW), and time-reversal symmetry breaking (TRSB) phases. Specifically in RbV3Sb5, two transitions have been well-identified for CDW and superconductivity: TCDW = 104K, and TC = 0.8K. Another transition has been observed around Tx = 50K by muon-spin rotation measurements, but it is by far the least understood transition out of the three due to a limited amount of data. Here, we provide additional evidence for this transition at Tx = 50K through nuclear magnetic resonance (NMR) and zero field nuclear quadrupole resonance (NQR).

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Domain wall engineering in distorted Kagome magnet

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In condensed matter, nontrivial topological states, electron correlations, and magnetism are central ingredients to realize quantum properties including unconventional superconductivity, charge and spin density waves, and spin liquid/ice state, multiferroicity, etc. Kagome materials can host these phenomena due to their unique lattice and band structure. [1] Interestingly, materials with noncoplanar antiferromagnetic spin structures also exhibit anomalous Hall effect (AHE) and under the applied field domain wall can be observed, which are technologically important due to development of spintronic devices, data storage devices, magnetic sensors, etc. [2] Recently, *RTX* series (*R*: rare earth, *T*: transition metal, *X*: Ge, Sn, Al) with ZrNiAl structure have gained attention due to possessing kagome lattice continuously breaking translation symmetry i.e., distorted kagome lattice. Intriguingly, HoAgGe has been predicted to have a kagome spin ice state originating from the geometric frustration resulting due to the arrangement of Ho-spins and electronic transport is found to break time reversal like symmetry and show two degenerate states in anomalous Hall effect. [3, 4] Along this line, we have synthesized single crystals of TbAgGe to investigate the magnetic and electrical transport properties in detail. It crystallizes in a hexagonal crystal structure with space group *P-62m*. It exhibits long-range AFM ordering of Tb3+ ions at Néel temperature T_{N1} ~ 29K, T_{N2} ~ 25K and T_{N3} ~ 20K. Further, it shows metamagnetic transitions when $H \parallel c$, which might result in a non-coplanar spin structure in the system and goes to ferromagnetic (FM) state at high fields. Moreover, it shows significant anomalous Hall effect near the metamagnetic transitions, which is attributed to originating from the magnetic domain walls. Our findings suggest that RTX family with distorted kagome lattice can be an excellent platform to study the interplay of domain wall magnetism and topology.

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Visualizing the kagome origin of the heavy-Fermion-like phenomenology in Ni_3In

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Flat bands around Fermi energy result in various electronic instabilities and exotic phenomena [1]. Particularly, in heavy-fermion materials, the interaction between partially filled *f*-states and the *spd*-conduction electrons results in the hybridization of flat and wide bands around the Fermi level, leading to quantum criticality [2,3]. This Kondo lattice description has also been used recently in moiré physics [4]. Here, using scanning tunneling microcopy/spectroscopy, we investigate Ni_3In, a kagome metal that hosts an active flat band that crosses Dirac states, presenting a heavy-fermion-like phenomenology [5,6]. We find in scanning tunneling spectroscopy a zero-bias peak-dip structure, which evolves with magnetic fields and temperature according to the reported Doniach phase diagram. We identify that the peak has its origin in compact molecular orbitals formed by destructive interference over the Kagome sites, resulting in emergent *f*-shell-like localized moments [7-9]. Finally, using quasi-particle interference, we visualize its interaction with the Dirac light bands. We unveil that the heavy-fermion description is applicable more universally than previously thought, in which there are certain commonalities as well as distinctions, that are unique to the specific flat band platform.

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Tailoring electronic structure of the AV_3Sb_5 kagome metals by pressure

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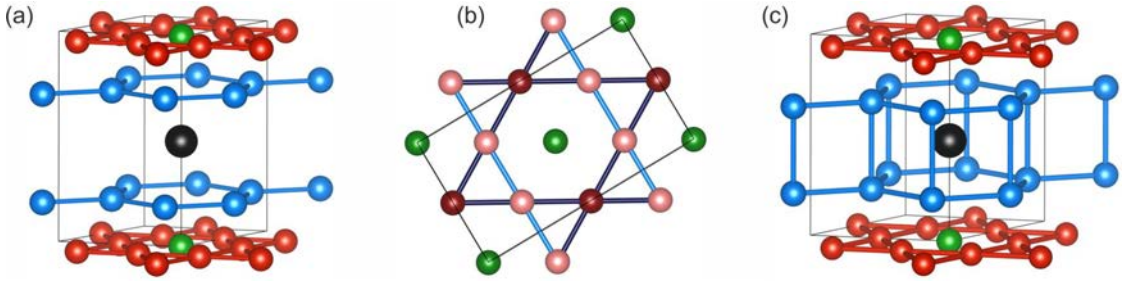
Kagome metals show interesting features of the electronic structure – most notably, Dirac points, flat bands, and van Hove singularities – along with exotic quantum states, such as unconventional density waves with loop current order and superconductivity. Most of this interesting phenomenology has been recently observed experimentally for the first time in the family of AV_3Sb_5 kagome metals with A = K, Rb, Cs [1]. In contrast to other kagome metals, which are the robust 3D intermetallic compounds with a very strong bonding between the kagome planes, the AV_3Sb_5 layered solids are highly sensitive to the applied pressure and show an intriguing pressure-induced behavior, including reentrant superconductivity.

In this talk, experimental structural evolution of AV_3Sb_5 under hydrostatic and nonhydrostatic pressure will be presented. We will show how structural changes induced by pressure can be used to manipulate the electronic structure of these materials. The primary effect is the 2D-3D crossover induced by the large compression perpendicular to the kagome layers with the formation of interlayer Sb-Sb bonds [2]. It leads to a distinct reconstruction of the Fermi surface, which is correlated with the reentrance of superconductivity in CsV_3Sb_5. Details of this reconstruction strongly depend on the alkaline metal, and additional distortion modes can be activated by switching between the quasi-hydrostatic and nonhydrostatic pressure conditions [3]. Our results highlight pressure as a versatile tuning parameter for kagome metals and demonstrate how different distortion modes of the superconducting kagome network can be achieved experimentally.



Crystal structures of CsV_3Sb_5 at 0 GPa (a) and 20 GPa (c) show the formation of interlayer Sb-Sb bonds under pressure. (b) An additional distortion caused by the nonhydrostatic pressure breaks down the six-fold symmetry in the kagome plane.

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Pressure-induced Lifshitz transitions in magnetic kagome metal Fe_3Sn_2 traced via structural and electronic changes

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Kagome metals emerged as a promising playground merging the field of strongly correlated localized electrons, topology, and non-trivial Dirac fermions [1]. The tunability of these different contributions via external means opens interesting new directions in the research of kagome metals. In this presentation, we present the pressure evolution of the electronic structure in ferromagnetic kagome metal Fe_3Sn_2 revealed by single-crystal XRD, high-pressure infrared and pump-probe spectroscopies, and density-functional calculations (DFT).

Different contributions to the optical spectra have been discussed and compared with the DFT calculations, which use the experimental high-pressure crystal structure. Infrared spectra reveal the signatures of the conventional and unconventional charge carriers in the compound [2]. While the low-energy spectral range reflects the response of the mobile charge carriers and is significantly modified with increasing pressure, the high-energy range shows the modest modification of the interband transitions in the compound.

The plasma frequency reflecting the carrier density in the compound shows a gradual increase with pressure, albeit small anomalies can be identified at ~10 and 16 GPa. Our DFT calculations reveal the appearance of new Fermi surfaces at the identified pressures creating a direct link with the IR studies and the pressure-induced Lifshitz transitions. Furthermore, the unconventional carrier dynamics present a non-monotonous change with the pressure that we can link to the morphology of the kagome network that is resolved with the XRD studies.

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Phenomenology of bond and flux orders in kagome metals

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Despite much experimental and theoretical work, the nature of the charge order in the kagome metals belonging to the family of materials AV_3Sb_5 (A = Cs,Rb,K) remains controversial. A crucial ingredient for the identification of the ordering in these materials is their response to external perturbations, such as strain or magnetic fields. To this end, we provide a comprehensive symmetry classification of the possible charge orders in kagome materials with a 2 × 2 increase of the unit cell. Motivated by the experimental reports of time-reversal symmetry breaking and rotational anisotropy, we consider the interdependence of flux and bond orders. Deriving the relevant Landau free energy for possible orders, we study the effect of symmetry-breaking perturbations such as strain and magnetic fields. Our results thus provide a road map for future tests of these intricate orders.

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The Complex Magnetic Structure and Giant Topological Hall Conductivity in Kagome Metal $YnMn_6Sn_6$

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The discovery of topological Kagome magnets attracts enormous interest. The flat bands and the Dirac point of the Kagome lattice might induce many intriguing phenomena. Furthermore, the interaction between the noncolinear magnetic structures and band topology deserves further exploration. In this work, by using first-principles calculations and spin Hamiltonian analysis, we investigated the magnetic phases with the increasing external field and discussed the origin of topological Hall conductivity for YMn6Sn6. This material is an ideal platform to understand the complex magnetic structures and topological properties of Kagome magnets.

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Optical study of ATi$_3$Bi$_5$ (A = Rb, Cs) compounds

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The AV$_3$Sb$_5$ compounds (where A = K, Rb, or Cs) display remarkable properties, such as charge density wave (CDW) order, superconductivity, and electronic nematicity. These properties are thought to be driven by the presence of nested van Hove singularities (VHS) near the Fermi level [1].
In contrast, the ATi$_3$Bi$_5$ family (A = Rb, Cs) shares the same crystal structure but has a different electronic band structure, lacking the band saddle points near the Fermi level [2]. This difference leads to the absence of CDW order at low temperatures, although electronic nematicity is still observed [3]. Using infrared spectroscopy, we study the temperature-dependent electronic structure of ATi$_3$Bi$_5$ (A =Rb, Cs) in a broad energy range of 6 meV - 2.25 eV. Aided by DFT calculations, we discuss the low-energy interband transitions and the influence of the band structure.

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Emergent Loop Current Order in the Kagome Lattice

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Recent experimental investigations have identified fascinating electronic orders in kagome materials, such as intriguing superconductivity, charge density wave (CDW) and nematicity. Notably, there is evidence of spontaneous time-reversal symmetry (TRS) breaking within the CDW phase, though its origins remain elusive. In our work, we comprehensively explore the competitive instabilities in the spinless kagome model with nonlocal interactions at the van Hove filling. We thoroughly analyze in intrinsic onsite and bond charge fluctuations within the kagome lattice, uncovering their intimate relations with the sublattice texture on the Fermi surface [1,2]. We find that, at the nesting vector, the onsite charge order will be significantly suppressed, while the bond charge order get enhanced owing to the sublattice interference effects. We also observe that next nearest-neighbor bonds are characterized by significant intrinsic imaginary bond fluctuations. The 2x2 loop current order (LCO) emerges as the ground state when the next NN repulsion is strong. Moreover, this TRS breaking LCO characterized by nontrivial Chern bands, reminiscent of the Haldane model, is also identified through functional renormalization group calculations for the first time [2]. While, sufficiently strong nonlocal interactions give rise to a nematic sublattice CDW. We further explore the possible superconductivity deviating from van Hove filling, where p- and f -wave pairings appear from bond charge fluctuations. Potential experimental implications are also discussed.

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Microscopic insights into the chiral flux phase of CsV3Sb5

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The layered compounds AV3Sb5 (A = K, Rb, and Cs) with a vanadium kagome lattice exhibit various interesting electronic phases, such as superconductivity [1] and a 2x2 charge density wave (CDW) [2]. Most notably, CsV3Sb5 was found to exhibit a time-reversal symmetry (TRS) broken state without the presence of local magnetic moments [3]. A chiral flux phase that arises within the 2x2 CDW state has been proposed as a possible TRS breaking mechanism. Direct experimental evidence for the chiral flux phase would be desirable to better understand the rich phenomenology of quantum states in these kagome compounds. We present results from cryogenic scanning tunneling microscopy experiments on cleaved bulk crystals of CsV3Sb5. The goal of our study is to shed light on the “pseudo gap” phase that appears in the low energy local density of states of the 2x2 CDW state. To this end, we combine high-resolution spectroscopy and quasi-particle interference with scattering experiments in which we study the response of the chiral flux phase phase to atomic scale perturbations. We compare our observations with results from microscopic model calculations with the focus on the spectral features of the chiral flux phase. We gratefully acknowledge funding support by the Croucher foundation.

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