



# ***Book of abstracts***

## **International Conference on Strongly Correlated Electron Systems (SCES)**

which took place in Amsterdam,  
the Netherlands from  
24 – 29 July 2022



*Anne Visser*  
Anne Visser  
Conference chair

*A. McCollam*  
Alix McCollam  
Conference chair



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# ***Program at a glance***

**International Conference on Strongly  
Correlated Electron Systems (SCES)**

Time	Forum	Room E107-E108	Room E104-E105	Room E103	Ruby Lounge and Room E102
<b>Monday 25 July</b>					
08.30 – 08.45	Welcome and opening				
	Plenary session MonP				
	Session Chair: Annah Hallas				
08.45 – 09.30	<b>Hae Young Kee</b> (University of Toronto): <i>Kitaev Materials</i>				
09.30 – 10.15	<b>Nicola Spaldin</b> (ETH Zurich): <i>Hidden magnetoelectric multipoles</i>				
			Coffee break		
	Parallel sessions MonPA1				
	Focus session: AdS/CFT correspondence for correlated electron systems. Session Chair: Erik van Heumen	Quantum magnetism (1): Kitaev spin liquid physics. Session Chair: Kwang-Yong Choi	Strong correlations in Dirac and Weyl systems Session Chair: Frank Kruger	Multiferroics and related materials. Session Chair: Kee-Hoon Kim	
10.45 – 11.00	<b>Johanna Erdmenger</b> (University of Würzburg): <i>Turbulent hydrodynamics in strongly correlated Kagome metals</i>	<b>Natalia Perkins</b> (University of Minnesota): <i>Non-London-Fleury Raman scattering in spin-orbit coupled Mott insulators</i>	<b>Young-Woo Son</b> (Korea Institute for Advanced Study): <i>Effects of Coulomb interactions in Dirac and Weyl semimetallic two-dimensional crystals</i>	<b>Sándor Bordács</b> (Budapest University of Technology and Economics): <i>Detection and manipulation of antiferromagnetic orders via the magnetoelectric effect</i>	
11.00 – 11.15					
11.15 – 11.30	<b>Mark Golden</b> (University of Amsterdam): <i>Momentum dependent scaling exponents of cuprate strange-metal self energies: ARPES meets semi-holography</i>	<b>Fazel Tafti</b> (Boston College): <i>Tuning competing interactions in Kitaev magnets via topochemical reactions</i>	<b>Qimiao Si</b> (Rice University): <i>Weyl-Kondo semimetals and their symmetry-based design</i>	<b>Sergey Artyukhin</b> (Italian Institute of Technology): <i>Topologically protected unidirectional magnetoelectric switching in a multiferroic</i>	Plenary (45 min)
11.30 – 11.45					
11.45 – 12.00	<b>Arata Tanaka</b> (Hiroshima University): <i>Planckian metallic state in the two-dimensional Hubbard model</i>	<b>Aprem Joy</b> (University of Cologne): <i>Dynamics of Visons and Thermal Hall effect in Perturbed Kitaev Models</i>	<b>Mario Modia Piva</b> (Max Planck Institute for Chemical Physics of Solids, Dresden): <i>Pressure-tuning the magnetic noncentrosymmetric Weyl semimetals CeAlSi and CeAlGe</i>	<b>Marine Verseils</b> (Synchrotron SOLEIL): <i>Strength and temperature range enhancement of electromagnon in CuO under pressure</i>	Invited (30 min)
12.00 – 12.15	<b>Jan Zaanen</b> (Leiden University): <i>Quantum supreme matter: the strange metals according to holography</i>	<b>Etienne Lefrançois</b> (University of Sherbrooke): <i>Evidence of a Phason Hall Effect in the Kitaev Spin Liquid Candidate <math>\alpha</math>-RuCl<sub>3</sub></i>	<b>Siobhan Tobin</b> (University of Oxford): <i>Spin dynamics and topological nature of the semimetal YbMnSb<sub>2</sub></i>	<b>Sanne Kristensen</b> (High Field Magnet Laboratory, Radboud University): <i>Exploration of multiferroic quantum phase transition in TbMnO<sub>3</sub></i>	
12.15 – 12.30		<b>Kyusung Hwang</b> (Korea Institute for Advanced Study): <i>Identification of a Kitaev Quantum Spin Liquid by Magnetic Field Angle Dependence</i>	<b>Maarten van Delft</b> (Radboud University): <i>Sondheimer oscillations as a probe of non-phonic flow in WP2 crystals</i>	<b>Ryunosuke Takahashi</b> (University of Hyogo): <i>Optically-induced magnetization switching in NiCo<sub>2</sub>O<sub>4</sub> thin films</i>	Contributed (15 min)
			Lunch break		
13.30 – 13.45					Poster session MonPO1
13.45 – 14.00					Poster numbers 1 to 104
14.00 – 14.15					
14.15 – 14.30					
14.30 – 14.45					
14.45 – 15.00					
15.00 – 15.15					
			Coffee break		
	Parallel sessions MonPA2				
	Heavy Fermions (1). Session Chair: William Knafo	Quantum Magnetism (2): 2-D frustrated magnets. Session Chair: Toru Sakai	Low dimensional materials and devices with strong correlations. Session Chair: Corentin Morice		
15.45 – 16.00	<b>Jonathan Dentinger</b> (Lawrence Berkeley National Laboratory): <i>Temperature evolution of electronic structures of paradigm Ce 4f and U 5f materials</i>	<b>Quentin Barthélemy</b> (University of Paris, University of Sherbrooke): <i>Specific heat of the kagome antiferromagnet herbertsmithite in high magnetic fields</i>	<b>Chuan Li</b> (University of Twente): <i>Axion electrodynamics induced <math>e/4</math> fractional charge of a superconducting vortex</i>		
16.00 – 16.15					
16.15 – 16.30	<b>Cristian Batista</b> (Oak Ridge National Laboratory): <i>A microscopic Kondo lattice model for the heavy fermion antiferromagnet CeIn<sub>3</sub></i>	<b>Julio Larrea Jimenez</b> (University of São Paulo): <i>Exotic critical points in a pure spin system SrCu<sub>2</sub>(BO<sub>3</sub>)<sub>2</sub></i>	<b>Mucio Continentino</b> (Centro Brasileiro de Pesquisas Físicas): <i>Thermoelectric properties of topological chains coupled to a quantum dot</i>		
16.30 – 16.45			<b>Hikaru Watanabe</b> (RIKEN Center for Emergent Matter Science): <i>Magnetic photocurrent response assisted by quantum geometry in solid</i>		
16.45 – 17.00	<b>Marcin Raczkowski</b> (University of Würzburg): <i>Zooming in on heavy fermions in Kondo lattice models</i>	<b>Kamil Kolincio</b> (Gdansk University of Technology): <i>Spin chirality induced by thermal fluctuations</i>	<b>Marta Gilbert</b> (Vienna University of Technology): <i>Critical length scales at metal-insulator and magnetic oxide interfaces</i>		
17.00 – 17.15	<b>Georg Poelchen</b> (ESRF, Grenoble): <i>Surface interlayer coupling with a 2D Kondo lattice and bulk underdamped spin excitations in CeCo<sub>2</sub>P<sub>2</sub></i>	<b>Kirill Povarov</b> (ETH Zurich): <i>Directly Probing S=1/2 Chain Spinon Backscattering with Electron Spin Resonance</i>			
17.15 – 17.30	<b>Ernst Bauer</b> (Vienna University of Technology): <i>Low temperature magnetic instabilities in the ternary Kondo lattice YbPtSb<sub>2</sub></i>	<b>Michel Kenzelmann</b> (Paul Scherrer Institute): <i>Quantum fluctuations and tunable magnetic excitations in the two-dimensional honeycomb materials YbBr<sub>3</sub> and ErBr<sub>3</sub></i>	<b>Jasper van Wezel</b> (University of Amsterdam): <i>Coexisting charge-ordered states with distinct driving mechanisms in monolayer VSe<sub>2</sub></i>		
17.30 – 17.45	<b>Jeroen Custers</b> (Charles University Prague): <i>Studying the interplay of Magnetism and Superconductivity in the Heavy Fermion Compound Ce<sub>3</sub>PtIn<sub>11</sub></i>	<b>Kotaro Shimizu</b> (University of Tokyo): <i>Phase degree of freedom and topological properties in multiple-Q spin textures</i>	<b>Steffen Wirth</b> (Max-Planck Institute for Chemical Physics of Solids, Dresden): <i>Scanning tunneling microscopy and spectroscopy on rare-earth hexaborides</i>		
				Sponsored session MonSP	
				Technical Innovation	
				Session Chair: Mark Golden.	
18.00 – 18.10				Welcome and Introduction	
18.10 – 18.30				<b>Laura Folkers</b> (STCE & Cie GmbH): <i>X-ray diffraction as a useful tool to research strongly correlated electron systems</i>	
18.30 – 18.50				<b>Hannes Kuehne</b> (Helmholtz-Zentrum Dresden-Rossendorf): <i>Two-axis rotator "Rotax": Out of the lab – for the lab</i>	
18.50 – 19.10				<b>Stefan Böttcher</b> (SPECS Surface Nano Analysis GmbH): <i>New Developments in Deflector Analyzer Technology for ARPES</i>	
19.10 – 19.30				<b>Rik Groenen</b> (DEMCON TSST BV): <i>Customised system solutions for thin film research</i>	

Plenary (45 min)

Invited (30 min)

Contributed (15 min)

Posters

Sponsored invited

Time	Forum	Room E107-E108	Room E104-E105	Room E103	Ruby Lounge and Room E102
<b>Tuesday 26 July</b>					
	Plenary session TuesPL Session Chair: Priscila Rosa				
08.45 – 09.30	<b>Vidya Madhavan</b> (University of Illinois Urbana Champaign): <i>Edge states and charge density wave orders in UTe2</i>				
09.30 – 10.15	<b>Youichi Yanase</b> (Kyoto University): <i>Parity transition, parity violation, and topological superconductivity in UTe2 and CeRh2As2</i>				
	Coffee break				
	Parallel sessions TuesPA1				
	Theoretical models for strong correlations (1) Session Chair: Nicola Spaldin	Unconventional superconductivity (1). Session Chair: André Strydom	Quantum phase transitions and quantum critical points (1). Session Chair: Mucio Continentino	Non-equilibrium phenomena in strongly correlated systems (1). Session Chair: Lea Santos	
10.45 – 11.00	<b>Yukitoshi Motome</b> (University of Tokyo): <i>Kitaev spin liquid materials as a Majorana platform</i>	<b>Seunghyun Khim</b> (Max-Planck Institute for Chemical Physics of Solids): <i>Muon spin relaxation (<math>\mu</math>SR) studies on the heavy-fermion superconductor CeRh2As2</i>	<b>Matthew Cook</b> (University College London): <i>Magnetotransport of pyrochlore spin ice Sm2/2O7 across the pressure-induced quantum-critical phase boundary</i>	<b>Maria Carolina de Oliveira Aguiar</b> (Federal University of Minas Gerais): <i>Quench dynamics and relaxation of a spin coupled to interacting leads</i>	
11.00 – 11.15		<b>Lev Levitin</b> (Royal Holloway University of London): <i>Interplay of superconductivity and magnetism in YbRh2Si2</i>			
11.15 – 11.30	<b>Roser Valenti</b> (University of Frankfurt): <i>Topological phases in kagome-based materials</i>	<b>Dai Aoki</b> (Tohoku University): <i>Electronic states and superconductivity in UTe2</i>	<b>Kee-Hoon Kim</b> (Seoul National University): <i>Pressure-induced quantum critical point of strong coupling charge density wave order in a 2H-Pd0.05TaSe2 superconductor</i>	<b>Jingwen Li</b> (ETH Zurich): <i>Light-induced magnetization dynamics in a ferromagnetic semiconductor</i>	
11.30 – 11.45			<b>Cornelius Krellner</b> (Goethe University Frankfurt/Main): <i>Isotopically pure YbRh2Si2 single crystals with 171Yb, 173Yb, and 174Yb</i>	<b>Satoshi Ejima</b> (University of Greifswald): <i>Photoinduced phase transitions in one-dimensional Mott insulators</i>	
11.45 – 12.00	<b>Ryota Ono</b> (Italian Institute of Technology): <i>Computing exchange anisotropy in a half-filled eg system from Wannier tight-binding model</i>	<b>Jean-Pascal Brison</b> (Univ. Grenoble Alpes, CEA, IRIG-Phelias): <i>Field-induced superconducting phases in UTe2</i>	<b>Devashibhai Adroja</b> (Rutherford Appleton Laboratory): <i>Quantum Critical Spin-Liquid in Geometrically Frustrated Kagome Lattice Investigated by Muon Spin Relaxation and Neutron Scattering</i>	<b>Houda Koussir</b> (University of Lille): <i>Volatile and non-volatile insulator-to-metal transition in narrow gap Mott insulator GaMn4S8</i>	
12.00 – 12.15	<b>Purevdorj Munkhbaatar</b> (Jeonbuk National University): <i>Theory of infrared absorption and Raman spectroscopy for orbital wave</i>	<b>Atsushi Miyake</b> (University of Tokyo): <i>First-order metamagnetic transition in UTe2 studied by magnetoresistance measurements</i>	<b>Stephen Julian</b> (University of Toronto): <i>Peering past spin density wave order at quantum criticality in SrRu2O7</i>	<b>Kacper Wrzesniewski</b> (Adam Mickiewicz University): <i>Dynamical quantum phase transition in a mesoscopic superconducting system</i>	
12.15 – 12.30	<b>Ryota Iwazaki</b> (Saitama University): <i>Spin-orbital dynamics of localized electrons</i>	<b>Kenji Ishida</b> (Kyoto University): <i>Spin-susceptibility behavior in Uranium-based Superconductor UTe2 investigated with Knight-shift measurements</i>	<b>Natalia Chepur</b> (Delft University of Technology): <i>From SU(2)<sub>5</sub> to SU(2)<sub>3</sub> Wess-Zumino-Witten transitions in a frustrated spin-3/2 chain</i>	<b>Chia-Jung Yang</b> (ETH Zurich): <i>Critical slowing down of fermionic quasiparticles in YbRh2Si2 by terahertz time-domain spectroscopy</i>	
	Lunch break				
13.30 – 13.45					Poster session TuesPO2
13.45 – 14.00					Poster numbers 105 to 202
14.00 – 14.15					
14.15 – 14.30					
14.30 – 14.45					
14.45 – 15.00					
15.00 – 15.15					
	Coffee break				
	Parallel sessions TuesPA2				
	MITs in strongly correlated systems. Session Chair: Matthe Grosche	Focus Session: UTe2. Session Chair: Kenji Ishida	Unconventional superconductivity (2). Session Chair: Sven Badoux		
15.45 – 16.00	<b>Kazushi Kanoda</b> (University of Tokyo): <i>Pressure-induced BEC-BCS crossover in a doped spin liquid candidate</i>	<b>Priscila Rosa</b> (Los Alamos National Laboratory): <i>Single thermodynamic transition at 2 K in superconducting UTe2 single crystals</i>	<b>Jake Ayres</b> (University of Bristol): <i>Incoherent Transport and the Evolution of Power-Law Scaling of the Magnetoresistance in Cuprate Superconductors</i>		
16.00 – 16.15					
16.15 – 16.30	<b>Martin Dressel</b> (Universität Stuttgart): <i>Electrodynamics at the Mott transition: the disappearance of Landau's quasiparticles</i>	<b>Katsuki Kinjo</b> (Kyoto University): <i>NMR study of magnetic and superconducting properties on UTe2 under pressure</i>	<b>Catherine Pepin</b> (IphT, CEA-Paris-Saclay): <i>Charge orders and strange metal in cuprate superconductors</i>		
16.30 – 16.45	<b>Claude Ederer</b> (ETH Zurich): <i>Charge disproportionation and "Hund's insulating" behavior in different transition metal oxides by DFT+DMFT</i>	<b>Georg Knebel</b> (CEA Grenoble): <i>High pressure properties of UTe2</i>			
16.45 – 17.00	<b>Tanusri Saha-Dasgupta</b> (S. N. Bose National Centre): <i>Nickelates: A Tale of Two Stories</i>	<b>Stéphane Raymond</b> (CEA-Grenoble): <i>Magnetic excitation spectrum of the unconventional superconductor UTe2</i>	<b>Dalia Bounoua</b> (Université Paris-Saclay, CNRS-CEA): <i>Hidden magnetic texture in the pseudogap phase of high-Tc YBaCuO3:6.6</i>		
17.00 – 17.15			<b>José Lorenzana</b> (Istituto dei Sistemi Complessi, CNR): <i>Mimicking cuprates with silver and fluorine</i>		
17.15 – 17.30	<b>Henrik Jacobsen</b> (University of Copenhagen): <i>Magnetically induced metal-insulator transition in Pb2CaOsO6</i>	<b>Shanta Saha</b> (University of Maryland): <i>Recent development in the spin-triplet superconductor UTe2</i>	<b>Haoyu Hu</b> (Rice University): <i>Unconventional and high-Tc superconductivity from Fermi surface fluctuations in strongly correlated metals</i>		
17.30 – 17.45	<b>Liu Hao Tjeng</b> (Max Planck Institute for Chemical Physics of Solids): <i>Orbital imaging of the spin state transition in LaCoO3</i>	<b>Riku Yamamoto</b> (Los Alamos National Laboratory): <i>NMR studies of local magnetism in UTe2 under pressure</i>	<b>Caitlin Duffy</b> (High Field Magnet Laboratory, Redboud University): <i>Current pulses, critical currents, and cuprates: a novel means of exploring the ground state</i>		

Plenary (45 min)

Invited (30 min)

Contributed (15 min)

Posters

Time	Forum	Room E107-E108	Room E104-E105	Room E103	Ruby Lounge and Room E102
<p><b>Wednesday 27 July</b></p> <p>Plenary session WedPL Session Chair: Qimiao Si</p>					
08:45 – 09:00	SCES 2022 Prize Ceremony Chair: Hisatomo Harima				
09:00 – 09:30	Bernard Coqblin prize winner. <b>Pascoal Pagliuso</b> (IFGW-Unicamp): <i>Electron Spin Resonance in SCES materials and the SCES 2020/21 conference: Two hard tasks in my career</i>				
09:30 – 10:15	<b>Ja-Geun Park</b> (Seoul National University): <i>New materials platform for two-dimensional magnetism and strong correlation studies: van der Waals magnets</i>				
Coffee break					
Parallel sessions WedPA1					
Materials design and advanced Materials. Session Chair: Tanusri Saha-Dasgupta		Quantum phase transitions and quantum critical points (2). Session Chair: Sven Friedemann	Low dimensional materials with strong correlations. Session Chair: Jasper van Wezel	Strong correlations in actinides. Session Chair: Jeroen Custers	
10:45 – 11:00	Bryan R. Coles prize winner. <b>Alannah Hallas</b> (University of British Columbia): <i>Entropy engineering and tunable magnetic order in the spinel high entropy oxide</i>	<b>Sooheon Shin</b> (Paul Scherrer Institute): <i>Field-induced quantum critical behavior in topological antiferromagnet CePtAlGe<sub>2</sub></i>	<b>Siddarth Saxena</b> (University of Cambridge): <i>Emergent Magnetic and Electronic Phases in Pressure-Tuned van der Waals Antiferromagnets</i>	<b>Marie-aude Measson</b> (Institut Néel, Grenoble): <i>Kondo anisotropy in URu<sub>2</sub>Si<sub>2</sub></i>	
11:00 – 11:15		<b>Bryan Vissar</b> (Technical University of Vienna): <i>Pressure tuned quantum phase transition in Fe(Ga<sub>1-x</sub>Gex)<sub>3</sub></i>			
11:15 – 11:30	<b>Silke Buehler-Paschen</b> (Technical University of Vienna): <i>Weyl-Kondo semimetals: Ce<sub>3</sub>Bi<sub>4</sub>Pd<sub>3</sub> and beyond</i>	<b>Andreas Wendl</b> (Technical University of Munich): <i>Mesoscale Quantum Phase Transitions in LiHoF<sub>4</sub></i>	<b>Rüdiger Klingeler</b> (Heidelberg University): <i>Uniaxial pressure effects, magnon excitations and the emerging anisotropic nature of short-range order in CrI<sub>3</sub></i>	<b>Peter Riseborough</b> (Temple University): <i>Orbitally Selective Enhanced Spin-Orbit Coupling in Itinerant Actinides</i>	Plenary (45 min)
11:30 – 11:45		<b>Shiyu Deng</b> (University of Cambridge): <i>Dynamics of the critical phonon modes in quantum paraelectric SrTiO<sub>3</sub></i>	<b>Björn Salzmann</b> (University of Fribourg): <i>Spontaneous and strain induced metallic phase due to modified interlayer stacking in 1T-TaS<sub>2</sub></i>	<b>Edwin Herrera Vasco</b> (Universidad Autónoma de Madrid): <i>Quantum-well states at the surface of the heavy fermion URu<sub>2</sub>Si<sub>2</sub></i>	
11:45 – 12:00	<b>Sarah Krebber</b> (Goethe University, Frankfurt): <i>Search for new europium-based intermetallic 122 materials with non-trivial topological properties</i>	<b>Rebecca Flint</b> (Iowa State University): <i>Two channel Kondo physics in one dimension, algebraic hysteric order and remnants of quantum criticality</i>	<b>Jian Liu</b> (University of Tennessee): <i>Emergent phenomena in structurally engineered square-lattice iridates</i>	<b>Hisatomo Harima</b> (Kobe University): <i>Hidden-orders of uranium compounds</i>	Invited (30 min)
12:00 – 12:15	<b>Matthew Cook</b> (Los Alamos National Laboratory): <i>Single crystal optimization and electrical transport in antiferromagnetic semiconductor EuIn<sub>2</sub>Si<sub>6</sub></i>			<b>Andres Marino</b> (Max Planck Institute for Chemical Physics of Solids): <i>Crystal-field ground state wave function of UGa<sub>2</sub> probed with Resonant &amp; Non-resonant Inelastic X-ray Scattering</i>	
12:15 – 12:30	<b>Samikshya Sahu</b> (University of British Columbia): <i>Chemical tuning effects on the extreme magnetoresistance of Dirac nodal arc semimetals</i>	<b>Saheli Sarkar</b> (Karlsruhe Institute of Technology): <i>Quantum criticality on a compressible lattice</i>	<b>Rebecca Cervasio</b> (Paris-Saclay University, Synchrotron SOLEIL): <i>Optical Properties of Superconducting Nd<sub>0.85</sub>Sr<sub>0.15</sub>O<sub>2</sub>Nickelate</i>	<b>David Hovancik</b> (Charles University Prague): <i>Alloying-driven transition between ferromagnetism and antiferromagnetism in UTcE compounds: UCo<sub>1-x</sub>Ir<sub>x</sub>Ge</i>	Contributed (15 min)
Lunch break					
Parallel sessions WedPA2					
Unconventional superconductivity (3). Session Chair: Hermann Suderow		Focus session: Orbital Kondo effect. Session Chair: Marie-aude Measson	Non-equilibrium phenomena in strongly correlated systems (2). Session Chair: Maria Carolina de Oliveira Aguiar		
13:45 – 14:00	Nevill F. Mott prize winner. <b>Aline Ramires</b> (Paul Scherrer Institute): <i>Unconventional properties of unconventional superconductors: the concept of superconducting fitness</i>	<b>Yong-Baek Kim</b> (University of Toronto): <i>Non-Fermi liquids and quantum criticality in multipolar Kondo Systems</i>	<b>Lea Santos</b> (Yeshiva University): <i>Equilibration time in many-body quantum systems</i>		
14:00 – 14:15					
14:15 – 14:30	<b>Yuan Cao</b> (Harvard University): <i>Superconductivity in Magic-angle Graphene Family</i>	<b>Andriy Nevidomskyy</b> (Rice University): <i>Quadrupolar Kondo Effect and Generalized Doniach Phase Diagram for Non-Kramers Ions: Praseodymium Heavy Fermion Materials</i>	<b>Dirk Manske</b> (Max Planck Institute for Solid State Research, Stuttgart): <i>Higgs spectroscopy of superconductors</i>		
14:30 – 14:45		<b>Takahiro Onimaru</b> (Hiroshima University): <i>Two-channel Kondo problem in non-Kramers doublet systems</i>	<b>Hector Pablo Ojeda Collado</b> (Sapienza University of Rome): <i>Emergent dynamical phases in periodically driven BCS systems</i>		
14:45 – 15:00	<b>Anushree Datta</b> (Instituto de Ciencia de Materiales de Madrid): <i>Accuracy of moiré Wannier function models for twist bilayer graphene</i>		<b>Kristin Klemm</b> (Goethe University Frankfurt): <i>Exchange scaling of ultrafast angular momentum transfer in 4f antiferromagnets</i>		
15:00 – 15:15	<b>Koen Bastiaans</b> (Delft University of Technology): <i>Direct evidence for Cooper pairing without a spectral gap in a disordered superconductor above T<sub>c</sub></i>	<b>Philipp Gegenwart</b> (University of Augsburg): <i>Symmetrized quadrupolar expansivity as sensitive probe of the quadrupolar Kondo effect: diluted Pr<sub>1-x</sub>R<sub>2x</sub>N<sub>2</sub>O</i>	<b>Girish Settur</b> (Indian Institute of Technology, Guwahati): <i>Non-chiral bosonization of strongly inhomogeneous Luttinger liquids driven out of equilibrium</i>		
Coffee break					
Parallel sessions WedPA3					
Theoretical models for strong correlations (2). Session Chair: Philippe Corboz		CEF effects and multipolar ordering in SCES. Session Chair: Stephen Julian	Quantum Magnetism (3): Emergent magnetic quasiparticles. Session Chair: Katia Pappas		
15:45 – 16:00	<b>Olivier Parcollet</b> (Flatiron Institute, Université Paris-Saclay): <i>Planckian Metal at a Doping-Induced Quantum Critical Point</i>	<b>Tatsuya Yanagisawa</b> (Hokkaido University): <i>Electric Quadrupolar Response in the Magnetic Phases of UNi<sub>4</sub>B</i>	<b>Hyeonsik Cheong</b> (Sogang University): <i>Optical Spectroscopy of 2-Dimensional van der Waals Antiferromagnets</i>		
16:00 – 16:15					
16:15 – 16:30	<b>Vikram Tripathi</b> (TIFR Mumbai): <i>Quasiparticle metamorphosis in a doped random J-J model: a many-body localization perspective</i>	<b>Femke Bangma</b> (High Field Magnet Laboratory, Radboud University): <i>Hyperfine interactions and antiferroquadrupolar order: their role in PrOs<sub>4</sub>Sb<sub>12</sub></i>	<b>Haijing Zhang</b> (Max Planck Institute for Chemical Physics of Solids): <i>Observation of the Rashba-driven anomalous Hall effect in an antiferromagnetic metal</i>		
16:30 – 16:45			<b>Johanna Jochum</b> (Technical University of Munich): <i>Large topological Hall effect from fluctuating Skyrmion textures</i>		
16:45 – 17:00	<b>Piotr Wrzosek</b> (University of Warsaw): <i>The fate of the spin polaron in the 1D J-J model</i>	<b>Dmytro Inosov</b> (Technical University of Dresden): <i>Field-space anisotropy of magnetic phases and excitations in cubic Ce<sup>3+</sup> compounds</i>	<b>Paul Goddard</b> (University of Warwick): <i>Scattering from magnetic monopoles and antiferromagnetic domain manipulation in a frustrated pyrochlore iridate</i>		
17:00 – 17:15	<b>Blaise Goutéraux</b> (Ecole Polytechnique): <i>Charge transport in pinned, gapless charge density waves</i>	<b>Yosuke Arai</b> (University of Tokyo): <i>Multipole polaron in the devil's staircase of CeSb</i>			
17:15 – 17:30	<b>Callin Walsh</b> (Royal Holloway University of London): <i>Information-theoretic measures of superconductivity in a two-dimensional doped Mott insulator</i>	<b>Leonid Pourousski</b> (CNRS, Ecole Polytechnique): <i>Hidden order, magnetic excitations and multipolar exchange striction in neptunium dioxide</i>	<b>Flavien Museur</b> (Université Grenoble Alpes - Institut Néel): <i>New fragmented state in pyrochlore ruthenate Ho<sub>2</sub>Ru<sub>2</sub>O<sub>7</sub></i>		
17:30 – 17:45	<b>Boris Ponsioen</b> (University of Amsterdam): <i>Automatic differentiation applied to the excitations with projected entangled-pair states</i>	<b>Sophie de Brion</b> (Institut Néel, Grenoble): <i>From spin ices to quadrupolar ices: the enigmatic case of the magnetic pyrochlore Tb<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub></i>	<b>Evgenii Barts</b> (University of Groningen): <i>Magnetic particles and strings in iron langasites</i>		
18:00 – 22:00	Canal cruise and conference dinner				

Time	Forum	Room E107-E108	Room E104-E105	Room E103	Ruby Lounge and Room E102
<b>Thursday 28 July</b>					
	Plenary session ThuPL Session Chair: Roger Valentí				
08.45 – 09.30	<b>Amalia Coldea</b> (University of Oxford): <i>Electronic, superconducting and quantum critical signatures of iron-chalcogenides tuned by chemical and hydrostatic pressures</i>				
09.30 – 10.15	<b>Harold Hwang</b> (Stanford University): <i>Superconductivity in infinite-layer nickelates</i>				
	Parallel sessions ThuPA1				
	Unconventional superconductivity (4). Session Chair: Antony Carrington	Fermi surfaces and electronic structure (1). Session Chair: Ilya Sheikin	Non-Fermi liquids and novel metallic phases. Session Chair: Catherine Pepin	Correlated topological phases (1). Session Chair: Sarah Grefe	
10.45 – 11.00 11.00 – 11.15	<b>Audrey Grockowiak</b> (Centro Nacional de Pesquisa em Energia e Materiais): <i>Hot Hydride Superconductivity above 550 K</i>	<b>Bin Shen</b> (University of Augsburg): <i>Fermi surface of heavy fermion ferromagnet CeRhGe4</i>	<b>Andrew Huxley</b> (University of Edinburgh): <i>Extended Non-Fermi-Liquid Phases</i>	<b>John Saunders</b> (Royal Holloway University of London): <i>Topological superfluid <math>^3\text{He}</math> under mesoscopic confinement: from quasi-2D chiral superfluid to pair density wave.</i>	
11.15 – 11.30	<b>Victor Baldent</b> (Paris Saclay University): <i>Pressure phase diagram of unidimensional iron based superconductor BaFeSe3</i>	<b>Jiazhong Chen</b> (University of Cambridge): <i>Fermi surface and mass renormalization in the iron-based superconductor YFe2Ge2</i>	<b>Frank Kruger</b> (University College London): <i>Field control of fluctuation-driven modulated magnetism in the metallic ferromagnet PtPtAl</i>	<b>Jean Carlo Souza</b> (University of Campinas): <i>Surface states evolution in half-Heusler systems Y(Pd,Pt)Bi</i>	
11.30 – 11.45	<b>Konstantin Semeniuk</b> (Max Planck Institute for Chemical Physics of Solids, Dresden): <i>Pressure tuning of the low-temperature states of CeRh2As2</i>		<b>Gaël Grissonanche</b> (Cornell University): <i>T-linear resistivity from an isotropic Planckian scattering rate</i>	<b>Gloria Platero</b> (Materials Science Institute of Madrid): <i>Simulation of chiral topological phases in driven quantum dot arrays</i>	
11.45 – 12.00	<b>Sven Badoux</b> (Radboud University): <i>Interplay between CDW and superconductivity of underdoped YBa2Cu3O7-x</i>	<b>Roos Leenen</b> (High Field Magnet Laboratory, Radboud University): <i>The Fermi surface of the ferromagnetic superconductor UCoGe under external magnetic fields.</i>			
12.00 – 12.15	<b>Kristine Krighaar</b> (University of Copenhagen): <i>Evolution of magnetic stripes under uniaxial stress in La1.885Ba0.115CuO4 studied by neutron scattering</i>	<b>William Broad</b> (University of Bristol): <i>Quantum oscillations in heavy-fermion ferromagnet YbNi4P2 over many Zeeman induced Lifshitz transitions</i>	<b>Indrani Paul</b> (Université Paris Cité): <i>Pseudogap Induced Electronic Anisotropy in Underdoped Cuprates</i>	<b>Hiroki Tsuchiura</b> (Tohoku University): <i>Josephson effects between the Kitaev ladder superconductors</i>	
12.15 – 12.30	<b>Suguru Nakata</b> (University of Hyogo): <i>Normal-state charge transport of YBa2Cu3O6.67 under uniaxial stress</i>	<b>Gertrud Zwicknagl</b> (Technical University of Braunschweig): <i>Heavy quasiparticles in CeRh2As2: Renormalized bands, Fermi surfaces, and electronic instabilities</i>	<b>Yannick Klein</b> (Sorbonne University): <i>Fermi to non-Fermi liquid crossover in intercalated VVS2 with the NIAAS-defect structure</i>	<b>Paula Mellado</b> (Universidad Adolfo Ibáñez): <i>Intrinsic topological magnons in arrays of magnetic dipoles</i>	
			Lunch break		
13.30 – 13.45 13.45 – 14.00 14.00 – 14.15 14.15 – 14.30 14.30 – 14.45 14.45 – 15.00 15.00 – 15.15					Poster session ThuPO3 Poster numbers 203 to 309
	Parallel sessions ThuPA2				
	Focus session: Novel phases in Fe-based systems. Session Chair: Santiago Grigera	Kondo effect and valence fluctuations. Session Chair: Gertrud Zwicknagl	Unconventional Superconductivity (5). Session Chair: Kim Lefmann		
15.45 – 16.00 16.00 – 16.15	<b>Pascal Reiss</b> (Max Planck Institute for Solid State Research, Stuttgart): <i>Unconventional Transport Properties in the High-Pressure Phase of FeSe<sub>0.89</sub>S<sub>0.11</sub></i>	<b>Andrea Severing</b> (University of Cologne): <i>RIXS characterization of the giant crystal field in CeRh3B2</i>	<b>Eduardo Marino</b> (Federal University of Rio de Janeiro): <i>A Testable Theory for High-Tc Superconductivity in Cuprates</i>		
16.15 – 16.30	<b>Johanna Palmstrom</b> (Los Alamos National Laboratory): <i>Investigating a putative nematic quantum critical point using high magnetic field elastoresistivity measurements</i>	<b>Nikola Maksimovic</b> (UC Berkeley): <i>Evidence for a delocalization transition without symmetry breaking in CeCoIn5</i>	<b>Clò Ethimía Agrapidis</b> (University of Warsaw): <i>Unravelling the Nature of Spin Excitations Disentangled from Charge Contributions in a Doped Cuprate Superconductor</i>		
16.30 – 16.45			<b>Hannes Kuehne</b> (Hochfeld-Magnetlabor Dresden, Helmholtz-Zentrum Dresden-Rossendorf): <i>Order-parameter evolution in the Fulde-Ferrell-Larkin-Ovchinnikov phase probed by <math>^{13}\text{C}</math> NMR spectroscopy</i>		
16.45 – 17.00	<b>Heiko Pfau</b> (Penn State University): <i>Quasiparticle coherence in the nematic state of iron-based superconductors</i>	<b>David Tam</b> (Paul Scherrer Institute): <i>Study of multi-f electron Kondo effect and magnetic ordering in SmCoIn5</i>	<b>Puhua Wan</b> (University of Groningen): <i>Orbital FFLO State in a Layer-Coupled Ising Superconductor</i>		
17.00 – 17.15		<b>Monika Güttler</b> (Technical University of Dresden): <i>Visualization of the Kondo lattice crossover with temperature in YbRh2Si2 with high-resolution Compton scattering</i>	<b>Javier Landaeza</b> (Max Planck Institute for Chemical Physics of Solids, Dresden): <i>Field-angle dependence reveals odd-parity superconductivity in CeRh2As2</i>		
17.15 – 17.30	<b>Mads Fonager Hansen</b> (Université Grenoble-Alpes, Institut Néel): <i>LaFeSiO1-δ: a novel superconducting member of the Fe silicide family</i>	<b>Atsushi Hariki</b> (Osaka Prefecture University): <i>CaCu3Ru4O12: A High Kondo-Temperature Transition Metal Oxide</i>	<b>Maria Teresa Mercaldo</b> (Università di Salerno): <i>Orbital effects in spin-singlet superconductors: p-pairing, Edelstein effect, and orbital vortex phase</i>		
17.30 – 17.45	<b>Jose P. Rodriguez</b> (California State University at Los Angeles): <i>Quantum Monte Carlo Simulations of Iron-Selenide Superconductors with No Sign Problem</i>	<b>Tamaghna Hazra</b> (Ruigens University): <i>Triplet pairing mechanisms from Hund's-Kondo models: applications to heavy fermion superconductors</i>	<b>Akito Daido</b> (Kyoto University): <i>Theory of intrinsic superconducting diode effect</i>		

Plenary (45 min)

Invited (30 min)

Contributed (15 min)

Posters



Time	Forum	Room E107-E108	Room E104-E105	Room E103	Ruby Lounge and Room E102
Friday 29 July					
	Plenary session FriPL Session Chair: Silvio Buehler-Paschen				
08.45 – 09.30	<b>Cristiane de Moraes Smith</b> (Utrecht University); <i>Topological properties at fractal dimensions</i>				
09.30 – 10.15	<b>Peter Lijerth</b> (Aalto university); <i>Designer quantum states in van der Waals heterostructures</i>				
	Coffee break				
	Parallel sessions FHPA1				
	Heavy fermions (2). Session Chair: Ernst Bauer	Fermi surfaces and electronic structure (2). Session Chair: Andreas Rost	Correlated topological phases (2). Session Chair: Maarten van Delft	Novel techniques for SCES investigations. Session Chair: Doohee Cho	
10.45 – 11.00	<b>Jonathan Denlinger</b> (Lawrence Berkeley National Laboratory); <i>Anisotropic c-f hybridization in CeRhGe4 and CeCu2S2</i>	<b>Antony Carrington</b> (University of Bristol); <i>Hall effect in overdoped cuprates and its link to Fermi surface reconstruction</i>	<b>Debmalya Chakraborty</b> (Uppsala University); <i>Disorder-robust phase crystal in high-temperature superconductors from topology and strong correlations</i>	<b>Petr Čermák</b> (Charles University Prague); <i>ALSA – Automatic Laue Sample Aligner</i>	
11.00 – 11.15			<b>Marein Rahn</b> (Technical University of Dresden); <i>Topology, colossal magnetoresistance, and complex magnetic domains in Eu5In2Sb6</i>		
11.15 – 11.30	<b>Oliver Squire</b> (University of Cambridge); <i>Quantum critical point in the high-pressure structure of CeSb2</i>	<b>Roemer Hinlopen</b> (University of Bristol); <i>Cascade of Fermi surface reconstructions linked to superconductivity inside the CDW phase of TlSe2</i>	<b>Sarah Greife</b> (Los Alamos National Laboratory); <i>The Weyl-Kondo semimetal: high-harmonic generation and extreme topological tunability</i>	<b>Santiago Grigera</b> (Universidad Nacional de La Plata); <i>Integrating Machine Learning with Neutron Scattering</i>	
11.30 – 11.45	<b>Jan Knapp</b> (Royal Holloway University of London); <i>Electro-nuclear transition in YbRh2S2; evidence for a spin density wave</i>	<b>Andrew Hunter</b> (University of Geneva); <i>Laser ARPES measurements of Sr2RuO4 under uniaxial strain</i>			
11.45 – 12.00	<b>Manuel Brando</b> (Max Planck Institute for Chemical Physics of Solids, Dresden); <i>The multi-phase heavy-fermion superconductor CeRh2As2</i>	<b>Mario Cuoco</b> (CNR-SPIN Salerno); <i>Orbital loop current phase at the surface of Sr2RuO4</i>	<b>Diana Kirschbaum</b> (Vienna University of Technology); <i>Physical properties of Ce3Bi4X3 beyond the X = Pt, Pd case: First study of Ce3Bi4Ni3</i>	<b>Isabel Guillamon</b> (Universidad Autónoma de Madrid); <i>STM at magnetic fields of 20 T: quasiparticle interference and vortex lattices of pnictide superconductors</i>	
12.00 – 12.15		<b>Wingyu Kang</b> (Massachusetts Institute of Technology); <i>Twofold van Hove singularity and origin of charge order in topological Kagome superconductors CsV3Sb5</i>	<b>Diego Zocco</b> (Vienna University of Technology); <i>Effects of hydrostatic pressure on the Weyl-Kondo semimetal candidate CeRu4Sb6</i>		
12.15 – 12.30	<b>Kosuke Nogaki</b> (Kyoto University); <i>Novel parity transition in strongly correlated superconductor: relation to CeRh2As2</i>	<b>Andre Dayenling</b> (Technical University Munich); <i>Electronic structure of CeTAI3 (T=Ag, Au, Cu, Pd, Pt) studied with density functional theory</i>	<b>Elena Gati</b> (Max-Planck-Institute for Chemical Physics of Solids, Dresden); <i>Pressure-induced ferromagnetism in the topological semimetal EuCu2As2</i>	<b>Maximilian Peily</b> (University of St Andrews); <i>Quantum oscillations and magnetostriction in Sr3Ru2O7 studied by a novel capacitive dilatometer</i>	
	Lunch break				
	Conference highlights. Session Chair: Alik McCollam				
13.30 – 13.45	<b>Rebecca Flint</b> (Iowa State University) Theory highlights.				
13.45 – 14.00	<b>Stephen Julian</b> (University of Toronto) Experiment highlights.				
14.00 – 14.15	Closing and announcements.				
14.15 – 14.30	<b>Anne de Visser</b>				

Plenary (45 min)

Invited (30 min)

Contributed (15 min)



# ***ORAL Program***

**International Conference on Strongly  
Correlated Electron Systems (SCES)**



## Monday 25 July

<b>FORUM</b> <b>08:30 - 08.45</b>	<b>Welcome and opening</b> Chair: Anne de Visser
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<b>FORUM</b> <b>08:45 - 10.15</b>	<b>Plenary session</b> Chair: Alannah Hallas
MonPL:01 - 08:45 <i>Plenary</i>	<b>Hae-Young Kee</b> <i>University of Toronto</i> Kitaev Materials
MonPL:02 - 09:30 <i>Plenary</i>	<b>Nicola Spaldin</b> <i>ETH Zurich</i> Hidden magnetoelectric multipoles

### COFFEE BREAK

<b>FORUM</b> <b>10.45 - 12.30</b>	<b>Focus session: AdS/CFT correspondence for correlated electron systems</b> Chair: Erik van Heumen
MonPA1:1.01 - 10:45 <i>Invited</i>	<b>Johanna Erdmegner</b> <i>University of Würzburg</i> Turbulent hydrodynamics in strongly correlated Kagome metals
MonPA1:1.02 - 11:15 <i>Invited</i>	<b>Mark Golden</b> <i>University of Amsterdam</i> Momentum dependent scaling exponents of cuprate strange-metal self energies: ARPES meets semi-holography
MonPA1:1.03 - 11:45 <i>Contributed</i>	<b>Arata Tanaka</b> <i>Hiroshima University</i> Planckian metallic state in the two-dimensional Hubbard model
MonPA1:1.04 - 12:00 <i>Invited</i>	<b>Jan Zaanen</b> <i>Leiden University</i> Quantum supreme matter: the strange metals according to holography.

<b>ROOM: E107-108</b>	<b>Parallel session: Quantum magnetism (1): Kitaev spin liquid physics</b>
<b>10.45 - 12.30</b>	Chair: Kwang-Yong Choi
MonPA1:2.01 - 10:45	<b>Natalia Perkins</b> <i>Invited</i> University of Minnesota Non-Loudon-Fleury Raman scattering in spin-orbit coupled Mott insulators
MonPA1:2.02 - 11:15	<b>Fazel Tafti</b> <i>Invited</i> Boston College Tuning competing interactions in Kitaev magnets via topochemical reactions
MonPA1:2.03 - 11:45	<b>Aprem Joy</b> <i>Contributed</i> University of Cologne Dynamics of Visons and Thermal Hall effect in Perturbed Kitaev Models
MonPA1:2.04 - 12:00	<b>Etienne Lefrancois</b> <i>Contributed</i> University of Sherbrooke Evidence of a Phonon Hall Effect in the Kitaev Spin Liquid Candidate $\alpha$ -RuCl <sub>3</sub>
MonPA1:2.05 - 12:15	<b>Kyusung Hwang</b> <i>Contributed</i> Korea Institute for Advanced Study Identification of a Kitaev Quantum Spin Liquid by Magnetic Field Angle Dependence

<b>ROOM: E104-105</b>	<b>Parallel session: Strong correlations in Dirac and Weyl systems</b>
<b>10.45 - 12.30</b>	Chair: Frank Kruger
MonPA1:3.01 - 10.45	<b>Young-Woo Son</b> <i>Invited</i> Korea Institute for Advanced Study Effects of Coulomb interactions in Dirac and Weyl semimetallic two-dimensional crystals
MonPA1:3.02 - 11.15	<b>Qimiao Si</b> <i>Invited</i> Rice University Weyl-Kondo semimetals and their symmetry-based design
MonPA1:3.03 - 11.45	<b>Mario Moda Piva</b> <i>Contributed</i> Max Planck Institute for Chemical Physics of Solids, Dresden Pressure-tuning the magnetic noncentrosymmetric Weyl semimetals CeAlSi and CeAlGe
MonPA1:3.04 - 12.00	<b>Siobhan Tobin</b> <i>Contributed</i> University of Oxford Spin dynamics and topological nature of the semimetal YbMnSb <sub>2</sub>
MonPA1:3.05 - 12.15	<b>Maarten van Delft</b> <i>Contributed</i> Radboud University Sondheimer oscillations as a probe of non-ohmic flow in WP <sub>2</sub> crystals

<b>ROOM: E103</b>	<b>Parallel session: Multiferroics and related materials</b>
<b>10.45 - 12.30</b>	Chair: Kee Hoon Kim
MonPA1:4.01 - 10.45	<b>Sándor Bordács</b> <i>Invited</i> <i>Budapest University of Technology and Economics</i> Detection and manipulation of antiferromagnetic orders via the magnetoelectric effect
MonPA1:4.02 - 11.15	<b>Sergey Artyukhin</b> <i>Invited</i> <i>Italian Institute of Technology</i> Topologically protected unidirectional magnetoelectric switching in a multiferroic
MonPA1:4.03 - 11.45	<b>Marine Verseils</b> <i>Contributed</i> <i>Synchrotron SOLEIL</i> Strength and temperature range enhancement of electromagnon in CuO under pressure
MonPA1:4.04 - 12.00	<b>Sanne Kristensen</b> <i>Contributed</i> <i>High Field Magnet Laboratory, Radboud University</i> Exploration of multiferroic quantum phase transition in TbMnO <sub>3</sub>
MonPA1:4.05 - 12.15	<b>Ryunosuke Takahashi</b> <i>Contributed</i> <i>University of Hyogo, Graduate school of material science</i> Optically-induced magnetization switching in NiCo <sub>2</sub> O <sub>4</sub> thin films

<b>12.30 - 13.30</b>	<b>LUNCH BREAK</b>
<b>13.30 - 15.15</b>	<b>POSTER SESSION</b>
<b>15.15 - 15.45</b>	<b>COFFEE BREAK</b>

<b>FORUM</b>	<b>Parallel session: Heavy Fermions (1)</b>
<b>15.45 - 17.45</b>	Chair: William Knafo
MonPA2:1.01 - 15.45	<b>Jonathan Denlinger</b> <i>Invited</i> <i>Lawrence Berkeley National Laboratory</i> Temperature evolution of electronic structures of paradigm Ce 4f and U 5f materials
MonPA2:1.02 - 16.15	<b>Cristian Batista</b> <i>Invited</i> <i>Oak Ridge National Laboratory</i> A microscopic Kondo lattice model for the heavy fermion antiferromagnet CeIn <sub>3</sub>
MonPA2:1.03 - 16.45	<b>Marcin Raczowski</b> <i>Contributed</i> <i>University of Würzburg</i> Zooming in on heavy fermions in Kondo lattice models
MonPA2:1.04 - 17.00	<b>Georg Poelchen</b> <i>Contributed</i> <i>ESRF, Grenoble</i> Surface interlayer coupling with a 2D Kondo lattice and bulk underdamped spin excitations in CeCo <sub>2</sub> P <sub>2</sub>
MonPA2:1.05 - 17.15	<b>Ernst Bauer</b> <i>Contributed</i> <i>Vienna University of Technology</i> Low temperature magnetic instabilities in the ternary Kondo lattice YbPt <sub>5</sub> B <sub>2</sub>
MonPA2:1.06 - 17.30	<b>Jeroen Custers</b> <i>Contributed</i> <i>Charles University Prague</i> Studying the Interplay of Magnetism and Superconductivity in the Heavy Fermion Compound Ce <sub>3</sub> PtIn <sub>11</sub>

<b>ROOM: E107-108</b>		<b>Parallel session: Quantum Magnetism (2): 2-D frustrated magnets</b>	
<b>15.45 - 17.45</b>		Chair: Toru Sakai	
MonPA2:2.01 - 15.45	<b>Quentin Barthélemy</b>	<i>Invited</i>	<i>University of Paris, University of Sherbrooke</i> Specific heat of the kagome antiferromagnet herbertsmithite in high magnetic fields
MonPA2:2.02 - 16.15	<b>Julio Larrea Jimenez</b>	<i>Invited</i>	<i>University of São Paulo</i> Exotic critical points in a pure spin system SrCu <sub>2</sub> (BO <sub>3</sub> ) <sub>2</sub>
MonPA2:2.03 - 16.45	<b>Kamil Kolincio</b>	<i>Contributed</i>	<i>Gdansk University of Technology</i> Spin chirality induced by thermal fluctuations
MonPA2:2.04 - 17.00	<b>Kirill Povarov</b>	<i>Contributed</i>	<i>ETH Zurich</i> Directly Probing S=1/2 Chain Spinon Backscattering with Electron Spin Resonance
MonPA2:2.05 - 17.15	<b>Michel Kenzelmann</b>	<i>Contributed</i>	<i>Paul Scherrer Institute</i> Quantum fluctuations and tunable magnetic excitations in the two-dimensional honeycomb materials YbBr <sub>3</sub> and ErBr <sub>3</sub>
MonPA2:2.06 - 17.30	<b>Kotaro Shimizu</b>	<i>Contributed</i>	<i>The University of Tokyo</i> Phase degree of freedom and topological properties in multiple-Q spin textures

<b>ROOM: E104-105</b>		<b>Parallel session: Low dimensional materials and devices with strong correlations</b>	
<b>15.45 - 17.45</b>		Chair: Corentin Morice	
MonPA2:3.01 - 15.45	<b>Chuan Li</b>	<i>Invited</i>	<i>University of Twente</i> Axion electrodynamics induced e/4 fractional charge of a superconducting vortex spectroscopy
MonPA2:3.02 - 16.15	<b>Mucio Amado Continentino</b>	<i>Contributed</i>	<i>Centro Brasileiro de Pesquisas Fisicas</i> Thermoelectric properties of topological chains coupled to a quantum dot
MonPA2:3.03 - 16.30	<b>Hikaru Watanabe</b>	<i>Contributed</i>	<i>RIKEN Center for Emergent Matter Science</i> Magnetic photocurrent response assisted by quantum geometry in solid
MonPA2:3.04 - 16.45	<b>Marta Gibert</b>	<i>Invited</i>	<i>Vienna University of Technology</i> Critical length scales at metal-insulator and magnetic oxide interfaces
MonPA2:3.05 - 17.15	<b>Jasper van Wezel</b>	<i>Contributed</i>	<i>University of Amsterdam</i> Coexisting charge-ordered states with distinct driving mechanisms in monolayer VSe <sub>2</sub>
MonPA2:3.06 - 17.30	<b>Steffen Wirth</b>	<i>Contributed</i>	<i>Max-Planck Institute for Chemical Physics of Solids Dresden</i> Scanning tunneling microscopy and spectroscopy on rare-earth hexaborides

<b>E103</b>		<b>Sponsored session: Technical Innovation</b>	
<b>18:00 - 19:30</b>		Chair: Mark Golden	
MonSP:00 - 18:00		Welcome and Introduction	
MonSP:01 - 18:10	<b>Laura Folkers</b>		
<i>Invited</i>	<i>STOE &amp; Cie GmbH</i>	X-ray diffraction as a useful tool to research strongly correlated electron systems	
MonSP:02 - 18:30	<b>Hannes Kuehne</b>		
<i>Invited</i>	<i>Helmholtz-Zentrum Dresden-Rossendorf</i>	Two-axis rotator "Rotax": Out of the lab - for the lab	
MonSP:03 - 18:50	<b>Stefan Böttcher</b>		
<i>Invited</i>	<i>SPECS Surface Nano Analysis GmbH</i>	New Developments in Deflector Analyzer Technology for ARPES	
MonSP:04 - 19:10	<b>Rik Groenen</b>		
<i>Invited</i>	<i>DEMCON TSST BV</i>	Customised system solutions for thin film research	

## Tuesday 26 July

<b>FORUM</b>	<b>Plenary session</b>
<b>08:45 - 10.15</b>	Chair: Priscila Rosa
<b>TuesPL:01 - 08.45</b>	<b>Vidya Madhavan</b>
<i>Plenary</i>	<i>University of Illinois Urbana Champaign</i> Edge states and Charge density wave orders in UTe2
<b>TuesPL:02 - 09.30</b>	<b>Youichi Yanase</b>
<i>Plenary</i>	<i>Kyoto University</i> Parity transition, parity violation, and topological superconductivity in UTe2 and CeRh2As2

### COFFEE BREAK

<b>FORUM</b>	<b>Parallel session: Theoretical models for strong correlations (1)</b>
<b>10.45 - 12.30</b>	Chair: Nicola Spaldin
<b>TuesPA1:1.01 - 10.45</b>	<b>Yukitoshi Motome</b>
<i>Invited</i>	<i>University of Tokyo</i> Kitaev spin liquid materials as a Majorana platform
<b>TuesPA1:1.02 - 11.15</b>	<b>Roser Valenti</b>
<i>Invited</i>	<i>University of Frankfurt</i> Topological phases in kagome-based materials
<b>TuesPA1:1.03 - 11.45</b>	<b>Ryota Ono</b>
<i>Contributed</i>	<i>Italian Institute of Technology</i> Computing exchange anisotropy in a half-filled eg system from Wannier tight-binding model
<b>TuesPA1:1.04 - 12.00</b>	<b>Purevdorj Munkhbaatar</b>
<i>Contributed</i>	<i>Jeonbuk National University</i> Theory of infrared absorption and Raman spectroscopy for orbital wave
<b>TuesPA1:1.05 - 12.15</b>	<b>Ryuta Iwazaki</b>
<i>Contributed</i>	<i>Saitama University</i> Spin-orbital dynamics of localized electrons

<b>ROOM: E107-108</b>	<b>Parallel session: Unconventional superconductivity (1)</b>
<b>10.45 - 12.30</b>	Chair: André Strydom
<b>TuesPA1:2.01 - 10.45</b>	<b>Seunghyun Khim</b>
<i>Contributed</i>	<i>Max-Planck Institute for Chemical Physics of Solids</i> Muon spin relaxation ( $\mu$ SR) studies on the heavy-fermion superconductor CeRh2As2
<b>TuesPA1:2.02 - 11.00</b>	<b>Lev Levitin</b>
<i>Contributed</i>	<i>Royal Holloway University of London</i> Interplay of superconductivity and magnetism in YbRh2Si2
<b>TuesPA1:2.03 - 11.15</b>	<b>Dai Aoki</b>
<i>Invited</i>	<i>Tohoku University</i> Electronic states and superconductivity in UTe2
<b>TuesPA1:2.04 - 11.45</b>	<b>Jean-Pascal Brison</b>
<i>Contributed</i>	<i>Univ. Grenoble Alpes, CEA, IRIG-Pheligs</i> Field-induced superconducting phases in UTe2



<b>TuesPA1:2.05 - 12.00</b>	<b>Atsushi Miyake</b>
<i>Contributed</i>	<i>University of Tokyo</i>
	First-order metamagnetic transition in UTe <sub>2</sub> studied by magnetostriction measurements
<b>TuesPA1:2.06 - 12.15</b>	<b>Kenji Ishida</b>
<i>Contributed</i>	<i>Kyoto University</i>
	Spin-susceptibility behavior in Uranium-based Superconductor UTe <sub>2</sub> investigated with Knight-shift measurements

<b>ROOM: E104-105</b>	<b>Parallel session: Quantum phase transitions and quantum critical points (1)</b>
<b>10.45 - 12.30</b>	Chair: Mucio Continentino

<b>TuesPA1:3.01 - 10.45</b>	<b>Matthew Coak</b>
<i>Invited</i>	<i>London Centre for Nanotechnology, University College London</i>
	Magnetotransport of pyrochlore spin ice Sm <sub>2</sub> Ir <sub>2</sub> O <sub>7</sub> across the pressure-induced quantum-critical phase boundary
<b>TuesPA1:3.02 - 11.15</b>	<b>Kee Hoon Kim</b>
<i>Contributed</i>	<i>Seoul National University</i>
	Pressure-induced quantum critical point of a strong coupling charge density wave order in a 2H-Pd <sub>0.05</sub> TaSe <sub>2</sub> superconductor
<b>TuesPA1:3.03 - 11.30</b>	<b>Cornelius Krellner</b>
<i>Contributed</i>	<i>Goethe University Frankfurt/Main</i>
	Isotopically pure YbRh <sub>2</sub> Si <sub>2</sub> single crystals with <sup>171</sup> Yb, <sup>173</sup> Yb and <sup>174</sup> Yb
<b>TuesPA1:3.04 - 11.45</b>	<b>Devashibhai Adroja</b>
<i>Contributed</i>	<i>Rutherford Appleton Laboratory</i>
	Quantum Critical Spin-Liquid in Geometrically Frustrated Kagome Lattice Investigated by Muon Spin Relaxation and Neutron Scattering
<b>TuesPA1:3.05 - 12.00</b>	<b>Stephen Julian</b>
<i>Contributed</i>	<i>University of Toronto</i>
	Peering past spin density wave order at quantum criticality in Sr <sub>3</sub> Ru <sub>2</sub> O <sub>7</sub>
<b>TuesPA1:3.06 - 12.15</b>	<b>Natalia Chepiga</b>
<i>Contributed</i>	<i>Delft University of Technology</i>
	From SU(2) <sub>5</sub> to SU(2) <sub>3</sub> Wess-Zumino-Witten transitions in a frustrated spin-5/2 chain

<b>ROOM: E103</b>	<b>Parallel session: Non-equilibrium phenomena in strongly correlated systems (1)</b>
<b>10.45 - 12.30</b>	Chair: Lea Santos

<b>TuesPA1:4.01 - 10.45</b>	<b>Maria Carolina de Oliveira Aguiar</b>
<i>Invited</i>	<i>Federal University of Minas Gerais</i>
	Quench dynamics and relaxation of a spin coupled to interacting leads
<b>TuesPA1:4.02 - 11.15</b>	<b>Jingwen Li</b>
<i>Contributed</i>	<i>ETH Zurich</i>
	Light-induced magnetization dynamics in a ferromagnetic semiconductor
<b>TuesPA1:4.03 - 11.30</b>	<b>Satoshi Ejima</b>
<i>Contributed</i>	<i>University of Greifswald</i>
	Photoinduced phase transitions in one-dimensional Mott insulators

<b>TuesPA1:4.04 - 11.45</b>	<b>Houda Koussir</b> <i>Contributed</i> University of Lille Volatile and non-volatile insulator-to-metal transition in narrow gap Mott insulator GaMo4S8
<b>TuesPA1:4.05 - 12.00</b>	<b>Kacper Wrześniewski</b> <i>Contributed</i> Adam Mickiewicz University Dynamical quantum phase transition in a mesoscopic superconducting system
<b>TuesPA1:4.06 - 12.15</b>	<b>Chia-Jung Yang</b> <i>Contributed</i> ETH Zurich Critical slowing down of fermionic quasiparticles in YbRh2Si2 by terahertz time-domain spectroscopy

<b>12.30 - 13.30</b>	<b>LUNCH BREAK</b>
<b>13.30 - 15.15</b>	<b>POSTER SESSION</b>
<b>15.15 - 15.45</b>	<b>COFFEE BREAK</b>

<b>FORUM</b>	<b>Parallel session: Metal-Insulator transitions in strongly correlated systems</b>
<b>15.45 - 17.45</b>	Chair: Malte Grosche
<b>TuesPA2:1.01 - 15.45</b>	<b>Kazushi Kanoda</b> <i>Invited</i> University of Tokyo Pressure-induced BEC-BCS crossover in a doped spin liquid candidate
<b>TuesPA2:1.02 - 16.15</b>	<b>Martin Dressel</b> <i>Contributed</i> Universität Stuttgart Electrodynamics at the Mott transition: the disappearance of Landau's quasiparticles
<b>TuesPA2:1.03 - 16.30</b>	<b>Claude Ederer</b> <i>Contributed</i> ETH Zurich Charge disproportionation and "Hund's insulating" behavior in different transition metal oxides by DFT+DMFT
<b>TuesPA2:1.04 - 16.45</b>	<b>Tanusri Saha-Dasgupta</b> <i>Invited</i> S. N. Bose National Centre Nickelates: A Tale of Two Stories
<b>TuesPA2:1.05 - 17.15</b>	<b>Henrik Jacobsen</b> <i>Contributed</i> University of Copenhagen Magnetically induced metal-insulator transition in Pb2CaOsO6
<b>TuesPA2:1.06 - 17.30</b>	<b>Liu Hao Tjeng</b> <i>Contributed</i> Max Planck Institute for Chemical Physics of Solids Orbital imaging of the spin state transition in LaCoO3

<b>ROOM: E107-108 Focus Session: UTe<sub>2</sub></b>	
<b>15.45 - 17.45</b> Chair: Kenji Ishida	
TuesPA2:2.01 - 15.45	<b>Priscila Rosa</b> <i>Invited</i> Los Alamos National Laboratory Single thermodynamic transition at 2 K in superconducting UTe <sub>2</sub> single crystals
TuesPA2:2.02 - 16.15	<b>Katsuki Kinjo</b> <i>Contributed</i> Kyoto University NMR study of magnetic and superconducting properties on UTe <sub>2</sub> under pressure
TuesPA2:2.03 - 16.30	<b>Georg Knebel</b> <i>Contributed</i> CEA Grenoble High pressure properties of UTe <sub>2</sub>
TuesPA2:2.04 - 16.45	<b>Stéphane Raymond</b> <i>Invited</i> CEA-Grenoble Magnetic excitation spectrum of the unconventional superconductor UTe <sub>2</sub>
TuesPA2:2.05 - 17.15	<b>Shanta Saha</b> <i>Contributed</i> University of Maryland Recent development in the spin-triplet superconductor UTe <sub>2</sub>
TuesPA2:2.06 - 17.30	<b>Riku Yamamoto</b> <i>Contributed</i> Los Alamos National Laboratory NMR studies of local magnetism in UTe <sub>2</sub> under pressure

<b>ROOM: E104-105 Parallel session: Unconventional superconductivity (2)</b>	
<b>15.45 - 17.45</b> Chair: Sven Badoux	
TuesPA2:2.01 - 15.45	<b>Jake Ayres</b> <i>Invited</i> University of Bristol Incoherent Transport and the Evolution of Power-Law Scaling of the Magnetoresistance in Cuprate Superconductors
TuesPA2:2.02 - 16.15	<b>Catherine Pepin</b> <i>Invited</i> IphT, CEA- Paris-Saclay Charge orders and strange metal in cuprate superconductors
TuesPA2:2.03 - 16.45	<b>Dalila Bounoua</b> <i>Contributed</i> Université Paris-Saclay, CNRS-CEA Hidden magnetic texture in the pseudogap phase of high-T <sub>c</sub> YBa <sub>2</sub> Cu <sub>3</sub> O <sub>6.6</sub>
TuesPA2:2.04 - 17.00	<b>José Lorenzana</b> <i>Contributed</i> Istituto dei Sistemi Complessi, CNR Mimicking cuprates with silver and fluorine
TuesPA2:2.05 - 17.15	<b>Haoyu Hu</b> <i>Contributed</i> Rice University Unconventional and high-T <sub>c</sub> superconductivity from Fermi surface fluctuations in strongly correlated metals
TuesPA2:2.06 - 17.30	<b>Caitlin Duffy</b> <i>Contributed</i> High Field Magnet Laboratory, Radboud University Current pulses, critical currents, and cuprates: a novel means of exploring the ground state

## Wednesday 27 July

<b>FORUM</b> <b>08:45 - 09:00</b>	<b>SCES 2022 Prize Ceremony</b> Chair: Hisatomo Harima
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<b>FORUM</b> <b>09:00 - 10:15</b>	<b>Plenary session</b> Chair: Qimiao Si
WedPL:01 - 09.00 <i>Prize winner</i>	<b>Bernard Coqblin Prize winner: Pascoal Pagliuso</b> <i>IFGW-Unicamp</i> Electron Spin Resonance in SCES materials and the SCES 2020/21 conference: Two hard tasks in my career
WedPL:02 - 09.30 <i>Plenary</i>	<b>Je-Geun Park</b> <i>Seoul National University</i> New materials platform for two-dimensional magnetism and strong correlation studies: van der Waals magnets

### COFFEE BREAK

<b>FORUM</b> <b>10:45 - 12:30</b>	<b>Parallel session: Materials design and advanced Materials</b> Chair: Tanusri Saha-Dasgupta
WedPA1:1.01 - 10.45 <i>Prize winner</i>	<b>Bryan R. Coles prize winner: Alannah Hallas</b> <i>University of British Columbia</i> Entropy engineering and tunable magnetic order in the spinel high entropy oxide
WedPA1:1.02 - 11.15 <i>Invited</i>	<b>Silke Buehler-Paschen</b> <i>Technical University of Vienna</i> Weyl-Kondo semimetals: Ce <sub>3</sub> Bi <sub>4</sub> Pd <sub>3</sub> and beyond
WedPA1:1.03 - 11.45 <i>Contributed</i>	<b>Sarah Krebber</b> <i>Goethe University, Frankfurt</i> Search for new europium-based intermetallic 122 materials with non-trivial topological properties
WedPA1:1.04 - 12.00 <i>Contributed</i>	<b>Matthew Cook</b> <i>Los Alamos National Laboratory</i> Single crystal optimization and electrical transport in antiferromagnetic semiconductor Eu <sub>5</sub> In <sub>2</sub> Sb <sub>6</sub>
WedPA1:1.05 - 12.15 <i>Contributed</i>	<b>Samikshya Sahu</b> <i>University of British Columbia</i> Chemical tuning effects on the extreme magnetoresistance of Dirac nodal arc semimetals

<b>ROOM: E107-108</b>		<b>Parallel session: Quantum phase transitions and quantum critical points (2)</b>	
<b>10.45 - 12.30</b>		Chair: Sven Friedemann	
WedPA1:2.01 - 10.45	<b>Sooheon Shin</b>	<i>Contributed</i>	<i>Paul Scherrer Institute</i> Field-induced quantum critical behavior in topological antiferromagnet CePtAl <sub>4</sub> Ge <sub>2</sub>
WedPA1:2.02 - 11.00	<b>Bryan Vlaar</b>	<i>Contributed</i>	<i>Technical University of Vienna</i> Pressure tuned quantum phase transition in Fe(Ga <sub>1-x</sub> Gex) <sub>3</sub>
WedPA1:2.03 - 11.15	<b>Andreas Wendl</b>	<i>Contributed</i>	<i>Technical University of Munich</i> Mesoscale Quantum Phase Transitions in LiHoF <sub>4</sub>
WedPA1:2.04 - 11.30	<b>Shiyu Deng</b>	<i>Contributed</i>	<i>University of Cambridge</i> Dynamics of the critical phonon modes in quantum paraelectric SrTiO <sub>3</sub>
WedPA1:2.05 - 11.45	<b>Rebecca Flint</b>	<i>Invited</i>	<i>Iowa State University</i> Two channel Kondo physics in one dimension: algebraic hastatic order and remnants of quantum criticality
WedPA1:2.06 - 12.15	<b>Saheli Sarkar</b>	<i>Contributed</i>	<i>Karlsruhe Institute of Technology</i> Quantum criticality on a compressible lattice

<b>ROOM: E104-105</b>		<b>Parallel session: Low dimensional materials with strong correlations</b>	
<b>10.45 - 12.30</b>		Chair: Jasper van Wezel	
WedPA1:3:01 - 10.45	<b>Siddarth Saxena</b>	<i>Invited</i>	<i>University of Cambridge</i> Emergent Magnetic and Electronic Phases in Pressure-Tuned van der Waals Antiferromagnets
WedPA1:3:02 - 11.15	<b>Rüdiger Klingeler</b>	<i>Contributed</i>	<i>Heidelberg University</i> Uniaxial pressure effects, magnon excitations and the emerging anisotropic nature of short-range order in CrI <sub>3</sub>
WedPA1:3:03 - 11.30	<b>Björn Salzmänn</b>	<i>Contributed</i>	<i>University of Fribourg</i> Spontaneous and strain induced metallic phase due to modified interlayer stacking in 1T-TaS <sub>2</sub>
WedPA1:3:04 - 11.45	<b>Jian Liu</b>	<i>Invited</i>	<i>University of Tennessee</i> Emergent phenomena in structurally engineered square-lattice iridates
WedPA1:3:05 - 12.15	<b>Rebecca Cervasio</b>	<i>Contributed</i>	<i>Paris-Saclay University, Synchrotron SOLEIL</i> Optical Properties of Superconducting Nd <sub>0.8</sub> Sr <sub>0.2</sub> NiO <sub>2</sub> Nickellate

<b>ROOM: E103</b>	<b>Parallel session: Strong correlations in actinides</b>
<b>10.45 - 12.30</b>	Chair: Jeroen Custers
WedPA1:4:01 - 10.45	<b>Marie-aude Measson</b> <i>Invited</i> Institut Néel, Grenoble Kondo anisotropy in URu2Si2
WedPA1:4:02 - 11.15	<b>Peter Riseborough</b> <i>Contributed</i> Temple University Orbitally Selective Enhanced Spin-Orbit Coupling in Itinerant Actinides
WedPA1:4:03 - 11.30	<b>Edwin Herrera Vasco</b> <i>Contributed</i> Universidad Autónoma de Madrid Quantum-well states at the surface of the heavy fermion URu2Si2.
WedPA1:4:04 - 11.45	<b>Hisatomo Harima</b> <i>Contributed</i> Kobe University Hidden-orders of uranium compounds
WedPA1:4:05 - 12.00	<b>Andrea Marino</b> <i>Contributed</i> Max Planck Institute for Chemical Physics of Solids Crystal-field ground state wave function of UGa2 probed with Resonant & Non-resonant Inelastic X-ray Scattering
WedPA1:4:06 - 12.15	<b>Dávid Hovančík</b> <i>Contributed</i> Charles University Prague Alloying-driven transition between ferromagnetism and antiferromagnetism in UTGe compounds: UCo1-xIrxGe

**12.30 - 13.30 LUNCH BREAK**

<b>FORUM</b>	<b>Parallel session: Unconventional superconductivity (3)</b>
<b>13.45 - 15.15</b>	Chair: Hermann Suderow
WedPA2:1.01 - 13.45	<b>Nevill F. Mott prize winner: Aline Ramires</b> <i>Prize winner</i> Paul Scherrer Institute Unconventional properties of unconventional superconductors: the concept of superconducting fitness
WedPA2:1.02 - 14.15	<b>Yuan Cao</b> <i>Invited</i> Harvard University Superconductivity in Magic-angle Graphene Family
WedPA2:1.03 - 14.45	<b>Anushree Datta</b> <i>Contributed</i> Instituto de Ciencia de Materiales de Madrid Accuracy of moiré Wannier function models for twist bilayer graphene
WedPA2:1.04 - 15.00	<b>Koen Bastiaans</b> <i>Contributed</i> Delft University of Technology Direct evidence for Cooper pairing without a spectral gap in a disordered superconductor above Tc

<b>ROOM: E107-108</b>		<b>Focus session: Orbital Kondo effect</b>	
<b>13.45 - 15.15</b>		Chair: Marie-aude Measson	
WedPA2:2.01 - 13.45	<b>Yong-Baek Kim</b>	<i>Invited</i>	<i>University of Toronto</i> Non-Fermi liquids and quantum criticality in multipolar Kondo Systems
WedPA2:2.02 - 14.15	<b>Andriy Nevidomskyy</b>	<i>Contributed</i>	<i>Rice University</i> Quadrupolar Kondo Effect and Generalized Doniach Phase Diagram for Non-Kramers Ions: Praseodymium Heavy Fermion Materials
WedPA2:2.03 - 14.30	<b>Takahiro Onimaru</b>	<i>Invited</i>	<i>Hiroshima University</i> Two-channel Kondo problem in non-Kramers doublet systems
WedPA2:2.04 - 15.00	<b>Philipp Gegenwart</b>	<i>Contributed</i>	<i>University of Augsburg</i> Symmetrized quadrupolar expansivity as sensitive probe of the quadrupolar Kondo effect: diluted PrIr <sub>2</sub> Zn <sub>20</sub>

<b>ROOM: E104-105</b>		<b>Non-equilibrium phenomena in strongly correlated systems (2)</b>	
<b>13.45 - 15.15</b>		Chair: Maria Carolina de Oliveira Aguiar	
WedPA2:3.01 - 13.45	<b>Lea Santos</b>	<i>Invited</i>	<i>Yeshiva University</i> Equilibration time in many-body quantum systems
WedPA2:3.02 - 14.15	<b>Dirk Manske</b>	<i>Contributed</i>	<i>Max Planck Institute for Solid State Research, Stuttgart</i> Higgs spectroscopy of superconductors
WedPA2:3.03 - 14.30	<b>Hector Pablo Ojeda Collado</b>	<i>Contributed</i>	<i>Sapienza University of Rome</i> Emergent dynamical phases in periodically driven BCS systems
WedPA2:3.04 - 14.45	<b>Kristin Kliemt</b>	<i>Contributed</i>	<i>Goethe University Frankfurt</i> Exchange scaling of ultrafast angular momentum transfer in 4f antiferromagnets
WedPA2:3.05 - 15.00	<b>Girish Setlur</b>	<i>Contributed</i>	<i>Indian Institute of Technology, Guwahati</i> Non-chiral bosonization of strongly inhomogenous Luttinger liquids driven out of equilibrium

15.15 - 15.45

COFFEE BREAK

<b>FORUM</b>	<b>Parallel sessions: Theoretical models for strong correlations (2)</b>
<b>15.45 - 17.45</b>	Chair: Philippe Corboz
WedPA3:1.01 - 15.45	<b>Olivier Parcollet</b> <i>Invited</i> Flatiron Institute, Université Paris-Saclay Planckian Metal at a Doping-Induced Quantum Critical Point
WedPA3:1.02 - 16.15	<b>Vikram Tripathi</b> <i>Invited</i> TIFR Mumbai Quasiparticle metamorphosis in a doped random t-J model: a many-body localization perspective
WedPA3:1.03 - 16.45	<b>Piotr Wrzosek</b> <i>Contributed</i> University of Warsaw The fate of the spin polaron in the 1D t-J model
WedPA3:1.04 - 17.00	<b>Blaise Goutéraux</b> <i>Contributed</i> Ecole Polytechnique Charge transport in pinned, gapless charge density waves
WedPA3:1.05 - 17.15	<b>Caitlin Walsh</b> <i>Contributed</i> Royal Holloway University of London Information-theoretic measures of superconductivity in a two-dimensional doped Mott insulator
WedPA3:1.06 - 17.30	<b>Boris Ponsioen</b> <i>Contributed</i> University of Amsterdam Automatic differentiation applied to excitations with projected entangled-pair states

<b>ROOM: E107-108</b>	<b>Parallel session: CEF effects and multipolar ordering in SCES</b>
<b>15.45 - 17.45</b>	Chair: Stephen Julian
WedPA3:2:01 - 15.45	<b>Tatsuya Yanagisawa</b> <i>Invited</i> Hokkaido University Electric Quadrupolar Response in the Magnetic Phases of UNi4B
WedPA3:2:02 - 16.15	<b>Femke Bangma</b> <i>Invited</i> High Field Magnet Laboratory, Radboud University Hyperfine interactions and antiferroquadrupolar order: their role in PrOs4Sb12
WedPA3:2:03 - 16.45	<b>Dmytro Inosov</b> <i>Contributed</i> Technical University of Dresden Field-space anisotropy of magnetic phases and excitations in cubic Ce <sup>3+</sup> compounds
WedPA3:2:04 - 17.00	<b>Yosuke Arai</b> <i>Contributed</i> University of Tokyo Multipole polaron in the devil's staircase of CeSb
WedPA3:2:05 - 17.15	<b>Leonid Pourovskii</b> <i>Contributed</i> CNRS, Ecole Polytechnique Hidden order, magnetic excitations and multipolar exchange striction in neptunium dioxide
WedPA3:2:06 - 17.30	<b>Sophie de Brion</b> <i>Contributed</i> Institut Néel, Grenoble From spin ices to quadrupolar ices: the enigmatic case of the magnetic pyrochlore Tb <sub>2</sub> Ti <sub>2</sub> O <sub>7</sub>



**ROOM: E104-105** **Parallel session: Quantum Magnetism (3): Emergent magnetic quasiparticles**

**15.45 - 17.45** Chair: Katia Pappas

WedPA3:3.01 - 15.45 **Hyeonsik Cheong**

*Invited*

*Sogang University*

Optical Spectroscopy of 2-Dimensional van der Waals Antiferromagnets

WedPA3:3.02 - 16.15 **Haijing Zhang**

*Contributed*

*Max Planck Institute for Chemical Physics of Solids*

Observation of the Rashba-driven anomalous Hall effect in an antiferromagnetic metal

WedPA3:3.03 - 16.30 **Johanna Jochum**

*Contributed*

*Technical University of Munich*

Large topological Hall effect from fluctuating Skyrmion textures

WedPA3:3.04 - 16.45 **Paul Goddard**

*Invited*

*University of Warwick*

Scattering from magnetic monopoles and antiferromagnetic domain manipulation in a frustrated pyrochlore iridate

WedPA3:3.05 - 17.15 **Flavien Museur**

*Contributed*

*Université Grenoble Alpes - Institut Néel*

New fragmented state in pyrochlore ruthenate  $\text{Ho}_2\text{Ru}_2\text{O}_7$

WedPA3:3.06 - 17.30 **Evgenii Barts**

*Contributed*

*University of Groningen*

Magnetic particles and strings in iron langasites

**18.00 - 22.00**

**CANAL CRUISE AND CONFERENCE DINNER**

## Thursday 28 July

<b>FORUM</b>	<b>Plenary session</b>
<b>08:45 - 10.15</b>	Chair: Roser Valenti
<b>ThuPL:01 - 08.45</b> <i>Plenary</i>	<b>Amalia Coldea</b> <i>University of Oxford</i> Electronic, superconducting and quantum critical signatures of iron-chalcogenides tuned by chemical and hydrostatic pressures
<b>ThuPL:02 - 09.30</b> <i>Plenary</i>	<b>Harold Hwang</b> <i>Stanford University</i> Superconductivity in infinite-layer nickelates

### COFFEE BREAK

<b>FORUM</b>	<b>Parallel session: Unconventional superconductivity (4)</b>
<b>10.45 - 12.30</b>	Chair: Antony Carrington
<b>ThuPA1:1.01 - 10.45</b> <i>Invited</i>	<b>Audrey Grockowiak</b> <i>Centro Nacional de Pesquisa em Energia e Materiais</i> Hot Hydride Superconductivity above 550 K
<b>ThuPA1:1.02 - 11.15</b> <i>Contributed</i>	<b>Victor Balédent</b> <i>Paris Saclay University</i> Pressure phase diagram of unidimensional iron based superconductor BaFeSe3
<b>ThuPA1:1.03 - 11.30</b> <i>Contributed</i>	<b>Konstantin Semeniuk</b> <i>Max Planck Institute for Chemical Physics of Solids, Dresden</i> Pressure tuning of the low-temperature states of CeRh2As2
<b>ThuPA1:1.04 - 11.45</b> <i>Contributed</i>	<b>Sven Badoux</b> <i>Radboud University</i> Interplay between CDW and superconductivity of underdoped YBa2Cu3O7-x
<b>ThuPA1:1.05 - 12.00</b> <i>Contributed</i>	<b>Kristine Krighaar</b> <i>University of Copenhagen</i> University of Evolution of magnetic stripes under uniaxial stress in La1.885Ba0.11CuO4 studied by neutron scattering
<b>ThuPA1:1.06 - 12.15</b> <i>Contributed</i>	<b>Suguru Nakata</b> <i>University of Hyogo</i> Normal-state charge transport of YBa2Cu3O6.67 under uniaxial stress

<b>ROOM: E107-108</b>	<b>Parallel session: Fermi surfaces and electronic structure (1)</b>
<b>10.45 - 12.30</b>	Chair: Ilya Sheikin
<b>ThuPA1:2.01 - 10.45</b> <i>Invited</i>	<b>Bin Shen</b> <i>Augsburg University</i> Fermi surface of heavy fermion ferromagnet CeRh6Ge4
<b>ThuPA1:2.02 - 11.15</b> <i>Invited</i>	<b>Jiasheng Chen</b> <i>University of Cambridge</i> Fermi surface and mass renormalization in the iron-based superconductor YFe2Ge2

<b>ThuPA1:2.03 - 11.45</b>	<b>Roos Leenen</b> <i>Contributed</i>	<i>High Field Magnet Laboratory, Radboud University</i> The Fermi surface of the ferromagnetic superconductor UCoGe under external magnetic fields.
<b>ThuPA1:2.04 - 12.00</b>	<b>William Broad</b> <i>Contributed</i>	<i>University of Bristol</i> Quantum oscillations in heavy-fermion ferromagnet YbNi <sub>4</sub> P <sub>2</sub> over many Zeeman induced Lifshitz transitions
<b>ThuPA1:2.05 - 12.15</b>	<b>Gertrud Zwicknagl</b> <i>Contributed</i>	<i>Technical University of Braunschweig</i> Heavy quasiparticles in CeRh <sub>2</sub> As <sub>2</sub> : Renormalized bands, Fermi surfaces, and electronic instabilities

<b>ROOM: E104-105</b>	<b>Parallel session: Non-Fermi liquids and novel metallic phases</b>	
<b>10.45 - 12.30</b>	Chair: Catherine Pepin	
<b>ThuPA1:3:01 - 10.45</b>	<b>Andrew Huxley</b> <i>Invited</i>	<i>University of Edinburgh</i> Extended Non-Fermi-Liquid Phases
<b>ThuPA1:3:02 - 11.15</b>	<b>Frank Kruger</b> <i>Contributed</i>	<i>University College London</i> Field control of fluctuation-driven modulated magnetism in the metallic ferromagnet PrPtAl
<b>ThuPA1:3:03 - 11.30</b>	<b>Gaël Grissonanche</b> <i>Invited</i>	<i>Cornell University</i> T-linear resistivity from an isotropic Planckian scattering rate
<b>ThuPA1:3:04 - 12.00</b>	<b>Indranil Paul</b> <i>Contributed</i>	<i>Université Paris Cité</i> Pseudogap Induced Electronic Anisotropy in Underdoped Cuprates
<b>ThuPA1:3:05 - 12.15</b>	<b>Yannick Klein</b> <i>Contributed</i>	<i>Sorbonne University</i> Fermi to non-Fermi liquid crossover in intercalated VxVS <sub>2</sub> with the NiAs-defect structure

<b>ROOM: E103</b>	<b>Parallel session: Correlated topological phases (1)</b>	
<b>10.45 - 12.30</b>	Chair: Sarah Grefe	
<b>ThuPA1:4.01 - 10.45</b>	<b>John Saunders</b> <i>Invited</i>	<i>Royal Holloway University of London</i> Topological superfluid <sup>3</sup> He under mesoscopic confinement: from quasi-2D chiral superfluid to pair density wave.
<b>ThuPA1:4.02 - 11.15</b>	<b>Jean Carlo Souza</b> <i>Contributed</i>	<i>University of Campinas</i> Surface states evolution in half-Heusler systems Y(Pd,Pt)Bi
<b>ThuPA1:4.03 - 11.30</b>	<b>Gloria Platero</b> <i>Invited</i>	<i>Materials Science Institute of Madrid</i> Simulation of chiral topological phases in driven quantum dot arrays

ThuPA1:4.04 - 12.00	<b>Hiroki Tsuchiura</b> <i>Contributed</i> Tohoku University Josephson effects between the Kitaev ladder superconductors
ThuPA1:4.05 - 12.15	<b>Paula Mellado</b> <i>Contributed</i> Universidad Adolfo Ibáñez Intrinsic topological magnons in arrays of magnetic dipoles

12.30 - 13.30	LUNCH BREAK
13.30 - 15.15	POSTER SESSION
15.15 - 15.45	COFFEE BREAK

<b>FORUM</b>	<b>Focus session: Novel phases in Fe-based systems</b>
<b>15.45 - 17.45</b>	Chair: Santiago Grigera
ThuPA2:1.01 - 15.45	<b>Pascal Reiss</b> <i>Invited</i> Max Planck Institute for Solid State Research, Stuttgart Unconventional transport properties in the high-pressure phase of FeSe <sub>0.89</sub> S <sub>0.11</sub>
ThuPA2:1.02 - 16.15	<b>Johanna Palmstrom</b> <i>Invited</i> Los Alamos National Laboratory Investigating a putative nematic quantum critical point using high magnetic field elastoresistivity measurements
ThuPA2:1.03 - 16.45	<b>Heike Pfau</b> <i>Invited</i> Penn State University Quasiparticle coherence in the nematic state of iron-based superconductors
ThuPA2:1.04 - 17.15	<b>Mads Fonager Hansen</b> <i>Contributed</i> Université Grenoble-Alpes, Institut Néel LaFeSiO1-δ: a novel superconducting member of the Fe silicide family
ThuPA2:1.05 - 17.30	<b>Jose P. Rodriguez</b> <i>Contributed</i> California State University at Los Angeles Quantum Monte Carlo Simulations of Iron-Selenide Superconductors with No Sign Problem

<b>ROOM: E107-108</b>	<b>Parallel session: Kondo effect and valence fluctuations</b>
<b>15.45 - 17.45</b>	Chair: Gertrud Zwicknagl
ThuPA2:2.01 - 15.45	<b>Andrea Severing</b> <i>Invited</i> University of Cologne RIXS characterization of the giant crystal field in CeRh3B2
ThuPA2:2.02 - 16.15	<b>Nikola Maksimovic</b> <i>Invited</i> UC Berkeley Evidence for a delocalization transition without symmetry breaking in CeCoIn5
ThuPA2:2.03 - 16.45	<b>David Tam</b> <i>Contributed</i> Paul Scherrer Institute Study of multi-f electron Kondo effect and magnetic ordering in SmCoIn5
ThuPA2:2.04 - 17.00	<b>Monika Güttler</b> <i>Contributed</i> Technical University of Dresden Visualization of the Kondo lattice crossover with temperature in YbRh2Si2 with high-resolution Compton scattering

ThuPA2:2.05 - 17.15	<b>Atsushi Hariki</b>
<i>Contributed</i>	<i>Osaka Prefecture University</i> CaCu <sub>3</sub> Ru <sub>4</sub> O <sub>12</sub> : A High Kondo-Temperature Transition Metal Oxide
ThuPA2:2.06 - 17.30	<b>Tamaghna Hazra</b>
<i>Contributed</i>	<i>Rutgers University</i> Triplet pairing mechanisms from Hund's-Kondo models: applications to heavy fermion superconductors

<b>ROOM: E104-105</b>	<b>Parallel session: Unconventional Superconductivity (5)</b>
<b>15.45 - 17.45</b>	Chair: Kim Lefmann

ThuPA2:3:01 - 15.45	<b>Eduardo Marino</b>
<i>Invited</i>	<i>Federal University of Rio de Janeiro</i> A Testable Theory for High-Tc Superconductivity in Cuprates
ThuPA2:3:02 - 16.15	<b>Cliò Efthimia Agrapidis</b>
<i>Contributed</i>	<i>University of Warsaw</i> Unravelling the Nature of Spin Excitations Disentangled from Charge Contributions in a Doped Cuprate Superconductor
ThuPA2:3:03 - 16.30	<b>Hannes Kuehne</b>
<i>Contributed</i>	<i>Hochfeld-Magnetlabor Dresden, Helmholtz-Zentrum Dresden-Rossendorf</i> Order-parameter evolution in the Fulde-Ferrell-Larkin-Ovchinnikov phase probed by <sup>13</sup> C NMR spectroscopy
ThuPA2:3:04 - 16.45	<b>Puhua Wan</b>
<i>Contributed</i>	<i>University of Groningen</i> Orbital FFLO State in a Layer-Coupled Ising Superconductor
ThuPA2:3:05 - 17.00	<b>Javier Landaeta</b>
<i>Contributed</i>	<i>Max Planck Institute for Chemical Physics of Solids, Dresden</i> Field-angle dependence reveals odd-parity superconductivity in CeRh <sub>2</sub> As <sub>2</sub>
ThuPA2:3:06 - 17.15	<b>Maria Teresa Mercaldo</b>
<i>Contributed</i>	<i>Università di Salerno</i> Orbital effects in spin-singlet superconductors: pi-pairing, Edelstein effect, and orbital vortex phase
ThuPA2:3:07 - 17.30	<b>Akito Daido</b>
<i>Contributed</i>	<i>Kyoto University</i> Theory of intrinsic superconducting diode effect

# Friday 29 July

<b>FORUM</b>	<b>Plenary session</b>
<b>08.45 - 10.15</b>	Chair: Silke Buehler-Paschen
<b>FriPL:01 - 08:45</b> <i>Plenary</i>	<b>Cristiane de Morais Smith</b> <i>Utrecht University</i> Topological properties at fractal dimensions
<b>FriPL:02 - 09.30</b> <i>Plenary</i>	<b>Peter Liljeroth</b> <i>Aalto University</i> Designer quantum states in van der Waals heterostructures

## COFFEE BREAK

<b>FORUM</b>	<b>Parallel session: Heavy fermions (2)</b>
<b>10.45 - 12.30</b>	Chair: Ernst Bauer
<b>FriPA1:1.01 - 10.45</b> <i>Invited</i>	<b>Jonathan Denlinger</b> <i>Lawrence Berkeley National Laboratory</i> Anisotropic c-f hybridization in CeRh <sub>6</sub> Ge <sub>4</sub> and CeCu <sub>2</sub> S <sub>2</sub>
<b>FriPA1:1.02 - 11.15</b> <i>Contributed</i>	<b>Oliver Squire</b> <i>University of Cambridge</i> Quantum critical point in the high-pressure structure of CeSb <sub>2</sub>
<b>FriPA1:1.03 - 11.30</b> <i>Contributed</i>	<b>Jan Knapp</b> <i>Royal Holloway University of London</i> Electro-nuclear transition in YbRh <sub>2</sub> Si <sub>2</sub> ; evidence for a spin density wave
<b>FriPA1:1.04 - 11.45</b> <i>Invited</i>	<b>Manuel Brando</b> <i>Max Planck Institute for Chemical Physics of Solids, Dresden</i> The multi-phase heavy-fermion superconductor CeRh <sub>2</sub> As <sub>2</sub>
<b>FriPA1:1.05 - 12.15</b> <i>Contributed</i>	<b>Kosuke Nogaki</b> <i>Kyoto University</i> Novel parity transition in strongly correlated superconductor: relation to CeRh <sub>2</sub> As <sub>2</sub>

<b>ROOM: E107-108</b>	<b>Parallel session: Fermi surfaces and electronic structure (2)</b>
<b>10.45 - 12.30</b>	Chair: Andreas Rost
<b>FriPA1:2.01 - 10.45</b> <i>Invited</i>	<b>Antony Carrington</b> <i>University of Bristol</i> Hall effect in overdoped cuprates and its link to Fermi surface reconstruction
<b>FriPA1:2.02 - 11.15</b> <i>Contributed</i>	<b>Roemer Hinlopen</b> <i>University of Bristol</i> Cascade of Fermi surface reconstructions linked to superconductivity inside the CDW phase of TiSe <sub>2</sub>
<b>FriPA1:2.03 - 11.30</b> <i>Contributed</i>	<b>Andrew Hunter</b> <i>University of Geneva</i> Laser ARPES measurements of Sr <sub>2</sub> RuO <sub>4</sub> under uniaxial strain
<b>FriPA1:2.04 - 11.45</b> <i>Contributed</i>	<b>Mario Cuoco</b> <i>CNR-SPIN Salerno</i> Orbital loop current phase at the surface of Sr <sub>2</sub> RuO <sub>4</sub>

<a href="#">FriPA1:2.05 - 12.00</a>	<b>Mingu Kang</b> <i>Contributed</i>	<i>Massachusetts Institute of Technology</i> Twofold van Hove singularity and origin of charge order in topological kagome superconductors CsV3Sb5
<a href="#">FriPA1:2.06 - 12.15</a>	<b>Andre Deyerling</b> <i>Contributed</i>	<i>Technical University Munich</i> Electronic structure of CeTAl3 (T=Ag, Au, Cu, Pd, Pt) studied with density functional theory

<b>ROOM: E104-105</b> <b>10.45 - 12.30</b>	<b>Parallel session: Correlated topological phases (2)</b> Chair: Maarten van Delft	
<a href="#">FriPA1:3:01 - 10.45</a>	<b>Debmalya Chakraborty</b> <i>Contributed</i>	<i>Uppsala University</i> Disorder-robust phase crystal in high-temperature superconductors from topology and strong correlations
<a href="#">FriPA1:3:02 - 11.00</a>	<b>Marein Rahn</b> <i>Contributed</i>	<i>Technical University of Dresden</i> Topology, colossal magnetoresistance, and complex magnetic domains in Eu5In2Sb6
<a href="#">FriPA1:3:03 - 11.15</a>	<b>Sarah Grefe</b> <i>Invited</i>	<i>Los Alamos National Laboratory</i> The Weyl-Kondo semimetal: high-harmonic generation and extreme topological tunability
<a href="#">FriPA1:3:04 - 11.45</a>	<b>Diana Kirschbaum</b> <i>Contributed</i>	<i>Vienna University of Technology</i> Physical properties of Ce3Bi4X3 beyond the X = Pt, Pd case: First study of Ce3Bi4Ni3
<a href="#">FriPA1:3:05 - 12.00</a>	<b>Diego Zocco</b> <i>Contributed</i>	<i>Vienna University of Technology</i> Effects of hydrostatic pressure on the Weyl-Kondo semimetal candidate CeRu4Sn6
<a href="#">FriPA1:3:06 - 12.15</a>	<b>Elena Gati</b> <i>Contributed</i>	<i>Max-Planck-Institute for Chemical Physics of Solids, Dresden</i> Pressure-induced ferromagnetism in the topological semimetal EuCd2As2

<b>ROOM: E103</b> <b>10.45 - 12.30</b>	<b>Parallel session: Novel techniques for SCES investigations</b> Chair: Doohee Cho	
<a href="#">FriPA1:4.01 - 10.45</a>	<b>Petr Čermák</b> <i>Invited</i>	<i>Charles University Prague</i> ALSA - Automatic Laue Sample Aligner
<a href="#">FriPA1:4.02 - 11.15</a>	<b>Santiago Grigera</b> <i>Invited</i>	<i>Universidad Nacional de La Plata</i> Integrating Machine Learning with Neutron Scattering
<a href="#">FriPA1:4.03 - 11.45</a>	<b>Isabel Guillamon</b> <i>Invited</i>	<i>Universidad Autónoma de Madrid</i> STM at magnetic fields of 20 T: quasiparticle interference and vortex lattices of pnictide superconductors
<a href="#">FriPA1:4.04 - 12.15</a>	<b>Maximilian Pelly</b> <i>Contributed</i>	<i>University of St Andrews</i> Quantum oscillations and magnetostriction in Sr3Ru2O7 studied by a novel capacitive dilatometer

12.30 - 13.30

LUNCH BREAK

**FORUM**      **Conference highlights**

**13.30 - 14.00**      Chair: Alix McCollam

13:30

**Rebecca Flint**

*Iowa State University*

Theory Highlights

13:45

**Stephen Julian**

*University of Toronto*

Experiment Highlights

**FORUM**

**Closing and announcements**

**14.00 - 14.30**      Chair: Anne de Visser



# Kitaev Materials

Hae-Young Kee<sup>1,2</sup>

<sup>1</sup>*Department of Physics, University of Toronto, Toronto, Ontario, Canada*

<sup>2</sup>*Canadian Institute for Advanced Research, Quantum Materials Program, Toronto, Ontario, Canada*

Fascinating features of two-dimensional van der Waals magnetic materials have attracted much attention from theoretical and experimental researchers. Among them, spin models for two-dimensional honeycomb Mott insulators beyond the standard Heisenberg interaction have been developed and several Kitaev candidate materials have been recently proposed. The Kitaev model on honeycomb lattice is a rare example of exactly solvable model, which exhibits non-Abelian anyons under a magnetic field.[1] However, in real materials there are non-Kitaev interactions, and most notable one is another type of bond-dependent interaction named Gamma. A minimal Kitaev-Gamma model has been investigated by various numerical techniques under a magnetic field, but definite conclusions about field-induced Kitaev quantum spin liquids remain elusive. The phase diagrams of the Kitaev-Gamma model in the presence of a magnetic field will be presented [2]. Its connection to possible spin liquids in the two-dimensional limit will be discussed. A microscopic derivation of higher-spin Kitaev interaction and experimental strategy to extract the Kitaev interaction out of a full spin model using the symmetry of Hamiltonian [3] will be also presented.

\*This work is supported by the NSERC of Canada and Canada Research Chair Program

[1] A. Kitaev, *Annals of Physics* **321**, 2 (2006).

[2] J. Gordon *et al.*, *Nature Communications* **10**, 2470 (2019); E. Sorensen *et al.*, *Phys. Rev. X* **11**, 011013 (2021).

[3] P. Stavropoulos *et al.*, *Phys. Rev. Lett.* **123**, 037203 (2019); J. Cen and H.-Y. Kee, arXiv:2203.06193.

## Hidden magnetoelectric multipoles

Nicola A. Spaldin<sup>1</sup>

<sup>1</sup>*Materials Department, ETH Zürich*

The concept of magnetic dipolar order -- for example ferro, ferri or antiferromagnetic -- is at the core of our understanding of the behavior of magnetic materials, and is invaluable in explaining their behavior and in selecting and tailoring them for applications. Sometimes, however, magnetic materials surprise us, and behave in ways that cannot be captured within our established paradigms, suggesting additional kinds of magnetic order that are not yet identified. In this talk, I will discuss the relevance of the so-called magnetoelectric multipoles, which form the next-order term, after the magnetic dipole, in the multipolar expansion of the energy of a magnetization density in a magnetic field. First, I will describe how magnetoelectric multipoles underlie multiferroic behavior and in particular how they determine the magnetic response to applied electric fields. Then I will discuss signatures of hidden magnetoelectric multipolar order and possibilities for its direct measurement. I will close with an analysis of how antiferromagnets that contain ferroically ordered magnetoelectric multipoles are fundamentally different from those that do not, in particular in their surface magnetic properties.

## Turbulent hydrodynamics in strongly correlated Kagome metals

Domenico Di Sante<sup>1</sup>, Johanna Erdmenger<sup>1</sup>, Martin Greiter<sup>1</sup>, Ioannis Matthaiakakis<sup>1</sup>, René Meyer<sup>1</sup>, David Rodríguez Fernández<sup>1</sup>, Ronny Thomale<sup>1</sup>, Erik van Loon<sup>2</sup> & Tim Wehling<sup>2</sup>  
*<sup>1</sup>Institut für Theoretische Physik und Astrophysik and Würzburg-Dresden Cluster of Excellence ct.qmat, Julius-Maximilians-Universität Würzburg, Am Hubland, 97074 Würzburg, Germany*

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*Authors in alphabetical order.*

So far, graphene is the material of choice for experimentally realizing hydrodynamic behaviour of strongly coupled electrons in a solid. However, in graphene the effective electron-electron coupling is only of order one, still far away from the infinite coupling limit studied in holographic hydrodynamics using gauge/gravity duality. We propose a new Dirac material, Scandium-substituted Herbertsmithite, in which the electron-electron coupling is enhanced by a factor 3.2 as compared to graphene [1]. Using a holographic approach that involves finite-coupling higher-curvature corrections to the famous holographic result of  $1/4 \pi$  for the ratio of shear viscosity over entropy density ( $\eta/s$ ), we then estimate  $\eta/s$  in the coupling regime of the proposed new material. The associated range of Reynolds numbers even puts turbulent behaviour within reach. - Moreover, I will briefly report on recent results for the Hall viscosity and its impact for electron flows in channel geometries [2].

\*This work is supported by SFB 1170 ToCoTronics and the Cluster of Excellence ct.qmat.

[1] D. Di Sante, J. Erdmenger, M. Greiter, I. Matthaiakakis, R. Meyer, D. Rodríguez Fernández, R. Thomale, E. Van Loon and T. Wehling, *Nat Commun* **11**, 3997 (2020).

[2] Z.-Y. Xian, S. Danz, I. Matthaiakakis, D. Rodríguez Fernández, R. Klees, C. Tutschku, J. Erdmenger, R. Meyer and E. Hankiewicz, *to appear*.

# Momentum dependent scaling exponents of cuprate strange-metal self energies: ARPES meets semi-holography

S. Smit<sup>1</sup>, E. Mauri<sup>2</sup>, L. Bawden<sup>1</sup>, F. Heringa<sup>1</sup>, F. Gerritsen<sup>1</sup>, E. van Heumen<sup>1</sup>, Y.K. Huang<sup>1</sup>, T. Kondo<sup>3</sup>, T. Takeuchi<sup>4</sup>, N. E. Hussey<sup>5,6</sup>, M. Allan<sup>7</sup>, T.K. Kim<sup>8</sup>, C. Cacho<sup>9</sup>, A. Krikun<sup>9</sup>, K. Schalm<sup>10</sup>, H.T.C. Stoof<sup>2</sup>, M.S.Golden<sup>1,11</sup>

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<sup>3</sup> *Institute for Solid State Physics, University of Tokyo*

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<sup>5</sup> *High Field Magnet Laboratory (HFML-EMFL) and Institute for Molecules and Materials, Radboud University, Nijmegen*

<sup>6</sup> *H. H. Wills Physics Laboratory, University of Bristol*

<sup>7</sup> *Leiden Institute of Physics, Leiden University*

<sup>8</sup> *Diamond Light Source*

<sup>9</sup> *NORDITA, KTH Royal Institute of Technology and Stockholm University*

<sup>10</sup> *Institute-Lorentz for Theoretical Physics, Leiden University*

<sup>11</sup> *Dutch Institute for Emergent Phenomena (DIEP), 1098 XH Amsterdam*

High resolution ARPES enables the precise experimental determination of the electronic self-energy. Here we present high quality data from the strange metal single-layer cuprate  $(\text{Pb,Bi})_2\text{Sr}_{2-x}\text{La}_x\text{CuO}_{6+\delta}$ , measured over a wide range in  $\omega$ - and  $T$  in the nodal direction. Constant energy cuts through the spectral function have a non-Lorentzian lineshape, meaning the nodal self-energy is  $k$  dependent. These experimental data provide a new test for aspiring theories.

We go on to show that the experimental data are captured remarkably well by a power law with a  **$k$ -dependent scaling exponent**, smoothly evolving with doping, a description that emerges naturally from AdS/CFT-based semi-holography, putting a spotlight on holographic methods for the quantitative modelling of strongly interacting quantum materials like the cuprate strange metals [1].

[1] [arxiv.org/pdf/2112.06576](https://arxiv.org/pdf/2112.06576).

# Planckian metallic state in the two-dimensional Hubbard model

Arata Tanaka

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In this study the Hubbard model on the square lattice is investigated using the dual fermion approximation [1] to understand the origin of the  $T$ -linear dependence of the resistivity with the Planckian dissipation limit [2] in the strange metallic state of cuprate superconductors, where the transport scattering rate is represented by  $1/\tau = \alpha k_B T/\hbar$  with  $\alpha \sim 1$ .

It is found that because of the two-dimensional antiferromagnetic fluctuation, the temperature dependence of electron scattering rate  $\gamma_k = -\text{Im} \Sigma_k(\omega = 0)$  at  $\mathbf{k}$  around the X point of the Brillouin zone of the square lattice is proportional to  $T$  in wide range of  $T$  in the non-Fermi liquid phase, which is located between electron densities at the end of the pseudo-gap phase around  $n_{\text{PG}} \sim 0.8$  and the antiferromagnetic quantum critical point  $n_{\text{QCP}}$ . The coefficient  $a$  of  $\gamma_k \sim aT$  is several times larger than unity without quasi-particle renormalization factor  $Z_k$ . However, with  $Z_k$  the coefficient  $a'$  of  $\gamma_k^* \equiv Z_k \gamma_k \sim a'T$  is always reduced to unity within 10% deviation at low temperatures within the reasonable parameter range for the cuprate superconductors. This shows that the non-Fermi liquid state in the Hubbard model, which corresponds to the strange metallic state of cuprate superconductors, is indeed at the Planckian dissipation limit.

[1] A. Tanaka, Phys. Rev. B **99**, 205133 (2019).

[2] J. A. N. Bruin *et al.*, Science **339**, 804 (2013).

## **Quantum supreme matter: the strange metals according to holography.**

J. Zaanen<sup>1</sup>

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Quantum supreme matter refers to forms of matter that are densely many-body entangled with the ramification that the quantum supremacy of the quantum computer is required to enumerate the way it works [1]. Strange metals are a prime candidate, with the Fermion sign problem driving the dense entanglement. The holographic duality of string theory appears to offer a mathematical entry into these realms revealing new general principles, suggesting both novel forms of “covariant” renormalization flows in finite density fermion systems but also exhibiting an eerie capacity to predict dissipation phenomena in terms of first principle quantum thermalization. Holography revolves around the map of the quantum physics to an equivalent gravitational black hole problem in one higher dimension. The present frontier is associated with breaking the spatial translational symmetry that requires solving the Einstein equations in their full glory as a system of highly non-linear partial differential equations. This is closely related to the computation of black hole mergers, requiring supercomputer facilities. In our Leiden effort we are focusing on the influence of large periodic (Umklapp) potentials and we find results having an eerie resemblance with famous properties such as the “Planckian dissipation” linear resistivity.

### **References**

[1]. J. Zaanen, arXiv:2110.00961 (2021).

# Non-Loudon-Fleury Raman scattering in spin-orbit coupled Mott insulators

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We revisit the theory of magnetic Raman scattering in Mott insulators with strong spin-orbit coupling, with a major focus on Kitaev materials. We show that Kitaev materials with bond-anisotropic interactions are generally expected to show both one- and two-magnon responses. It is further shown that to obtain the correct leading contributions to the Raman operator, one must consider the precise, photon-assisted microscopic hopping processes of the electrons and that, in systems with multiple hopping paths, the Raman operator contains terms beyond those appearing in the traditional Loudon-Fleury theory. Most saliently, a numerical implementation of the revised formalism to the case of the three-dimensional hyperhoneycomb Kitaev material  $\beta$ -Li<sub>2</sub>IrO<sub>3</sub> reveals that the non-Loudon-Fleury scattering terms dominate the Raman intensity. In addition, they induce a qualitative modification of the polarization dependence, including, e.g., the emergence of a sharp one-magnon peak at low energies which is not expected in the traditional Loudon-Fleury theory. This peak is shown to arise from microscopic photon-assisted tunneling processes that are of similar type with the ones leading to the symmetric off-diagonal interaction  $\Gamma$  (known to be present in many Kitaev materials) but take the form of a bond-directional magnetic dipole term in the Raman vertex. These results are expected to apply across all Kitaev materials and mark a drastic change of paradigm for the understanding of Raman scattering in materials with strong spin-orbit coupling and multiple exchange paths.

\*This work is supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award No. DE-SC0018056.

[1] A. Yang Yang, Mengqun Li, Ioannis Rousochatzakis, and Natalia B. Perkins, Phys. Rev. B 104, 144412 (2021).

[2] Yang Yang, Yiping Wang, Ioannis Rousochatzakis, Alejandro Ruiz, James G. Analytis, Kenneth S. Burch, and Natalia B. Perkins, Phys. Rev. B 105, L2411011 (2020).

# Tuning competing interactions in Kitaev magnets via topochemical reactions

Faranak Bahrami<sup>1</sup>, Mykola Abramchuk<sup>1</sup>, Ying Ran<sup>1</sup>, Xiaodong Hu<sup>1</sup>, Michael Graf<sup>1</sup>, Eric Kenney<sup>1</sup>, Kemp W. Plumb<sup>2</sup>, Alberto de la Torre<sup>2</sup>, Adam Berlie<sup>3</sup>, Chennan Wang<sup>4</sup>, Oleg Lebedev<sup>5</sup>, Daniel Haskel<sup>6</sup> and Fazel Tafti<sup>1</sup>

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Honeycomb iridate materials have been intensely studied in the past two decades due to the potential realization of a Kitaev spin liquid phase. The basic ingredients of the Kitaev model including a honeycomb lattice, spin  $\frac{1}{2}$  ions, and bond-directional Ising-like interactions are present in materials such as  $\alpha$ -Li<sub>2</sub>IrO<sub>3</sub> and Na<sub>2</sub>IrO<sub>3</sub>. However, non-Kitaev interactions such as the Heisenberg and off-diagonal exchange are also present in real materials. These competing interactions create a complex phase diagram with non-collinear magnetic orders as well as the spin liquid phase. In this talk, we explain how topochemical methods can be used to tune the competing interactions and access different regimes in the phase diagram of Kitaev magnets. In a typical topochemical reaction, alkali ions are replaced by monovalent transition metal ions. As a result, the bond angles across the super-exchange paths change, providing a mechanism for tuning the relative strength of different exchange interactions and a potential route to discovering the quantum spin liquid phase. We will present several materials synthesized by topochemical reactions including Cu<sub>2</sub>IrO<sub>3</sub> that exhibits a competition between static and dynamic magnetism [1,2,3], Ag<sub>3</sub>LiIr<sub>2</sub>O<sub>6</sub> that exhibits thermodynamic evidence of proximity to the Kitaev spin liquid phase [4,5,6,7], and Ag<sub>3</sub>LiRh<sub>2</sub>O<sub>6</sub> that falls in a dramatically different region of the phase diagram far from the spin liquid phase [8].

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[1] M. Abramchuk *et al.*, J. Am. Chem. Soc. **139**, 15371 (2017)

[2] E. Kenney *et al.*, Phys. Rev. B **100**, 094418 (2019)

[3] S. K. Takahashi *et al.*, Phys. Rev. X **9**, 031047 (2019)

[4] F. Bahrami *et al.* Phys. Rev. Lett **123**, 237203 (2019)

[5] F. Bahrami *et al.* Phys. Rev. B **103**, 094427 (2021)

[6] J. Wang *et al.* Phys. Rev. B **103**, 214405 (2021)

[7] A. de la Torre, Phys. Rev. B **104**, L100416 (2021)

[8] F. Bahrami, Science Advances, **8**, eabl5671 (2022)



# Dynamics of visons and Thermal Hall effect in perturbed Kitaev models

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A vison is an excitation of the Kitaev spin liquid which carries a  $\mathbb{Z}_2$  gauge flux. While immobile in the pure Kitaev model, it becomes a dynamical degree of freedom in the presence of perturbations. We study an isolated vison in the isotropic Kitaev model in the gapless phase of the Kitaev honeycomb model perturbed by a small external magnetic field  $h$ , an offdiagonal exchange interactions  $\Gamma$  and a Heisenberg coupling  $J$ . In the ferromagnetic Kitaev model, the dressed vison obtains a dispersion linear in  $\Gamma$  and  $h$  and a fully universal low- $T$  mobility,  $\mu = 6 v_m^2 / T^2$ , where  $v_m$  is the velocity of Majorana fermions. In contrast, in the antiferromagnetic Kitaev model interference effects preclude coherent propagation and an incoherent Majorana-assisted hopping leads to a  $T$ -independent mobility. This explains the striking difference of ferro- and antiferromagnetic Kitaev models in the presence of these perturbations. The motion of a single vison due to Heisenberg interactions is strongly suppressed for both signs of the Kitaev coupling. Vison bands induced by  $h$  can be topological and may lead to signatures in thermal Hall effect.

[1] AP Joy and Achim Rosch, PRX (accepted), arxiv.2109.00250

# Evidence of a Phonon Hall Effect in the Kitaev Spin Liqui Candidate $\alpha$ - $\text{RuCl}_3$

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The material  $\alpha$ - $\text{RuCl}_3$  has been the subject of intense scrutiny as a potential Kitaev quantum spin liquid, predicted to display Majorana fermions as low energy excitations. In practice,  $\alpha$ - $\text{RuCl}_3$  undergoes a transition to a state with antiferromagnetic order below a temperature  $T_N \approx 7$  K, but this order can be suppressed by applying an external in-plane magnetic field of  $H_{\parallel} = 7$  T. Whether a quantum spin liquid phase exists just above that field is still an open question, but the reported observation of a quantized thermal Hall conductivity at  $H_{\parallel} > 7$  T by Kasahara and co-workers [1] has been interpreted as evidence of itinerant Majorana fermions in the Kitaev quantum spin liquid state. In this study, we re-examine the origin of the thermal Hall conductivity  $\kappa_{xy}$  in  $\alpha$ - $\text{RuCl}_3$ . Our measurements of  $\kappa_{xy}(T)$  on several different crystals yield a temperature dependence very similar to that of the phonon-dominated longitudinal thermal conductivity  $\kappa_{xx}(T)$ , for which the natural explanation is that  $\kappa_{xy}$  is also mostly carried by phonons. Upon cooling,  $\kappa_{xx}$  peaks at  $T \approx 20$  K, then drops until  $T_N$ , whereupon it suddenly increases again. The abrupt increase below  $T_N$  is attributed to a sudden reduction in the scattering of phonons by low-energy spin fluctuations as these become partially gapped when the system orders. The fact that  $\kappa_{xy}$  also increases suddenly below  $T_N$  is strong evidence that the thermal Hall effect in  $\alpha$ - $\text{RuCl}_3$  is also carried predominantly by phonons. This implies that any quantized signal from Majorana edge modes would have to come on top of a sizable – and sample-dependent – phonon background [2].

[1] Y. Kasahara *et al.*, Nature **559**, 227 (2018).

[2] É. Lefrançois *et al.*, arXiv:2111.05493, (2021).

# Identification of a Kitaev Quantum Spin Liquid by Magnetic Field Angle Dependence

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Quantum spin liquids realize massive entanglement and fractional quasiparticles from localized spins, proposed as an avenue for quantum science and technology. In particular, topological quantum computations are suggested in the non-abelian phase of Kitaev quantum spin liquid with Majorana fermions, and detection of Majorana fermions is one of the most outstanding problems in modern condensed matter physics. Here, we propose a concrete way to identify the non-abelian Kitaev quantum spin liquid by magnetic field angle dependence. Topologically protected critical lines exist on a plane of magnetic field angles, and their shapes are determined by microscopic spin interactions. A chirality operator plays a key role in demonstrating microscopic dependences of the critical lines. We also show that the chirality operator can be used to evaluate topological properties of the non-abelian Kitaev quantum spin liquid without relying on Majorana fermion descriptions. Experimental criteria for the non-abelian spin liquid state are provided for future experiments.

[1] K. Hwang, A. Go, J. H. Seong, T. Shibauchi, & E.-G. Moon, Nat. Commun. 13, 323 (2022).

[2] O. Tanaka, Y. Mizukami, R. Harasawa, K. Hashimoto, K. Hwang, N. Kurita, H. Tanaka, S. Fujimoto, Y. Matsuda, E.-G. Moon, T. Shibauchi, Nat. Phys. (2022).

# Effects of Coulomb interactions in Dirac and Weyl semimetallic two-dimensional crystals

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We present two examples displaying interesting effects of Coulomb interactions in two-dimensional crystals. First, we show that novel electronic features among carbon materials such as zone-center saddle point and peculiar type-II Dirac fermionic states are shown to exist in the low-energy electronic spectrum of a new planar carbon crystal formed through networking biphenylene molecules. The type-II state here has a nearly flat branch and is close to a transition to type I. Possible magnetic instabilities related to low-energy bands are discussed. Furthermore, with a moderate uniaxial strain, a pair of Dirac points merge with the zone-center saddle point, realizing concurrent Lifshitz transitions of van Hove singularity as well as pair annihilation of the Dirac fermions. Second, we will show the direct evidence of impacts of the Coulomb interaction in a prototypical Weyl semimetal, MoTe<sub>2</sub>, that alter its bare bands in a wide range of energy and momentum. Our quasiparticle interference patterns measured using scanning tunneling microscopy are shown to match the joint density of states of quasiparticle energy bands including momentum-dependent self-energy corrections, while electronic energy bands based on the other simpler local approximations of the Coulomb interaction fail to explain neither the correct number of quasiparticle pockets nor the shape of their dispersions observed in our spectrum. With this, we predict a transition between type-I and type-II Weyl fermions with doping and resolve its disparate quantum oscillation experiments, thus highlighting the critical roles of Coulomb interactions in layered Weyl semimetals.

# Weyl-Kondo semimetals and their symmetry-based design

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Strong correlations driving electronic topology has long been known in insulators, as exemplified by the fractional quantum Hall effect. Whether and how this happens in gapless (metallic) cases has been an outstanding question. In this talk, I will describe the progress we have made in going from the canonical correlation physics of quantum criticality [1] to the realization of electronic topology in strongly correlated metallic systems. The context of heavy fermion metals is particularly advantageous, because of the well-defined input about the effective degrees of freedom that describe the low-energy physics.

I will present the theoretical concept and salient properties of Weyl-Kondo semimetal [2,3]. They set the stage for a general approach, *viz.* to utilize the cooperation of crystalline symmetry with interactions to design new types of Weyl-Kondo semimetal phases and realize them in new (or, in some cases, old and yet to be explored) materials [4].

I will also describe models for gapless topological phases without any free-electron counterpart [5]: they have no Landau quasiparticles and show strange-metal behavior. The manifestation of such non-Fermi liquid topological matter will be presented, and their materials realization will be proposed [5].

Our results illustrate the potential of the proposed symmetry-correlation cooperation to guide the search for new topological matter in a broad range of strongly correlated systems.

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[1] S. Paschen & Q. Si, *Nat. Rev. Phys.* **3**, 9 (2021); S. Kirchner et al, *Rev. Mod. Phys.* **92**, 011002 (2020); Q. Si et al, *Nature* **413**, 804 (2001).

[2] H.-H. Lai, S. Grefe et al., *PNAS* **115**, 93 (2018); S. Grefe et al., *Phys. Rev. B* **101**, 075138 (2020).

[2] S. Dzsaber et al., *PNAS* **118**, e2013386118 (2021); *Phys. Rev. Lett.* **118**, 246601 (2017).

[3] L. Chen et al, arXiv:2107.10837 ( <https://arxiv.org/abs/2107.10837> ).

[4] H. Hu et al., arXiv:2110.06182 ( <https://arxiv.org/abs/2110.06182> ).

# Pressure-tuning the magnetic noncentrosymmetric Weyl semimetals CeAlSi and CeAlGe

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Chiral domain walls have great potential to enable new spintronic devices [1]. These domain walls occur in systems with broken space-inversion symmetry. Promising candidate materials belong to the family  $LnAlX$  ( $Ln$  = lanthanides,  $X$  = Ge, Si) with noncentrosymmetric crystalline structure ( $I41md$ ). In particular, introducing Ce on the lanthanide site produces more complex properties, such as the Kondo effect, which may pin electronic-band crossings of magnetic Weyl semimetals near the Fermi level [2], further enhancing the possibility of large spin currents.

Here we focus on the compounds CeAlSi and CeAlGe. In CeAlSi, chiral domain walls were recently observed in the magnetic phase [3,4], while in CeAlGe, domain walls were reported to be responsible for a singular angular magnetoresistance [5]. By applying hydrostatic pressure, we were able to modify the domain wall landscape of both compounds, revealing the fundamental role of domain walls for the nontrivial topological features observed in these materials. We explore hysteretic domain wall scattering as a possible source for anomalies seen in the Hall resistivity. For instance, in CeAlSi, a contribution of domain wall scattering to the anomalous Hall effect was observed, along with an unusual temperature evolution of the quantum oscillations amplitude. The suppression of both by external pressure and the negligible effect of pressure on the magnetism and the electronic bands structure hint at the importance of the domain wall landscape for the observed anomalous properties in CeAlSi [6].

[1] S.-H. Yang, R. Naaman, Y. Paltiel and S. S. P. Parkin, Nat. Rev. Phys. **3**, 328 (2021).

[2] S. E. Grefe, H.-H. Lai, S. Paschen, and Q. Si, Phys. Rev. B, **101**, 075138 (2020).

[3] B. Xu, *et al.*, Adv. Quantum Technol., **4**, 2000101 (2021).

[4] Y. Sun, *et al.*, Phys. Rev. B, **104**, 235119 (2021).

[5] T. Suzuki *et al.*, Science **365**, 377 (2019).

[6] M. M. Piva, *et al.*, arXiv:2111.05742 (2021).

# Spin dynamics and topological nature of the semimetal YbMnSb<sub>2</sub>

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The family of quantum materials  $AMnX_2$  ( $A = \text{Ca, Sr, Ba, Yb, Eu}$ ;  $X = \text{Sb, Bi}$ ) has demonstrated characteristics of topological semimetals. The quasi-2D plane formed by the Sb or Bi ‘square’ may host topological fermions [1-3], and the magnetic order of Mn could provide a mechanism to manipulate the band structure topology and quasiparticles [4]. Interactions between the electrons involved in quasiparticle behaviour, and those responsible for magnetism, can also influence quasiparticle characteristics: increasing spin-orbit coupling increases quasiparticle mass [1].

YbMnSb<sub>2</sub> belongs to the  $P4/nmm$  space group and shows evidence of a magnetic ordering transition involving the Mn moments at  $\sim 350$  K [1]. This is a relatively high Néel temperature among the family of materials  $AMnX_2$ . The compound YbMnSb<sub>2</sub> is of note due to its excellent thermoelectric properties [5]. The magnetic structure of YbMnSb<sub>2</sub> and its corresponding semimetal nature has been the subject of multiple investigations [1, 6–8]. Our recent report featuring neutron diffraction data [8] concluded that YbMnSb<sub>2</sub> displays C-type antiferromagnetism and is a gapped Dirac semimetal.

We have now measured the spin waves of YbMnSb<sub>2</sub> using triple-axis spectroscopy and will present the results here, along with a magnetization distribution for this material. The magnetic excitations of this material add a new layer of intrigue, as the exchange constants are larger than any previously reported for isostructural semimetals [9, 10]. In particular, the exchange between the  $c$  axis nearest neighbours is especially strong for this family. The implications of the out-of-plane magnetism, and for the in-plane quasiparticles and charge transport will be discussed.

- [1] Y.-Y. Wang, *et al.*, Phys. Rev. Mat. **2**, 021201 (2018).
- [2] J. Liu, *et al.*, Scientific Reports **6**, 30525 (2016).
- [3] J. B. He, *et al.*, Phys. Rev. B **95**, 045128 (2017).
- [4] H. Tsai, *et al.*, Nature **508**, 608 (2020).
- [5] Y. Pan, *et al.*, Advanced Materials **33**, 2003168 (2021).
- [6] R. Kealhofer, *et al.*, Phys. Rev. B **97**, 045109 (2018).
- [7] Z. Qiu, *et al.*, Phys. Rev. B **100**, 125136 (2019).
- [8] J.-R. Soh, *et al.*, Phys. Rev. B **104**, L161103 (2021).
- [9] J.-R. Soh, *et al.*, Phys. Rev. B **100**, 144431 (2019).
- [10] M. Rahn, *et al.*, Phys. Rev. B **95**, 134405 (2017).

## Sondheimer oscillations as a probe of non-ohmic flow in WP<sub>2</sub> crystals

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As conductors in electronic applications shrink, the detailed scattering processes may lead to deviations from Ohm's law. Depending on the length scales of momentum conserving ( $l_{mc}$ ) and relaxing ( $l_{mr}$ ) scattering and the device size ( $d$ ), current flow may shift from ohmic to ballistic or hydrodynamic regimes. So far, an in situ methodology to obtain these parameters within a micro/nanodevice is critically lacking.

Here we present Sondheimer oscillations (SO) as a method to obtain  $l_{mr}$  even when  $l_{mr} \gg d$ . SO manifest as periodic-in- $B$  oscillations of the resistivity due to the helical motion of carriers along a magnetic field. The field sets the cyclotron radius and thus determines at which point the helical motion is cut off by scattering from the device surface, making a positive or negative contribution to the conduction [1]. As this effect requires there to be no scattering in the bulk, it is sensitive to the mean-free-path and enables its extraction.

Using WP<sub>2</sub> as a test case, we demonstrate the presence of SO and extract  $l_{mr}$  over a wide range of temperatures and magnetic fields up to 30 T. Our data on  $\mu\text{m}$ -sized devices are in excellent agreement with experimental reports of the bulk  $l_{mr}$  and confirm that WP<sub>2</sub> can be microfabricated without degradation. These results conclusively establish Sondheimer oscillations as a quantitative probe of  $l_{mr}$  in micro-devices [2].

[1] V. L. Gurevich. Soviet Physics JETP 35(8): 3, 464-470 (1959)

[2] M. R. van Delft *et al.* Nature Communications 12, 4799 (2021)



# Detection and manipulation of antiferromagnetic orders via the magnetoelectric effect

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The concept of utilizing antiferromagnets (AFMs) in spintronic devices has attracted much attention recently. AFMs are appealing as the absence of net magnetization eliminates crosstalk between neighboring domains, the rich variety of antiferromagnetic orders offers new possibilities to encode information and their THz dynamics enables much faster manipulation compared to ferromagnets. However, the detection and manipulation of AFMs are notoriously difficult with the conventional methods that are based on the magnetization.

When the antiferromagnetic order breaks not only the time-reversal but also the spatial inversion symmetry, the magnetoelectric (ME) effect becomes allowed. This cross-coupling provides a new handle on the antiferromagnetic state. Moreover, in these compounds, the electric and magnetic dipoles are entangled at finite frequencies as well, thus, intriguing optical effects such as non-reciprocal light absorption and polarization rotation also emerge.

In this talk, we present our efforts to use these optical ME effects to detect antiferromagnetic orders. Using THz spectroscopy, we studied the antiferromagnetic resonances of LiCoPO<sub>4</sub>, an antiferromagnet with finite toroidal moment [1,2]. We found that some of the spin excitations are simultaneously electric and magnetic dipole active and show strong non-reciprocal light absorption. By cooling the sample in crossed electric and magnetic fields, we switched between the antiferromagnetic domains exhibiting different light absorption. In the easy-plane AFM, Ba<sub>2</sub>CoGe<sub>2</sub>O<sub>7</sub>, we also detected strong non-reciprocal light absorption in the THz frequency range [3]. The soft antiferromagnetic structure of this compound allowed us to demonstrate the in situ electric field control of the antiferromagnetic state.

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[1] V. Kocsis *et al.*, Phys. Rev. Lett. **121**, 057601 (2018).

[2] V. Kocsis *et al.*, Phys. Rev. B **100**, 155124 (2019).

[3] J. Vit *et al.*, Phys. Rev. Lett. **127**, 157201 (2021).

# Topologically protected unidirectional magnetoelectric switching in a multiferroic

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Electric control of magnetism and magnetic control of ferroelectricity can improve energy efficiency of magnetic memory and data processing devices. However, the necessary magnetoelectric switching is hard to achieve, and requires more than just a coupling between spin and charge degrees of freedom. We show that an application and subsequent removal of a magnetic field reverses the electric polarization of the multiferroic GdMn<sub>2</sub>O<sub>5</sub>, thus requiring two cycles to bring the system back to the original configuration. During this unusual hysteresis loop, four states with different magnetic configurations are visited by the system, with one half of all spins undergoing unidirectional full-circle rotation in increments of  $\sim 90^\circ$ . Therefore, GdMn<sub>2</sub>O<sub>5</sub> acts as a magnetic crankshaft converting the back-and-forth variations of the magnetic field into a circular spin motion. This peculiar four-state magnetoelectric switching emerges as a topologically protected boundary between different two-state switching regimes. Our findings establish a paradigm of topologically protected switching phenomena in ferroic materials.

# Strength and temperature range enhancement of electromagnon in CuO under pressure

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New exciting high-speed transmission technologies in which spin waves (SW) are vectors for processing information at the nanometer scale are now focused on finding more manageable magnetic quantum objects. Indeed, the traditional method in which SW are excited by dynamic magnetic fields generated by microwave currents significantly loses efficiency at the nanoscale due to parasitic couplings as the dimensions of the system decrease. Identifying alternative magnetic quantum objects that could be shaped and guided by electric field with minimal or no energy consumption is a highly promising pathway for SW applications. Such electroactive spin waves do exist in multiferroic materials and are called “electromagnons”, but they are usually weak quantum objects which are only present at cryogenic temperature making them unpractical to manipulate.

We demonstrated that in CuO, a relatively modest hydrostatic pressure (3GPa) allows an increase of the electromagnon strength by a factor 7 and an extension of its temperature range of existence by more than 40 K. Moreover, the extension of our data suggests that this excitation is present at room temperature around 10 GPa.

To obtain these results, we have pushed in its tracks the THz spectroscopy at the AILES beamline of synchrotron SOLEIL by probing such excitations of low absorption intensity (ten times smaller than phonons) on thin sample (less than 100  $\mu\text{m}$ ) suitable for high pressure measurements. This achievement is doubled by Monte-Carlo simulations based on a new effective Hamiltonian model and spin-waves dynamics which account for the first time for the complex magnetic phase diagram and allow to simulate the THz response of the CuO electromagnons in excellent agreement with our experimental results.

Our work highlights the possibility to place the CuO compound on the horizon of the spin waves-based technology roadmap.

# Exploration of multiferroic quantum phase transition in TbMnO<sub>3</sub>

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A multiferroic quantum phase transition (MQPT) occurs when two ferroic orders are simultaneously tuned to zero temperature in a single material [1,2]. In the case of a continuous MQPT, theory suggests that the overall critical fluctuations are governed by the order with the lower critical exponent, perhaps with additional corrections due to the specific interactions between the order parameter fields. However, this theory so far lacks experimental support.

TbMnO<sub>3</sub> is a magnetically driven multiferroic in which a spin spiral state develops below 28K, inducing ferroelectricity [3]. Previous work showed that the multiferroic order is suppressed to a paraelectric, canted AFM state when magnetic field is applied along the c-axis, with a low temperature re-entrant behaviour that suggests a magnetic field-tuned MQPT should be reached at high magnetic field [4].

In order to examine the behaviour of TbMnO<sub>3</sub> in the vicinity of this expected MQPT, we have measured the dielectric and magnetic susceptibilities with magnetic field parallel to the c-axis, up to 30 T and at temperatures down to 350 mK. Our results indicate that the multiferroic phase is fully suppressed at ~19.5 T. In addition, both susceptibilities show non-Curie-Weiss behaviour in a wide region of the phase diagram near the MQPT, suggesting that quantum fluctuations are important. I will present our magnetic field- and temperature dependent susceptibility results, as well as a comparison with theoretical predictions, which suggests that the MQPT is not simple biquadratic in nature, but has a more complex coupling between the ferroelectric and antiferromagnetic order parameters.

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[1] A. Narayan *et al.*, *Nature Materials* **18**, 223 (2019)

[2] C. Morice *et al.*, *Phys. Rev. B* **96**, 245104 (2017)

[3] T. Kimura *et al.* *Nature* **426**, 55 (2003)

[4] T. Kimura *et al.* *Phys. Rev. B* **71**, 224425 (2005)

# Optically-induced magnetization switching in NiCo<sub>2</sub>O<sub>4</sub> thin films

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Recently, all-optical magnetization control has been garnering considerable attention in realizing next-generation ultrafast magnetic information devices since ultrafast demagnetization within 1 ps was observed in Ni foils [1]. Ultrafast demagnetization was also observed in NiCo<sub>2</sub>O<sub>4</sub> thin films [2].

Here, employing a magneto-optical Kerr effect (MOKE) microscope, we observed the laser-induced magnetization switching of ferrimagnetic oxide NiCo<sub>2</sub>O<sub>4</sub> epitaxial thin films with perpendicular magnetic anisotropy [2,3], where the sample was pumped at 1030-nm laser pulses, and magnetic domain images were acquired via the MOKE microscope with a white light emitting diode. Laser pulses irradiated an NiCo<sub>2</sub>O<sub>4</sub> thin film at various temperatures from 300 K to 400 K while altering the parameters of pulse interval, fluence, and the number of pulses with the absence of the external magnetic field. We observed all-optical switching at 380 K and above when 10<sup>3</sup> or more pulses irradiated at 1-kHz repetition rates.

Our observation of oxide NiCo<sub>2</sub>O<sub>4</sub> thin films facilitates the realization of chemically stable magnetization switching using ultrafast lasers, and without applying a magnetic field.

[1] E. Beaurepaire *et al.*, Phys. Rev. Lett. **76**, 4250 (1996).

[2] R. Takahashi *et al.*, Appl. Phys. Lett. **119**, 102404 (2021).

[3] D. Kan *et al.*, Phys. Rev. B **101**, 224434 (2020).

# Temperature evolution of electronic structures of paradigm Ce 4f and U 5f materials

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The temperature evolution of the 4f Kondo lattice system CeCoIn<sub>5</sub> is investigated using angle-resolved photoemission spectroscopy (ARPES) with comparison to first principles dynamical mean field theory that include treatment of the crystalline electric field split 4f-states (DMFT+CEF). Measurement of the experimental three-dimensional Fermi surface (FS) is enabled by ARPES mapping of two orthogonal (001) and (100) cleaved surfaces [1]. Observation of a complex hole-like topology centered on the Z point, which exists only in f-localized density functional theory (DFT), and yet hosts strong T-dependent f spectral weight, highlights the deficiencies of both f-itinerant and f-localized DFT for this material.

The DMFT+CEF calculations are able to capture the surprising Z-point FS. They also agree with the general experimental finding of 4f FS participation far above the transport coherence temperature, and make new predictions for the T-dependent evolution of CEF states above  $E_F$  including visualization of a CEF degeneracy crossover [1].

For the 5f material URu<sub>2</sub>Si<sub>2</sub> a new model is introduced for the underlying physics of its famous hidden order phase transition and its various related doping phase diagrams. The model is motivated by the theoretical existence of an extended U 5f saddle-point dispersion at the N-point, thermally active at the 17.5K transition because it is located only a few meV below  $E_F$ . ARPES measurements of this N-point region do indeed reveal a strongly T-dependent evolution of incommensurate nesting hotspots lying along Z-N-Z [2] and also provide signatures distinguishing an f-orbital-ordered phase from the magnetically ordered ground states achieved by substitutional doping.

In collaboration with M.B. Maple, J.W. Allen, Ji Hoon Shim, Ryan Baumbach and others.

[1] S. Jang *et al.*, PNAS **117**, 23467 (2020).

[2] J. D. Denlinger *et al.*, Electron. Struct. **4**, 013001 (2022).

# A microscopic Kondo lattice model for the heavy fermion antiferromagnet CeIn<sub>3</sub>

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Electrons at the border of localization generate exotic states of matter across all classes of strongly correlated electron materials. Heavy electron metals are a model example, in which magnetic interactions arise from the opposing limits of localized and itinerant electrons. This remarkable duality is intimately related to the emergence of a plethora of novel quantum matter states, such as unconventional superconductivity, electronic-nematic, hidden order and most recently topological states, including skyrmion crystals, topological Kondo insulators and putative chiral superconductors. The outstanding challenge is that the archetypal Kondo lattice model that captures the underlying electronic dichotomy is notoriously difficult to solve for real materials. Using the prototypical strongly correlated antiferromagnet CeIn<sub>3</sub>, we will show that a multi-orbital periodic Anderson model embedded with input from ab initio band structure calculations can be reduced to a simple Kondo-Heisenberg model, which captures the magnetic interactions quantitatively. This tractable Hamiltonian is validated via high-resolution neutron spectroscopy that reproduces accurately the full magnon dispersion of CeIn<sub>3</sub>.

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## Zooming in on heavy fermions in Kondo lattice models

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Resolving the heavy fermion band in the conduction electron momentum resolved spectral function of the Kondo lattice model (KLM) is challenging since, in the weak coupling limit, its spectral weight is exponentially small. To alleviate this limitation we consider a composite fermion operator, consisting of a conduction electron dressed by spin fluctuations that shares the same quantum numbers as the electron.

Using auxiliary-field quantum Monte Carlo simulations we show that for the SU(2) spin-symmetric model on the square lattice at half filling, the quasiparticle residue of the composite fermion tracks the Kondo coupling  $J_k$  [1]. This result holds down to  $J_k/W = 0.025$ , with  $W$  the bandwidth, and confirms that magnetic ordering, present below  $J_k/W = 0.18$ , does not destroy the heavy quasiparticle. Next, we study the spectral function of the composite fermion at finite temperatures, for SU( $N$ ) generalizations of the KLM, as well as for ferromagnetic Kondo couplings, and compare our results to analytical calculations in the limit of high temperatures, large- $N$ , large- $S$ , and large  $J_k$ .

We also investigate the KLM on the honeycomb lattice and observe that the pole at the  $\Gamma=(0,0)$  point of the composite fermion spectral function gives way to incoherent weight below a critical value of  $J_k/W=0.1$  [2]. Our result provides an explicit example of a Kondo-breakdown transition within the magnetically ordered phase that sets in at  $J_k/W=0.22$ .

[1] B. Danu, Z. Liu, F. F. Assaad, and M. Raczkowski, Phys. Rev. B **104**, 155128 (2021).

[2] M. Raczkowski, B. Danu, and F. F. Assaad, in preparation.



# Surface interlayer coupling with a 2D Kondo lattice and bulk underdamped spin excitations in CeCo<sub>2</sub>P<sub>2</sub>

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In the surface region of strongly-correlated  $f$  materials, the electronic environment can be heavily modified with respect to the bulk leading to different properties and new energy scales. Using surface-sensitive angle-resolved photoemission spectroscopy (ARPES) on the P-terminated surface of the antiferromagnet CeCo<sub>2</sub>P<sub>2</sub>, we unveil the emergence of a subsurface two-dimensional Ce Kondo lattice, which couples ferromagnetically to the magnetically ordered Co sublattice [1]. In contrast to the  $4f$  physics observed at the surface, Ce in the bulk is passive and behaves tetravalently [2,3]. However, the symmetry breaking at the surface results in an effective magnetic field caused by an uncompensated ferromagnetic Co layer leading to a partial Ce  $4f$  occupation and spin-polarization in the subsurface layer which is observed in ARPES as a Ce  $4f$  admixture to the itinerant bands near the Fermi level. The temperature-dependent measurements reveal strong changes of the  $4f$  intensity at the Fermi level in accordance with the Kondo scenario.

While  $4f$  physics are absent in the bulk of CeCo<sub>2</sub>P<sub>2</sub>, instead large spin excitations on the Co sublattice can be observed with resonant inelastic X-ray scattering (RIXS) measurements. In contrast to most metallic systems, these spin excitations in the THz range show low damping and thus a weak electron-magnon interaction which is interesting for the field of magnonics where long lifetimes are desirable. We discuss these weakly damped magnons in comparison to the isostructural LaCo<sub>2</sub>P<sub>2</sub> where typical damping is observed.

[1] G. Poelchen *et al.*, ACS Nano **16**, 3573 (2022).

[2] M. Reehuis *et al.*, J. Alloys Comp. **266**, 54 (1998).

[3] K. Kliemt *et al.*, Cryst. Res. Technol. **55**, 1900116 (2020).

## Low temperature magnetic instabilities in ternary Kondo lattice $\text{YbPt}_5\text{B}_2$

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Numerous borides in many different material-families have been studied since decades, mainly because of an immense variety of ground states and sophisticated physical features that have been obtained, but also because of the vast range of daily-life-applications, reaching from steel to pharmaceuticals. Twenty years ago, in 2001,  $\text{MgB}_2$ , a binary boride with a quite simple hexagonal crystal structure, has been unexpectedly found as a high temperature superconductor ( $T_c \sim 40$  K).

Among the many families of borides, the rare earth (RE)-based ones are known for their diverse physical features like magnetically ordered phases, exotic types of ordering such as quadrupolar ordering, intermediate valence, Kondo-based or topologically protected materials, heavy fermion behavior or superconductivity in coexistence with long range magnetic order. Several of such features are observed in systems with  $\text{RE} = \text{Ce}, \text{Yb}$ , because of the respective unstable  $4f^1$  and  $4f^{13}$  electronic configurations.

Novel  $\text{YbPt}_5\text{B}_2$  and  $\text{LuPt}_5\text{B}_2$  (monoclinic, space group  $C2/m$ ) [1] have been synthesized by arc melting of constituent elements and annealed at 1020 K.  $\text{YbPt}_5\text{B}_2$  exhibits two magnetic phase transitions at  $T_{\text{mag}1} \sim 8$  K and  $T_{\text{mag}2} \sim 4$  K as deduced from specific heat, magnetostriction, electric resistivity and magnetization measurements, as well as two field induced phase transitions below  $T_{\text{mag}2}$ . Besides ordering, the ground state is governed by Kondo interactions in presence of strong crystalline electric field effects. The Kadowaki-Woods ratio of  $1.22 \cdot 10^{-5} \mu\Omega\text{cm}(\text{mol}\cdot\text{K}/\text{mJ})^2$  classifies  $\text{YbPt}_5\text{B}_2$  as a heavy fermion system. Nonmagnetic  $\text{LuPt}_5\text{B}_2$  is characterized by a simple metallic behavior.

[1] L. Salamakha *et al.*, Phys. Rev. B (2022), in press.

# Studying the Interplay of Magnetism and Superconductivity in the Heavy Fermion Compound $\text{Ce}_3\text{PtIn}_{11}$

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The properties of the heavy fermion compound  $\text{Ce}_3\text{PtIn}_{11}$  (tetragonal,  $P4/mmm$  structure) are enigmatic. At ambient pressure the compound displays two consecutive magnetic transitions into antiferromagnetic (AFM) states at  $T_{N1} = 2.2$  K and  $T_N = 2.0$  K, respectively. Below  $T_c = 0.32$  K superconductivity (SC) is found [1]. It has been speculated that the coexistence of AFM and SC results from the presence of two inequivalent Ce sites. The surrounding of the Ce1-ion is identical to Ce-atoms in  $\text{Ce}_2\text{TIn}_8$  with  $T$  being a transition element and is believed to be largely Kondo screened and responsible for SC. The Ce2-ion experiences a  $\text{CeIn}_3$ -like environment and hence, is assumed to order magnetically. Entropy analysis indeed conjectured this idea [1] and further support comes from  $^{115}\text{In}$  NQR experiments [2] revealing that the magnetic moment of Ce2 has to be 20 to 40 times larger than the moment of Ce1 [2,3]. More intriguing, in the NQR experiment a sudden drop of spin-relaxation rate  $1/T_1$  emerges upon entering the superconducting state suggesting a first order type of transition from the AFM state into the SC one [4]. Such would indicate a breaking of symmetry implying that magnetic order and superconductivity compete.

Here we discuss recent results on low temperature specific heat and magnetization measurements. In addition we conducted zero-field and longitudinal field  $\mu\text{SR}$  experiments from the paramagnetic state down to the SC state. The latter indicate the presence of a static or quasi-static internal field for  $T < T_c$ .

\*Samples were grown in MGML ([mgml.eu](http://mgml.eu)), which is supported within the program of Czech Research Infrastructures (project no. LM2018096)

[1] J. Prokleška, *et al.*, Phys. Rev. B **92**, 161114(R) (2015).

[2] H. Fukazawa *et al.*, Phys. Rev. B **102**, 165124 (2020).

[3] N. Shioda *et al.*, Phys. Rev. B **104**, 245119 (2021)

[4] S. Kambe *et al.*, Phys. Rev. B **101**, 081103(R) (2020).

# Specific heat of the kagome antiferromagnet herbertsmithite in high magnetic fields

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Herbertsmithite  $\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$  is an emblematic quantum spin liquid candidate because it is the closest materialization of the nearest neighbor  $S = 1/2$  kagome Heisenberg antiferromagnet ( $J \sim 190$  K) with a dynamical ground state. As main perturbations, we can mention copper ions on the zinc sites between the kagome planes and a finite out-of-plane Dzyaloshinskii-Moriya component ( $D_z \sim 0.06J$ ).

As a fundamental thermodynamic quantity, the low-temperature specific heat is a powerful probe of any low-energy excitation, which is both its strength and weakness. Indeed, for herbertsmithite in zero to moderate fields, the kagome contribution is masked by a contribution from magnetic defects.

The use of high magnetic fields allows us, for the first time, to get rid of this parasitic contribution and single out the kagome behavior. We show that this behavior is attributed to gapless excitations which are unaffected by the magnetic field, at variance with predictions for fermionic spinons. Our observations are well reproduced by state-of-the-art numerical methods but challenge all the existing models so far. The proposed spin liquid ground state remains enigmatic but our study provides a delimited path for future theoretical developments.

[1] Q. Barthélemy *et al.*, Phys. Rev. X **12**, 011014 (2022).

## Exotic critical points in a pure spin system $\text{SrCu}_2(\text{BO}_3)_2$

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We present exotic critical point-physics unveiled by the application of pressure and magnetic field on a geometrically frustrated quantum antiferromagnet  $\text{SrCu}_2(\text{BO}_3)_2$ , which is the near-exact realization of the paradigmatic Shastry–Sutherland model [1]. Combining high-precision specific-heat measurements and data interpretation with finite-temperature tensor-network methods we demonstrate that, as in water, the pressure–temperature phase diagram has a first-order transition line that separates phases with different local magnetic energy densities, and that terminates at an Ising critical point [2]. Our results further advance in the understanding of first-order quantum phase transitions in quantum magnetism, setting a benchmark for realization of strongly correlated electron materials with anisotropic spin interactions and topological properties.

\* J. L. J. acknowledges FAPESP-Young Investigator Grant (2018/08845-3).

[1] B. S. Shastry, et al. *Physica B+C* **108**, 1069 (1981).

[2] J. Larrea Jiménez *et al.*, *Nature* **592**, 370 (2021)

## Spin chirality induced by thermal fluctuations

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The term chirality originates from the word  $\chi\epsilon\acute{\iota}\rho$  - meaning *hand* in ancient Greek language. This term is used for the description of objects which, like a human hand, are distinguishable from their mirror reflection. In magnetic materials it refers to certain geometrical arrangements of spins, where magnetic moments are canted and have neither parallel nor antiparallel orientation. The resulting scalar spin chirality is the bridge between the microscopic details of the magnetic structure and the quantum-mechanical behavior of conduction electrons, whose anomalous motion can be directly measured in macroscopic samples through off-diagonal transport responses. Among these transport responses are electrical Hall and thermoelectric Nernst effects.

Apart from materials with static spin-chiral orderings, including skyrmionic systems, finite scalar spin chirality can be produced when averaging macroscopic ensembles of thermally fluctuating spins. The thermal averaging process can generate strong magneto-transport effects of quantum-mechanical origin, even far above the magnetic ordering temperature. We demonstrate this point in Nd<sub>3</sub>Ru<sub>4</sub>Al<sub>12</sub>, a highly metallic ferromagnet with breathing kagomé lattice structure [1]. Furthermore, we present a comparative analysis of the spin-chiral features in two model systems with distinct spin networks, namely in triangular and kagomé spin lattices. Our work illustrates the crucial role played by the geometry of the spin lattice in fostering spin-chiral phenomena induced by thermal fluctuations [2].

[1] K. K. Kolincio *et al.*, Proc. Natl. Acad. Sci. USA **118**, e2023588118 (2021).

[2] K. K. Kolincio *et al.*, submitted (2022).

# Directly Probing $S=1/2$ Chain Spinon Backscattering with Electron Spin Resonance

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The quantum spin chains are known to be fundamentally different from conventional antiferromagnets. For instance, in Heisenberg  $S=1/2$  chains the usual spin waves are replaced by pairs of fractionalized spinon excitations. These exotic fermionic quasiparticles are inevitably experiencing strong backscattering interaction in 1D geometry. Yet, this interaction is not directly manifest in the observables. The dramatic backscattering consequences for the dynamics of magnetized chains were realized only recently [1]: renormalization of the two-spinon continuum energies and emergence of a bound state, similar to Silin mode in conventional Fermi liquids. However, these details are challenging for observation, as they occur only in the magnetized state and at nonzero momenta. Here we demonstrate a direct measurement of the spinon continuum fine structure and associated backscattering interaction constant by means of Electron Spin Resonance [2]. This technique becomes an efficient spin dynamics probe at small non-zero momentum in the presence of Dzyaloshinskii-Moriya interaction, uniform between the sites of the chain. Such rare interaction pattern exists in our target material  $\text{K}_2\text{CuSO}_4\text{Br}_2$  [3,4]. The resulting ESR spectra are drastically different from the normal Larmor resonance, and exact solution-based quantitative analysis allows us to estimate the backscattering constant as  $2.38J$  in the Heisenberg exchange units. We also compare our results and the predictions of Renormalization Group approach [5].

\*This work has been supported by the SNSF Division II (ETHZ), the NSF CMMT grant DMR-1928919 (U. Utah), and the RSF Grant 17-12-01505 (Kapitza Institute).

- [1] A. Keselman, L. Balents, O. Starykh, *Phys. Rev. Lett.* **125**, 187201 (2020).
- [2] K. Povarov, T. Soldatov, R.-B. Wang *et al.*, arXiv:2108.02835 (2021) *accepted to PRL*.
- [3] M. Halg, W. Lorenz, K. Povarov *et al.*, *Phys. Rev. B* **90**, 174413 (2014).
- [4] A. Smirnov, T. Soldatov, K. Povarov *et al.*, *Phys. Rev. B* **92**, 134417 (2015).
- [5] S. Lukyanov, *Nucl. Phys. B* **522**, 533 (1998).

# Quantum fluctuations and tunable magnetic excitations in the two-dimensional honeycomb materials YbBr<sub>3</sub> and ErBr<sub>3</sub>

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Low-dimensional magnetism on the honeycomb lattice is expected to lead to a range of novel phases, some of which feature quantum spin liquid correlations or topological degrees of freedom. We studied two different van-der Waals rare-earth trihalides, YbBr<sub>3</sub> and ErBr<sub>3</sub>, using single-crystal neutron scattering to investigate the magnetic correlations and their excitations.

In YbBr<sub>3</sub> we find no magnetic order down to the lowest temperatures surveyed of about 100mK [1]. The correlations remain short-ranged, but feature relatively well-defined magnetic excitations. At the zone boundary of the reciprocal cell, we find broad continuum scattering as a function of wave-vector and energy that is consistent with hexagon plaquette quantum fluctuations. The magnetic excitations are the result of competing nearest and next-nearest antiferromagnetic exchange interaction that place YbBr<sub>3</sub> near a quantum critical point towards a quantum spin liquid phase.

In ErBr<sub>3</sub>, we find magnetic order below T=280mK and magnetic excitations that arise from purely dipolar magnetic interactions [2]. The magnetic ground state appears to include continuously degenerate non-collinear spin arrangements in the honeycomb plane. The magnon dispersion exhibit Dirac-like cones as long as time and inversion symmetry are respected, and a spin gap opening otherwise, with a finite Berry curvature near the Dirac points. These results illustrate that the spin-wave dispersion of magnetic dipoles on the honeycomb lattice may be reversibly controlled from a magnetic phase with Dirac cones to a topological phase with non-trivial magnon valley Chern numbers.

[1] C. Wessler et al. NPJ Quantum Materials **5**, 85 (2020).

[2] C. Wessler, B. Roessli, K.W. Krämer, U. Stuhr, A. Wildes, H.B. Braun and M.Kenzelmann, unpublished (2022).



# Phase degree of freedom and topological properties in multiple- $Q$ spin textures

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Topological spin textures, such as two-dimensional skyrmion lattices (SkLs) and three-dimensional hedgehog lattices (HLs) are approximately represented by superpositions of multiple spin density waves, and hence, called multiple- $Q$  spin textures. In such spin structures, the phase degree of freedom of the superposed waves plays an important role in the topological properties as well as the symmetry of the magnetic textures [1,2], but the systematic investigation has not been performed thus far.

In this study, we theoretically investigate the evolution of magnetic and topological properties in SkLs composed of three spin density waves ( $3Q$ -SkL) and HLs composed of four spin density waves ( $4Q$ -HL) while changing the phases as well as the magnetization [3]. By introducing a hyperspace to deal with the phase degree of freedom systematically, we find that the  $3Q$ -SkLs change their skyrmion number among -2, -1, 0, 1, and 2 depending on the phase and magnetization. In the case of the  $4Q$ -HLs, we obtain richer phase diagrams where the density and configuration of topological objects called hedgehogs and antihedgehogs change in a wide range. Our results of the complete phase diagrams for the phase shift provide good references to discuss how the actual systems experience the magnetic and topological transitions in an applied magnetic field.

[1] T. Kurumaji *et al.*, *Science* **365**, 914 (2019).

[2] S. Hayami, T. Okubo, and Y. Motome, *Nat. Commun.* **12**, 6927 (2021).

[3] K. Shimizu *et al.*, preprint (arXiv:2201.03290).

# **Axion electrodynamics induced $e/4$ fractional charge of a superconducting vortex**

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Fractional charge and coupled flux-charge quasiparticles are found in strongly correlated matter, such as fractional quantum Hall states.

The change in the topology across the surface of a strong topological insulator provides an extra  $E \cdot B$  coupling term in the effective action of electrodynamics, thereby called axion electrodynamics. A magnetic flux through the topological surface state is predicted to carry an electric charge. For a quantized superconducting flux,  $\phi_0 = h/2e$ , theory predicts a fractional charge of  $e/4$ .

We have experimentally realized Josephson junction arrays on top of thin film topological insulator  $B_{1-x}Sb_xTe_3$  and have performed interferometry of the Josephson vortex flow to measure the associated electric charge.

# Thermoelectric properties of topological chains coupled to a quantum dot

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Topological one-dimensional superconductors can sustain in their extremities zero energy modes that are protected by different kinds of symmetries. The observation of these excitations in the form of Majorana fermions is one of the most intensive quests in condensed matter physics. Their study is not only interesting in itself, but also because they have promising applications in the area of quantum computation. In this work we are interested in another class of one dimensional topological systems, namely topological insulators. These also present symmetry protected end modes with robust properties and do not require the low temperatures necessary for topological superconductivity. We consider the simplest kind of topological insulators, namely chains of atoms with hybridized sp orbitals. We study the transport properties of these chains in the trivial, non-trivial topological phases and at the quantum topological transition. We use a simple device consisting of two semi-infinite hybridized sp-chains connected to a quantum dot and obtain the thermoelectric properties of this system as a function of temperature and distance to the topological transition. We show that the electrical conductance and the Wiedemann-Franz ratio of the device at the topological transition have universal values at very low temperatures. The thermopower gives direct evidence of fractional charges in these systems.

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# Magnetic photocurrent response assisted by quantum geometry in solid

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The *photocurrent response* (photo-induced rectified current response) is of great interest in the light of basic science and engineering fields [1]. Apart from prototypical setups using a built-in asymmetric structure (e.g., p-n semiconductor junction), the response in bulk can appear due to the microscopic parity symmetry breaking. For instance, the photocurrent generation results from the noncentrosymmetric crystal structure and is strongly enhanced by the nontrivial quantum geometry found in such as (chiral) Weyl semimetals [2,3].

Numerous experimental and theoretical efforts have been devoted to the analysis of the photocurrent response of nonmagnetic materials. On the other, it has been scarcely investigated the role of time-reversal symmetry breaking of magnetic materials. Similar to the second-harmonic generation study [4], such *magnetic* photocurrent response may probe the magnetic symmetry in material and gets more tunable with the help of external magnetic fields.

Addressing this issue, we present a theory of photocurrent response enriched by magnetic parity breaking. We formulated the photocurrent response based on the established perturbation analysis and identified that nonmagnetic and magnetic photocurrent responses are distinguished by preserving antiunitary symmetries [5]. As a consequence of systematic classification, we predict the mechanism for circularly-polarized light-induced photocurrent which is the magnetic counterpart of the so-called shift mechanism [6]. We introduce the newly-discovered mechanism and demonstrate enhanced responses in a topological antiferromagnet [5] and a topological surface state [7].

\*This work was supported by JSPS KAKENHI Grants and by SPIRITS 2020 of Kyoto University.

[1] B. I. Sturman and V. M. Fridkin, *Photovoltaic and Photorefractive Effects in Noncentrosymmetric Materials* (Gordon and Breach, New York, 1992).

[2] J. Liu *et al.*, *Nat. Mater.* **19**, 830 (2020); J. Orenstein *et al.*, *Annu. Rev. Condens. Matter Phys.* **12**, 247 (2021).

[3] For theory, e.g., F. de Juan *et al.*, *Nat. Commun.* **8**, 15995 (2017).; J. Ahn *et al.*, *Phys. Rev. X* **10**, 041041 (2020).

[4] M. Fiebig *et al.*, *J. Opt. Soc. Am. B* **22**, 96 (2005).

[5] HW and Y. Yanase, *Phys. Rev. X* **11**, 011001 (2021)

[6] R. von Baltz and W. Kraut, *Phys. Rev. B* **23**, 5590 (1981); J. E. Sipe and A. I. Shkrebtii, *Phys. Rev. B* **61**, 5337 (2000).

[7] HW and N. Nagaosa, in preparation.

## Critical length scales at metal-insulator and magnetic oxide interfaces

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Atomically-engineered heterostructures constitute excellent model systems to investigate fundamental structure-property relations in transition metal oxides.

We will first focus on metal-insulator transitions (MITs). Despite their general interest, little is known about the characteristic lengths of the two phases involved. To that aim, we generate an artificially layered phase-separated system by alternating NdNiO<sub>3</sub> and SmNiO<sub>3</sub> layers, which undergo MITs at different temperatures in bulk. Transport measurements reveal that a minimum layer thickness of 3 nm is required to observe the two transitions separated; otherwise, the system behaves as one material with only one MIT. We show that this critical length scale is determined by balancing the energy cost of the boundary between a metal and an insulator and the bulk phase energies. [1]

The loss of the functionality of interest as the thickness is reduced to a few unit cells (u.c.) is another long-standing issue most oxides face. We show that films of La<sub>2</sub>NiMnO<sub>6</sub>, a ferromagnetic insulating double-perovskite [2], are still magnetic down to 2 u.c.. However, the magnetic properties of 2-5 u.c. La<sub>2</sub>NiMnO<sub>6</sub> films are affected beyond dimensionality effects due to an oxygen-vacancy-assisted electronic reconstruction occurring at the La<sub>2</sub>NiMnO<sub>6</sub>//substrate polar interfaces. By introducing a top electron-acceptor layer, the electron excess is redistributed, and the ferromagnetic properties of the ultrathin La<sub>2</sub>NiMnO<sub>6</sub> films are restored.

[1] C. Dominguez *et al.*, Nat. Mater. **19**, 1182 (2020)

[2] G. De Luca *et al.*, APL Mater. **9**, 081111 (2021)

# Coexisting charge-ordered states with distinct driving mechanisms in monolayer VSe<sub>2</sub>

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Thinning crystalline materials to two dimensions (2D) creates a rich playground for electronic phases, including charge, spin, superconducting and topological order. Bulk materials hosting charge density waves (CDWs), when reduced to ultrathin films, have shown CDW enhancement and tunability. However, charge order confined to only 2D remains elusive.

Here we report a distinct charge ordered state emerging in the monolayer limit of 1T-VSe<sub>2</sub>. Systematic scanning tunnelling microscopy experiments reveal that bilayer VSe<sub>2</sub> largely retains the bulk electronic structure, hosting a tri-directional CDW. However, monolayer VSe<sub>2</sub> exhibits a dimensional crossover, hosting two CDWs with distinct wavelengths. Electronic structure calculations reveal that while one CDW is bulk-like and arises from the well-known Peierls mechanism, the other is decidedly unconventional. The observed CDW-lattice decoupling and the emergence of a flat band suggest that the new CDW arises from enhanced electron-electron interactions in the 2D limit.

These findings establish monolayer-VSe<sub>2</sub> as the first host of coexisting charge orders with distinct origins, opening the door to tailoring electronic phenomena via emergent interactions in 2D materials.

[1] R. Chua, J. Henke, et al., *ACS Nano* **16**, 783 (2022). doi:[10.1021/acsnano.1c08304](https://doi.org/10.1021/acsnano.1c08304)

[2] J. Henke, F. Flicker, et al., *SciPost Phys* **9**, 056 (2020). doi:[10.21468/SciPostPhys.9.4.056](https://doi.org/10.21468/SciPostPhys.9.4.056)

[3] X. Feng, J. Henke, et al., *Phys. Rev. B* **104**, 165134 (2021). doi:[10.1103/PhysRevB.104.165134](https://doi.org/10.1103/PhysRevB.104.165134)

# Scanning tunneling microscopy and spectroscopy on rare-earth hexaborides\*

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The hexaborides of cubic structural type  $\text{CaB}_6$  ( $Pm\bar{3}m$ ) represent a very versatile class of compounds. The majority of the hexaborides with trivalent rare earths are highly conductive, with one charge carrier per rare-earth atom. Exceptions are divalent Eu and Yb resulting in materials with very low charge carrier densities, and  $\text{SmB}_6$  with intermediate valence.

Here we focus on  $\text{CeB}_6$ . At low temperatures, this compound features dense Kondo behavior, a complex magnetic phase diagram and quadrupolar order [1]. We use Scanning Tunneling Microscopy and Spectroscopy (STM/S) to gain local insight in the electronic structure of this material. A prerequisite for successful STS, however, are clean and atomically flat surfaces. To this end, we cleaved samples of  $\text{CeB}_6$  *in situ* and at low temperature. Similar to many other hexaborides,  $\text{CeB}_6$  is notoriously difficult to cleave and the resulting surfaces are surprisingly complex, despite the relatively simple crystallographic structure. In particular, we often encountered reconstructed surface areas. We compare the surface topographies to those obtained on  $\text{SmB}_6$  and  $\text{EuB}_6$  [2,3].

We also conducted STS on non-reconstructed surface areas (presumably of B termination) down to temperatures of 4.6 K. As expected for a dense Kondo system, the spectroscopic data can be described by a Fano resonance yielding a resonance width of the gap-like local conductance of about 42 meV, in line with earlier measurements on planar tunnel junctions [4].

\*This work is supported by the German Research Foundation, Project No. 449866704. Work at Los Alamos was supported by the Los Alamos Laboratory Directed Research and Development program through project 20220135DR.

[1] A. C. Cameron, G. Friemel and D. S. Inosov, Rep. Prog. Phys. **79**, 066502 (2016).

[2] S. Wirth *et al.*, Phys. Stat. Solidi B **258**, 2000022 (2021).

[3] S. Wirth and P. Schlottmann, Adv. Quantum Technol. **4**, 2100102 (2021).

[4] B. Amsler *et al.*, Phys. Rev. B **57**, 8747 (1998).

# X-ray diffraction as a useful tool to research strongly correlated electron systems.

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In strongly correlated systems, atoms can affect each other, for example by facilitating or preventing magnetic exchange coupling. Hence, knowledge of the precise position of atoms in the solid is imperative to understanding and predicting physical properties. X-ray diffraction (XRD) is THE method of choice to research atomic arrangements in the solid. It has been available for decades and is therefore highly developed to answer a plethora of research questions with the bonus of being non-destructive.

We discuss what can be learned from XRD in general and examine the following two cases in detail.

In a publication by Jia et al. [1] XRD is employed to exclude a connection between structure and physical properties. While a study by Bao et al. [2] applies XRD to correlate physical properties with the crystal structure. Both works use XRD as a natural given in their selection of analysis methods, highlighting its importance in the field of solid-state physics.

Finally, we will explore what STOE & Cie GmbH has to offer you in terms of high-quality XRD equipment.

## References:

[1] S. Jia, N. Ni, G. D. Samolyuk, A. Safa-Sefat, K. Dennis, H. Ko, G. J. Miller, S. L. Bud'Ko, P. C. Canfield, *Phys. Rev. B*, **2008**, 77, 104408.

[2] J-K. Bao, D. E. Bugaris, H. Zheng, K. Willa, U. Welp, D. Young Chung, M. G. Kanatzidis, *Phys. Rev. Mater.*, **2019**, 3, 024802.



## **Two-axis rotator “Rotax”: Out of the lab – for the lab**

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The exact angular alignment of sample materials for the determination of their physical properties under cryomagnetic and other extreme environmental conditions is often difficult. In many experimental setups, the samples to be examined cannot be aligned directly because they are installed in a complex sample environment, and, thus, can only be aligned precisely by remote control. Nevertheless, a realization of all possible orientations is often required - with an available sample space that is usually only the size of a thimble.

At the Helmholtz-Zentrum Dresden-Rossendorf (HZDR), we have developed the "Rotax", a patented, filigree two-axis rotator that can do just that. The special feature of our Rotax is the simultaneous controllability of two rotational axes that are at right angles to each other and can be moved independently of each other. This makes it possible to precisely align the samples under investigation in a confined space for any orientation, e.g., with respect to an external magnetic field.

In my presentation, I will discuss the capabilities as well as some of the possible scientific applications of the Rotax, and also how we realized the technology transfer at the HZDR that ultimately allowed us to make the Rotax available to the scientific community as a commercial product through the HZDR Innovation GmbH.

# **New Developments in Deflector Analyzer Technology for ARPES**

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Electron-optical deflectors in the lenses of hemispherical analyzers have been changing the data acquisition strategies of ARPES significantly. Among other benefits, keeping the experimental conditions constant (the sample light geometry stays fixed) and enhanced acquisition precision (no mechanical movement is involved) have increased the data quality and acquisition speed. However, several aspects of the electron-trajectory manipulation have been unaddressed so far, such as field inhomogeneities in the deflector sections and distortions induced by deflecting the angular image. We present a new type of deflector technology for APRES measurements, enhancing the deflector precision and simultaneously overcoming existing limitations of deflector analyzers, such as angular acceptance, reliability of mechanical parts and electron optical distortions. We have characterized the analyzer in lab-based environments using well established standard samples and compared the results to cutting edge literature from synchrotron experiments.

## Customised system solutions for thin film research

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DEMCON TSST BV is a scientific instrumentation company specialized in custom designed, innovative thin-film deposition equipment with a focus on Pulsed Laser Deposition (PLD) equipment and complementary components such as high pressure RHEED and heating and target stages for upgrading existing systems. We share knowledge on thin-film growth by maintaining close relations with the scientific community, organizing courses and providing instructions on the client's systems.

Besides growth on conventional small samples, TSST offers system solutions for PLD growth on wafer scale, ensuring highly flexible PLD parameter tunability. The development of this wafer scale system solution follows from our extensive research on our experimental wafer scale PLD system, which is used to investigate and optimize growth of many complex oxides on 4" silicon wafers. Next to optimising plume scanning for homogeneous growth, suitable buffer layers have been optimised for epitaxial growth of epitaxial oxides[1].

From our expertise in all aspects of PLD film growth, we understand the importance of obtaining insight in fundamental growth characteristics, including initial nucleation processes at the surface of the sample. We are currently developing an in situ SPM tool, easily mounted to any deposition system, allowing SPM measurements during film growth. A sample is quickly and reproducibly moved between deposition position and SPM tip position, allowing SPM measurements even after a single PLD pulse, while the sample remains in growth deposition conditions, temperature and gas environment. We will outline the latest status of the development of this unique thin film growth characterisation solution.

[1] D. Pullini et al, ACS Appl. Mater. Interfaces, 9 (2017)

## Edge states and Charge density wave orders in $UTe_2$

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In the ongoing search for new phases of matter, the heavy fermion superconductor  $UTe_2$  which combines strong correlations and unconventional triplet-superconductivity with possible non-trivial topology, is an extremely promising system. In this talk I present scanning tunneling microscopy (STM) data on  $UTe_2$ . The STM data reveal signatures of coexisting Kondo effect and superconductivity which show competing spatial modulations within one unit-cell. STM spectroscopy at step edges show signatures of chiral in-gap states, predicted to exist at the boundaries of a topological superconductor. In addition, spatially resolve spectroscopic maps reveal multiple incommensurate charge density wave (CDW) orders. Interestingly, the CDW orders appear to be intertwined with superconductivity. I will discuss a possible explanation for this unusual CDW, by considering a Ginzburg-Landau theory of a superconductor with the symmetries of  $UTe_2$  coexisting with two triplet pair density wave (PDW) states. This theory naturally gives rise to daughter CDWs which would be sensitive to magnetic field due to their origin in a triplet PDW state.

\* The STM work at the University of Illinois was supported by DOE under Grant- DE-SC0022101 and Gordon and Betty Moore foundation EPiQS grant #9465.

[1] Lin Jiao et al., Nature 579, 523-527 (2020)

# Parity transition, parity violation, and topological superconductivity in $UTe_2$ and $CeRh_2As_2$

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Symmetry and topology are fundamental properties of quantum phases. I will discuss exotic superconductivity in  $UTe_2$  and  $CeRh_2As_2$ , focusing on symmetry, topology, and quantum criticality. Space inversion symmetry and time-reversal symmetry are essential for superconductors, and breaking either of them is a route to realizing topological superconductivity.

Traditionally, superconductivity has been classified based on the space inversion parity, as spin-singlet (spin-triplet) Cooper pairs lead to the even-parity (odd-parity) superconductivity in the usual setup. However, the recent discovery of two superconducting phases in  $CeRh_2As_2$  [1] renewed such traditional understanding, as the sublattice-antisymmetric Cooper pairs allow odd-parity spin-singlet superconductivity in locally noncentrosymmetric crystals. Consistent with the theoretical prediction [2], the phase diagram indicates the even-odd parity transition in superconducting  $CeRh_2As_2$ . I will review theoretical studies triggered by the experimental discovery [3] and predict topological superconductivity based on the first-principles band structure calculation [4].

I will discuss the symmetry and topology of superconductivity in  $UTe_2$  [5,6] based on the GGA+U band structure calculation [7] and an effective 24-band periodic Anderson model [8]. The Ising ferromagnetic spin correlation changes to antiferromagnetic when the c-f hybridization increases. Accordingly, the Eliashberg theory shows spin-singlet superconductivity and spin-triplet superconductivity. Interestingly, the spin-triplet superconductivity can be stabilized by antiferromagnetic fluctuation. Based on the results, experimentally observed multiple superconducting phases are interpreted, and topological superconductivity is predicted.

In  $CeRh_2As_2$  and  $UTe_2$ , spontaneous parity violation due to either magnetism or superconductivity has been proposed. I will discuss the mechanism and clarify some phenomena related to the parity violation.

[1] S. Khim *et al.*, *Science* **373**, 1012 (2021).

[2] T. Yoshida, M. Sigrist, and Y. Yanase, *Phys. Rev. B* **86**, 134514 (2012).

[3] For a review, M. H Fischer, M. Sigrist, D. F. Agterberg, Y. Yanase, arXiv:2204.02449.

[4] K. Nogaki, A. Daido, J. Ishizuka, Y. Yanase, *Phys. Rev. Research* **3**, L032071 (2021).

[5] S. Ran *et al.*, *Science* **365**, 684 (2019).

[6] For a review, D. Aoki *et al.*, *J. Phys.: Condens. Matter* **34**, 243002 (2022).

[7] J. Ishizuka, S. Sumita, A. Daido, Y. Yanase, *Phys. Rev. Lett.* **123**, 217001 (2019).

[8] Jun Ishizuka, Youichi Yanase, *Phys. Rev. B* **103**, 094504 (2021).

# Kitaev spin liquid materials as a Majorana platform

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The Kitaev model provides a canonical example of quantum spin liquids in more than one dimension, with the exact solution of the ground state and fractional Majorana excitations [1]. Since the proposal by Jackeli and Khaliullin [2], tremendous efforts have been made to realize it in materials [3]. While the recent discovery of half quantization of the thermal Hall conductivity in a candidate  $\alpha$ - $\text{RuCl}_3$  supports the existence of Majorana excitations [4], further exploration of the platform of the Kitaev spin liquid and the manipulation of fractional excitations is crucial for not only deeper understanding of quantum spin liquids but also their application to topological quantum computation. In this talk, we will highlight our recent efforts on the following topics in this direction: (i) a new candidate, iridium ilmenites  $A\text{IrO}_3$  ( $A=\text{Mg}$  and  $\text{Zn}$ ) [5], (ii) feasibility in ultracold polar molecules [6], (iii) higher-spin Kitaev spin liquids [7], and (iv) control of vortex excitations [8].

This work has been done in collaboration with K. Fukui, S.-H. Jang, Y. Kato, and J. Nasu.

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[1] A. Kitaev, *Ann. Phys. (NY)* **321**, 2 (2006).

[2] G. Jackeli and G. Khaliullin, *Phys. Rev. Lett.* **102**, 017205 (2009).

[3] For a review, see Y. Motome and J. Nasu, *J. Phys. Soc. Jpn.* **89**, 012002 (2020).

[4] Y. Kasahara *et al.*, *Nature* **559**, 227 (2018); T. Yokoi *et al.*, *Science* **373**, 568 (2021).

[5] S.-H. Jang and Y. Motome, *Phys. Rev. Materials* **5**, 104409 (2021).

[6] K. Fukui, Y. Kato, J. Nasu, and Y. Motome, preprint (arXiv:2204.06144).

[7] K. Fukui, Y. Kato, J. Nasu, and Y. Motome, in preparation.

[8] S.-H. Jang, Y. Kato, and Y. Motome, *Phys. Rev. B* **104**, 085142 (2021).

# Topological phases in kagome-based materials

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The recent surge of interest in kagome materials, often discussed in the context of frustrated magnetism and spin liquid phases, has been boosted by the discovery of the kagome metals AV<sub>3</sub>Sb<sub>5</sub> (A=K,Rb,Cs) undergoing successive charge density wave (CDW) and superconducting transitions upon lowering temperature. Recent experimental findings have reported the presence of unconventional charge orders in the enlarged (2×2) unit-cell of kagome metals AV<sub>3</sub>Sb<sub>5</sub> (A=K,Rb,Cs) and hinted towards specific topological signatures. In this talk I will discuss the types of topological phases that can be realized in such kagome materials by considering extended Hubbard models with inclusion of electron-phonon interactions [1] and will introduce a recently developed statistical method to predict topological phases in quantum materials [2,3].

This work has been done in collaboration with Francesco Ferrari, Thomas Mertz, Paul Wunderlich, Federico Becca and Shinibali Bhattacharyya.

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[1] F. Ferrari, F. Becca, R. Valenti, arXiv: 2204.10328

[2] T. Mertz, P. Wunderlich, S. Bhattacharyya, F. Ferrari, npj Comput. Mater. 8, 66 (2022)

[3] T. Mertz, R. Valenti, PRR 3, 013132 (2021)

# Computing exchange anisotropy in a half-filled $e_g$ system from Wannier tight-binding model

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Anisotropic interactions due to spin-orbit coupling in Mott-insulators give rise to complex spin structures. However, computation of a full spin Hamiltonian, including all anisotropic interactions from first-principle electronic structure calculations is a difficult problem. In this talk, combining the general form of transfer integrals and superexchange theory, we derive the analytical expression for the spin Hamiltonian, including Dzyaloshinskii-Moriya interaction and traceless symmetric anisotropy in a half-filled  $e_g$  model [1-3].

The result is applied to multiferroic  $\text{Ni}_3\text{TeO}_6$  that is a half-filled  $e_g$  magnet ( $S=1$ ) and may possess considerable anisotropic spin interactions due to strong spin-orbit coupling on Te atoms. All the magnetic parameters are calculated from the DFT-derived Wannier tight-binding Hamiltonian for  $e_g$  (two-orbital) model using mean field Coulomb interaction parameters  $U$  and  $J$ .

[1] T. Moriya, Phys. Rev. **120**, 91 (1960).

[2] L. Shekhtman, O. Entin-Wohlman, and A. Aharony, Phys. Rev. Lett. **69**, 836 (1992).

[3] T. Yildirim, A. B. Harris, A. Aharony, and O. Entin-Wohlman, Phys. Rev. B **52**, 10239 (1995).



# Theory of infrared absorption and Raman spectroscopy for orbital wave

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In LaMnO<sub>3</sub>, the interpretation of the phonon spectra remains as a long-standing debate after the collective orbital excitation (orbital wave) was suggested as the possible origin of the resonant peaks of the Raman scattering spectrum [1,2]. The orbital wave assignment has been regarded as a skeptical idea and the most critical point of the skepticism is how the orbital wave resonance are active both in Raman scattering and in the infrared conductivity. The rule of symmetry says that the vibrational modes of a centrosymmetric material should be either Raman active or infrared active but not both. Yet in LaMnO<sub>3</sub>, the 'orbital wave' resonances around 130~150 meV are active both in Raman and infrared spectrum. Furthermore, the resonance peak around 76 meV (~19 THz) in the stimulated Raman scattering spectrum shows strong light polarization dependence, which is another observation that should be explained by the orbital wave theory if the theory is correct. In the presentation, we will show the polarization-dependent Raman scattering cross-section spectra of LaMnO<sub>3</sub> calculated by using the orbital wave model [3]. We will also present the infrared conductivity spectrum of LaMnO<sub>3</sub> based on the same orbital wave model. Also we will show the stimulated Raman scattering spectra (experiment and theory) calculated by the same model considering the coupling between the orbital and the Jahn-Teller lattice distortion. We will demonstrate that the orbital wave model can answer to the long-standing debate about the reason why the Raman scattering and the infrared conductivity can be both active. Also we will explain the strong light polarization observed in the laser pulse pump-probe experiment by using the same model consistently.

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[1] E. Saitoh, S. Okamoto, T. K. Takahashi, K. Tobe, K. Yamamoto, T. Kimura, S. Ishihara, S. Maekawa, and Y. Tokura, *Nature* 410, 180 (2001); E. Saitoh, S. Okamoto, K. Tobe, K. Yamamoto, T. Kimura, S. Ishihara, S. Maekawa, and Y. Tokura, *ibid.* 418, 40 (2002).

[2] M. Grüninger, R. Rückamp, M. Windt, P. Reutler, C. Zobel, T. Lorenz, A. Freimuth, and A. Revcolevschi, *Nature* 418, 39 (2002).

[3] P. Munkhbaatar, and K. Myung-Whun, Orbital wave in the Raman scattering cross section of LaMnO<sub>3</sub>, *Phys. Rev. B* 97, 085101(2018)A. Author *et al.*, *Phys. Rev. B* 1, 1 (2020).

# Spin-orbital dynamics of localized electrons

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Multi-orbital systems, such as the  $d$ -electron systems, have various interesting physical properties since the spin-orbital degrees of freedom are entangled through the Coulomb interaction and spin-orbit coupling. In particular for  $5d$ -electronic systems, which host atoms having a large atomic number, the energy scales of the Coulomb interaction and the spin-orbit coupling are comparable, leading to rich physical phenomena, such as the cross correlation [1]. When we perform the material-based theoretical research, we should use the parameters obtained from first-principles calculation, and also should treat the Coulomb interaction and the spin-orbit coupling accurately, although it is highly difficult because of the huge computational cost. In the strongly correlated limit, however, the electrons are localized, and we can treat both of them at a reasonable numerical cost. In the case of the multi-orbital system, it is known as the Kugel-Khomskii model [2].

In the present study, we aim to analyze the ordered state of multi-orbital systems under the strongly correlated limit by constructing the effective model combined with the band structure. We established the framework to automatically construct the localized effective model for general multi-orbital systems by applying the perturbation theory using the matrix operations [3]. In the presentation, we will show the procedure of our analysis on pyrochlore oxides,  $\text{Cd}_2\text{B}_2\text{O}_7$ , which we have taken  $B=\text{Os}$ , as a test calculation. In addition, we show the result of the analysis using the mean field theory as well as the classical Monte Carlo simulation for the constructed model [4].

[1] for example, G. Cao and P. Schlottmann, Rep. Prog. Phys. **81**, 042502 (2018).

[2] K. I. Kugel and D. I. Khomskii, Zh. Eksp. Teor. Fiz. **64**, 1429 (1973) [Sov. Phys. JETP **37**, 725 (1973)].

[3] R. Iwazaki and S. Hoshino, Phys. Rev. B **103**, 235145 (2021).

[4] R. Iwazaki, H. Shinaoka and S. Hoshino, in preparation.

# Muon spin relaxation ( $\mu$ SR) studies on the heavy-fermion superconductor $\text{CeRh}_2\text{As}_2$

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We study the magnetic and superconducting (SC) properties of the unconventional heavy-fermion superconductor  $\text{CeRh}_2\text{As}_2$  [1,2] using muon spin rotation/relaxation ( $\mu$ SR) experiments. Zero-field  $\mu$ SR time spectra do not show any clear evidence of oscillations or an initial drop down to 0.27 K, but the deduced relaxation rate moderately increases below  $\approx 0.4$  K. This increase could potentially be associated with the suggested quadrupolar density wave order at  $T_0 \sim 0.4$  K [3], while the absence of any oscillations makes it unlikely that the order at  $T_0$  is due to a simple dipolar ordering. In transverse-field (TF) measurements, we observe a pronounced increase in the relaxation rate ( $\sigma_{\text{SC}}$ ) below  $T_c \approx 0.29$  K, in accordance with the onset of bulk superconductivity. Interestingly  $\sigma_{\text{SC}}$  becomes independent of temperature for  $T/T_c < 0.2$ , which is indicative of a fully gapped SC order parameter. Furthermore, TF- $\mu$ SR under an external field of 2 T shows a large exponential relaxation in the normal state above  $T_c$ . The corresponding relaxation rate  $\Lambda$  follows a power-law-like temperature dependence  $\Lambda \propto T^{-0.35}$  below 4 K, possibly connected to strong critical fluctuations [4]. Our observations suggest  $\text{CeRh}_2\text{As}_2$  to be a fully-gapped SC in the vicinity of a quantum critical point.

[1] S. Khim *et al.*, Science **373**, 1012 (2021).

[2] M. Kibune *et al.*, Phys. Rev. Lett. **128**, 057002 (2022).

[3] D. Hafner *et al.*, Phys. Rev. X **12**, 011023 (2022).

[4] S. Kitagawa *et al.*, J. Phys. Soc. Jpn. **91**, 043702 (2022).

## Interplay of superconductivity and magnetism in $\text{YbRh}_2\text{Si}_2$

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We report an electrical transport study of superconductivity of the heavy fermion metal  $\text{YbRh}_2\text{Si}_2$  [1]. High-resolution low-dissipation SQUID-based techniques were developed to measure the complex sample impedance down to 0.3 mK. This material is characterised by strong magnetic anisotropy and hyperfine interaction of its  $^{171}\text{Yb}$  and  $^{173}\text{Yb}$  isotopes. The superconductivity emerges from an antiferromagnetic Fermi liquid. A rich phase diagram is observed in magnetic field, applied both in the *ab* plane of the tetragonal crystals and along the *c* axis. Superconductivity beyond the Pauli limit for both field orientations points towards spin-triplet Cooper pairing. The existence of several distinct transport regimes, inferred from four transport signatures, opens the intriguing possibility of multiple superconducting phases. One of these signatures, an abrupt transition between two superconducting regimes with different sample inductance at  $T_A \approx 2$  mK, coincides with electro-nuclear magnetic transition, observed with calorimetry [2]. Below  $T_A$  a re-entrant resistive state is induced by magnetic field; above  $T_A$  re-entrant superconductivity manifests in fields close to the critical field of antiferromagnetism. Together these results demonstrate close interplay between the electro-nuclear magnetism and superconductivity and suggest spin-fluctuation-mediated Cooper pairing tunable with magnetic field.

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[1] E. Schuberth *et al.*, *Science* **351**, 485 (2016).

[2] J. Knapp *et al.*, this conference.

# Electronic states and superconductivity in UTe<sub>2</sub>

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Unconventional superconductivity of the heavy fermion paramagnet UTe<sub>2</sub> is one of the hottest topics in the strongly correlated electron systems[1]. Superconductivity occurs below  $T_c=1.5-2\text{K}$  with the large specific heat jump, indicating the strong coupling regime. The huge and anisotropic upper critical field  $H_{c2}$  resembles those observed in the ferromagnetic superconductors URhGe and UCoGe. However, the ferromagnetic fluctuations in UTe<sub>2</sub> are not experimentally established, instead the antiferromagnetic fluctuations with the incommensurate  $q$ -vector is directly observed in the inelastic neutron scattering experiments. One of the highlights of UTe<sub>2</sub> is the field-reentrant superconductivity, which appears up to  $H_m=35\text{T}$ , when the field is applied along the hard magnetization  $b$ -axis in the orthorhombic structure. Another remarkable point is the multiple superconducting phases under pressure, indicating the different superconducting order parameters. These significant properties are consistent with the spin-triplet state, which has the spin and orbital degree of freedom. A key experimental target is to determine the Fermi surface properties by means of the quantum oscillations experiments using high quality single crystals. In this talk, we review our recent results on UTe<sub>2</sub>. The focus is given on Fermi surfaces, multiple superconducting phases, and field-induced superconductivity. This work was done in collaboration with G. Knebel, D. Braithwaite, A. Pourret, J. P. Brison, Q. Niu, M. Valiska, G. Lapertot, S. Raymond, J. Flouquet, D.X. Li, F. Honda, A. Nakamura, Y. Shimizu, Y. Homma, Y. J. Sato, M. Kimata, A. Miyake, C. Paulsen, W. Knafo, I. Sheikin, H. Harima, Y. Yanase, Y. Haga, and H. Sakai.

[1] see a review paper, for example, D. Aoki, J. P. Brison, J. Flouquet, K. Ishida, G. Knebel, Y. Tokunaga, and Y. Yanase, *J. Phys.: Condens. Matter* 34, 243002 (2022).

## Field-induced superconducting phases in $\text{UTe}_2$

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$\text{UTe}_2$ , recently discovered to be superconducting [1,2], belongs to the rare class of superconductors presenting several different superconducting phases: this has been well established at finite pressures [3], and was long suspected at zero pressure owing to the behavior of the upper critical field, and the appearance of a re-entrant superconducting phase in the (partially) polarized phase, above the metamagnetic transition [4]. Moreover,  $\text{UTe}_2$  has also been claimed to present a double superconducting transition in zero field, required to explain a possible time-reversal symmetry breaking in the superconducting phase [5].

Here, based on our new thermodynamic measurements at ambient pressure up to 36T [6] showing clear evidence for two different superconducting phases at finite fields along the hard b-axis, we discuss the possible mechanisms for these different phases. We will explain the constraints imposed by these new experimental results, and their relation with the theoretical proposals for ambient and finite pressure phase diagrams [7,8,9], and notably the possible competition of spin-triplet and spin-singlet order parameters [9].

Last, we will discuss a possible mechanism for the field re-entrant phase in the polarized regime, inspired by the proposed mechanism for the field-reinforced phase along the b-axis.

[1] S. Ran et al. *Science* **365**, 684 (2019).

[2] D. Aoki, et al. *J. Phys. Soc. Jpn.* **88**, 043702 (2019).

[3] D. Aoki et al., *J. Phys. Condens. Matter* **34**. 243002 (2022).

[4] S. Ran, et al., *Nature Phys.* **15**, 1250 (2019)

[5] I.M. Hayes et al., *Science* **373**, 797 (2021).

[6] A. Rosuel et al., *ArXiv* (2022).

[7] J. Ishizuka and Y. Yanase, *Phys. Rev. Lett.* **123**, 217001 (2019).

[8] T. Shishidou et al. *Phys. Rev. B* **103**, 104504 (2021).

[9] J. Ishizuka et al. *Phys. Rev. B* **103**, 094504 (2021).

# First-order metamagnetic transition in UTe<sub>2</sub> studied by magnetostriction measurements

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The first-order metamagnetic transition of spin-triplet superconductor UTe<sub>2</sub> was studied thermodynamically. We revealed a discontinuous change in magnetostriction along all the principal orthorhombic axes across the metamagnetic transition at  $\mu_0 H_m \approx 35$  T for  $H \parallel b$ . The resultant volume magnetostriction changes discontinuously by  $\Delta V/V \approx -5.9 \times 10^{-4}$  at  $H_m$ . The initial pressure dependence of  $H_m$  estimated by the Clausius-Clapeyron's equation with  $\Delta V/V$  and the change in magnetization  $\Delta M \approx 0.5 \mu_B/U$  agrees with previous pressure measurements [1, 2, 3]. Further, significant anisotropic magnetostriction (AMS), derived by subtracting the averaged linear magnetostriction, was revealed. Contrary to the weakly field-dependent AMS along the  $a$ -axis, those along the  $b$  and  $c$  axes show strong field dependences with similar magnitude but opposite signs, indicating its lattice instability at  $H_m$ . The relationship between characteristic energy scales of magnetic fields and temperatures was discussed in terms of the Grüneisen parameters and compared to the other  $f$ -electron systems. The volume shrinkage in UTe<sub>2</sub> at  $H_m$  pushes to invoke the link with the valence instability related to the itinerant-localized dual nature of the U magnetism.

[1] A. Miyake *et al.*, J. Phys. Soc. Jpn. **88**, 063706 (2019).

[2] A. Miyake *et al.*, J. Phys. Soc. Jpn. **90**, 103702 (2021).

[3] G. Knebel *et al.*, J. Phys. Soc. Jpn. **89**, 053707 (2020).

# Spin-susceptibility behavior in Uranium-based Superconductor UTe<sub>2</sub> investigated with Knight-shift measurements

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UTe<sub>2</sub> is a recently-discovered superconductor with a superconducting (SC) transition temperature ( $T_c$ ) of 1.6 ~ 2.0 K[1,2]. Although UTe<sub>2</sub> does not exhibit ferromagnetism, it is considered as an end member of ferromagnetic (FM) superconductors owing to their similar physical characteristics, such as Ising anisotropy in the magnetic susceptibility, the phenomenon of SC upper critical field ( $H_{c2}$ ), and superconductivity boosted by a magnetic field ( $H$ ) above 20 T for  $H \parallel b$  (magnetic hard axis) *etc.* Thus, UTe<sub>2</sub> is anticipated to be a spin-triplet superconductor, similar to the FM superconductors[3].

In order to determine the SC order parameter, we measured Knight shifts in a low magnetic field  $H$  along the three crystalline axes, and reported that the dominant SC state is determined to be  $B_{3u}$ , in which the spin component of the SC pairing is along the  $a$  axis[4-6]. Thus, we claimed that UTe<sub>2</sub> is a spin triplet superconductor with the spin degrees of freedom. The important issue to be clarified is how the remaining spin degrees of freedom behave under strong magnetic field.

To investigate superconductivity boosted by  $H \parallel b$  above 20 T[7,8], we performed *in-situ*  $\chi_{AC}$  and Knight-shift measurement up to 24.8 T. We found the bulk superconductivity in the high- $H$  (HH) SC state and that the normal-state behavior continues to the HHSC state, implying unchanged spin susceptibility in the HHSC state. We discuss possible SC state in the HHSC state based on our experimental results.

[1] S. Ran *et al.*, Science **365**, 684 (2019).

[2] D. Aoki *et al.*, J. Phys. Soc. Jpn. **88**, 043702 (2019).

[3] D. Aoki *et al.*, arXiv 2110.10451.

[4] G. Nakamine *et al.*, J. Phys. Soc. Jpn. **88**, 113703 (2019).

[5] G. Nakamine *et al.*, Phys. Rev. B **103**, L100503 (2021).

[6] H. Fujibayashi *et al.*, J. Phys. Soc. Jpn. **91**, 043705 (2022).

[7] G. Knebel *et al.*, J. Phys. Soc. Jpn. **88**, 063707 (2019).

[8] S. Ran *et al.*, Nature Physics **15**, 1250 (2019).



# Magnetotransport of pyrochlore spin ice $\text{Sm}_2\text{Ir}_2\text{O}_7$ across the pressure-induced quantum-critical phase boundary

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The family of rare-earth pyrochlore iridates  $\text{Ln}_2\text{Ir}_2\text{O}_7$  comprise an ideal environment for investigating fundamental magnetism and correlated-electron physics. In addition to the all-in-all-out (AIAO) magnetism of the Ir ions, and associated metal-insulator transition, the rare-earth sublattice in these materials may also show interesting and correlated behavior. In  $\text{Dy}_2\text{Ir}_2\text{O}_7$  and  $\text{Ho}_2\text{Ir}_2\text{O}_7$ , the large rare-earth Ising moments are constrained along their local [111] axes and are coupled ferromagnetically via dipolar interactions, promoting spin-ice physics and the appearance of magnetic monopole quasiparticles.

We have measured the transport and magnetotransport properties of single-crystal  $\text{Sm}_2\text{Ir}_2\text{O}_7$  for the first time, then tuned them up to and beyond the pressure-induced quantum critical point for AIAO Ir order suppression at  $p_c = 63$  kbar previously identified by resonant X-ray scattering [1]. Contrary to prior predictions, we do not find a crossover from insulating to metallic behavior at low temperatures above  $p_c$ .

Instead, the metal-insulator transition temperature, which tracks the decrease in the AIAO ordering temperature for pressures up to 30 kbar, begins to increase under further application of pressure, pointing to the presence of an additional localization mechanism. The behavior of magnetotransport does track the Ir magnetism, however, with a strong hysteresis observed only within the AIAO phase boundary, similar to that found for  $\text{Ho}_2\text{Ir}_2\text{O}_7$  and attributed to plastic deformation of Ir domains [2].

Around  $p_c$  a new type of electronic behavior emerges, characterized by negative magnetoresistance with small hysteresis at the lowest temperatures, and hysteresis-free positive magnetoresistance above 5 K. The results are discussed in light of the Weyl semimetal and quadratic-band-touching phases predicted to occur in the vicinity of the quantum critical point.

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[1] Y. Wang, T. F. Rosenbaum, D. Prabhakaran, A. T. Boothroyd, and Y. Feng, *Physical Review B* 101, 220404(R) (2020).

[2] M. J. Pearce, K. Götze, A. Szabó, T. S. Sikkenk, M. R. Lees, A. T. Boothroyd, D. Prabhakaran, C. Castelnovo, and P. A. Goddard, *Nature Communications* 13, 444 (2022).

# Pressure-induced quantum critical point of a strong coupling charge density wave order in a $2H\text{-Pd}_{0.05}\text{TaSe}_2$ superconductor

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## Abstract

Although charge density wave (CDW) order and superconductivity (SC) are often found in quasi-two-dimensional metals, the relationship between the two phenomena, as well as the nature of the CDW itself, remains a subject of debate. Here, we address these long-standing issues by demonstrating a pressure-induced CDW quantum critical point (QCP) in a  $2H\text{-Pd}_{0.05}\text{TaSe}_2$  single crystal with  $T_{\text{CDW}} = 115$  K and a superconducting transition temperature  $T_c = 2.6$  K. Upon applied pressure, the  $T_{\text{CDW}}$  indicated by an anomaly in the in-plane resistivity shift towards lower temperature to  $P_c = 21.5$  GPa. Accordingly, a negative drop in the Hall coefficient due to the Fermi surface reconstruction disappears above  $P_c$ , indicating a CDW QCP of  $T_{\text{CDW}} = 0$  K at  $P_c$ . Furthermore, the pressure dependence of the two-phonon Raman mode unravels a strong correlation between local lattice distortions and the CDW order, supporting that the local lattice distortions at high temperature act as a precursor to the CDW phase. In contrast to the suppression of the CDW order, analysis of low-temperature resistivity measured at 9 T field exhibits a factor 5 enhancement of the quadratic power-law coefficient, indicating a large increase of the electronic density of states near the CDW QCP. Correspondingly, a superconducting dome is found with a maximum  $T_c = 8.5$  K. Our findings coherently suggest that the increase in the electronic density of states near the CDW QCP should be a key to reaching the maximum  $T_c$  in  $2H\text{-Pd}_{0.05}\text{TaSe}_2$ .

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## Isotopically pure YbRh<sub>2</sub>Si<sub>2</sub> single crystals with <sup>171</sup>Yb, <sup>173</sup>Yb, and <sup>174</sup>Yb

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A central question in strongly correlated electron systems concerns the interplay between quantum criticality and unconventional superconductivity. This interplay was extensively studied in Ce-based heavy-fermion systems. Superconductivity was also discovered in the Yb-based quantum-critical material YbRh<sub>2</sub>Si<sub>2</sub> at 2 mK [1]. The superconducting transition is accompanied by nuclear magnetic order of Yb, however, the interplay between electronic and nuclear moments and its impact on the superconductivity is not settled. Recently, pronounced differences were observed in the temperature-magnetic field phase diagrams for a <sup>174</sup>YbRh<sub>2</sub>Si<sub>2</sub> crystal in comparison to a crystal with a natural mixture of Yb-isotopes (70% of the Yb-isotopes do not carry a nuclear spin) [2]. For that reason, it is essential to further investigate YbRh<sub>2</sub>Si<sub>2</sub> crystals with well-defined Yb nuclear moments.

In this contribution, we present the successful growth of single crystals with three different nuclear spins I, <sup>171</sup>Yb (I = 1/2), <sup>173</sup>Yb (I = 5/2), and <sup>174</sup>Yb (I = 0). One crucial step towards isotope-pure crystals was the development of a metallothermic-reduction experiment, as the isotope pure Yb is only available as oxide. Subsequently, the single crystals were grown using the established high-temperature indium-flux method [3]. We determined the precise isotopic composition in the different crystals using the LA-ICPMS technique and confirmed an isotopic enrichment of 95.5%, 92.6%, and 99.2% for <sup>171</sup>Yb, <sup>173</sup>Yb, and <sup>174</sup>Yb, respectively. Heat-capacity measurements down to 20 mK with field along the c-direction were performed, to study the suppression of the electronic magnetic transition and the occurrence of quantum-critical behavior for the three different crystals.

[1] E. Schuberth *et al.*, *Science* **351**, 485 (2016).

[2] D. H. Nguyen *et al.*, *Nat. Commun.* **12**, 4341 (2021).

[3] C. Krellner *et al.*, *Philos. Magazine* **92**, 2508 (2012).

# Quantum Critical Spin-Liquid in Geometrically Frustrated Kagome Lattice Investigated by Muon Spin Relaxation and Neutron Scattering

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We present the results of muon spin relaxation ( $\mu$ SR) and neutron scattering on the frustrated quasi-Kagome lattice  $\text{CeRh}_{1-x}\text{Pd}_x\text{Sn}$  [1]. Our zero-field (ZF)  $\mu$ SR reveals the absence of static long-range magnetic order and spin freezing down to 0.05 K in  $x = 0.1$  and  $x = 0.2$ . The weak temperature-dependent plateaus of the dynamic spin fluctuations below 0.2 K in ZF- $\mu$ SR together with its longitudinal-field dependence indicate the presence of dynamic spin fluctuations persisting down  $T = 0.05$  K without static magnetic order. Further, the magnetic specific heat ( $C_{4f}$ ) for  $x = 0.1$  shows a nearly linear  $T$  dependence below 0.13 K and above it  $C_{4f}/T$  reveals the  $-\log T$  dependence. Low-energy inelastic neutron scattering (INS) study of  $x = 0.1$  and  $0.2$  reveals gapless magnetic excitations. Our high energy INS study reveals a very weak and broad scattering in  $x = 0$  and  $0.1$ , which transforms into well localized crystal field excitations for  $x = 0.5$ . We therefore attribute the observed behaviour for  $x = 0.1$  and  $0.2$  to a metallic spin-liquid ground state near the quantum critical point. The ZF- $\mu$ SR results for the  $x = 0.5$  sample are interpreted as a long-range antiferromagnetic ground state below  $T_N = 0.8$  K, which probably overcomes the frustration effect. The long-range magnetic ordering is also supported by evolution of magnetic Bragg peaks in  $x = 0.75$  sample observed below 5 K in the neutron diffraction data.

[1] C. L. Yang *et al.*, Phys. Rev. B 96, 045139 (2017).

## Peering past spin density wave order at quantum criticality in $\text{Sr}_3\text{Ru}_2\text{O}_7$

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At ambient pressure the bilayer ruthenate  $\text{Sr}_3\text{Ru}_2\text{O}_7$  displays a rare example of magnetic-field-induced spin density wave order, in connection with a metamagnetic transition at  $H_c \sim 8$  T. Above the SDW ordering temperature of  $\sim 1.1$  K,  $\text{Sr}_3\text{Ru}_2\text{O}_7$  shows  $T$ -linear resistivity [1] over a huge range of temperature. Recently, Lester et al. [2] have shown that fluctuations of the SDW order parameter can account for the specific heat at low temperatures for applied magnetic fields near  $H_c$  but outside the SDW phase.

We have measured the resistivity of  $\text{Sr}_3\text{Ru}_2\text{O}_7$  down to 100 mK in the region surrounding  $H_c$ . By applying modest pressure we can reduce the SDW transition temperature, allowing us to follow the  $T$ -linear resistivity to well below 1 K. We compare our results with the predictions of spin fluctuation theory, using the parametrization of the dynamical susceptibility obtained by Lester et al. [2].

[1] J.A.N. Bruin *et al.*, *Science* **339** (2013) 804.

[2] C. Lester *et al.*, *Nat. Commun.* **12**, 5798 (2021)

# From $SU(2)_5$ to $SU(2)_3$ Wess-Zumino-Witten transitions in a frustrated spin-5/2 chain

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We investigate the properties of a frustrated spin-5/2 chain with next-nearest neighbor two and three-site interactions, with two questions in mind: the nature of the transition into the dimerized phase induced by the three-site interaction, and the possible presence of a critical floating phase at intermediate values of the next-nearest neighbor interaction. We provide strong evidence that the continuous transition into the dimerized phase, which has been found to be generically in the Wess-Zumino-Witten  $SU(2)_{2S}$  universality class up to spin  $S = 2$ , is  $SU(2)_5$  only at two isolated points of the phase diagram, and that it is  $SU(2)_3$  in between, in agreement with the presence of two relevant operators allowed by symmetry for  $SU(2)_5$ , and with the conservation of the parity of the level index along the renormalization flow between  $SU(2)_k$  theories with different values of  $k$ . We also find that the dimerization induced by the next-nearest neighbor interaction is a three step process, with first a small partially dimerized phase followed by a broad critical floating phase with incommensurate correlations before the fully dimerized phase is reached. Implications for the iron oxide  $Bi_3FeMo_2O_{12}$  are briefly discussed.

## Quench dynamics and relaxation of a spin coupled to interacting leads

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We study a quantum quench in which a magnetic impurity is suddenly coupled to Hubbard chains, whose low-energy physics is described by Tomonaga-Luttinger liquid theory. In an earlier work [Physical Review B 103, 125152 (2021)], by using the time-dependent density-matrix renormalization-group (tDMRG) technique, we analyzed the propagation of charge, spin and entanglement in the chains after the quench and related the light-cone velocities to the dispersion of holons and spinons. We found that the local magnetization at the impurity site decays faster if we increase the interaction in the chains, even though the spin velocity decreases. We derived an analytical expression for the relaxation of the impurity magnetization which is in good agreement with the tDMRG results at intermediate timescales.

More recently, we have investigated the system transport properties and generalized the result for the magnetization at the impurity considering a broader time interval. If we turn off the interaction  $U$  in the chains, we find that in the steady state the charge current through the impurity is a function of the renormalized Kondo coupling, as it happens in the static problem [Pustilnik and Glazman, J. Phys. Condens. Matter 16, R513 (2004)]. In the weakly interacting case, we obtain an expression for the current that allows us to extract an analytical expression for the Kondo time  $t_K$  as a function of  $U$ , which indicates that the electronic interaction in the chains favors the formation of the Kondo cloud, in accordance with our previous numerical results. The magnetization at the impurity calculated at times  $t \ll t_K$  is not a function of the Kondo coupling, but its derivative, that is, the spin current, is. We believe that our results provide valuable insights into the time evolution of the Kondo screening cloud in interacting systems.

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# Light-induced magnetization dynamics in a ferromagnetic semiconductor

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Ferromagnetic semiconductors are a special class of materials that simultaneously show both ferromagnetic ordering of spins and semiconducting properties. This provides a new platform with spin degrees of freedom in electronic and/or optical devices. A prototype example is EuO, which is extensively investigated because of its remarkable magnetism-related properties such as the metal-insulator transition, the colossal magnetoresistance, and nearly 100% spin polarization in the ferromagnetic state [1]. In addition, an ultrafast carrier-density-controlled strengthening or quenching of the ferromagnetic order is demonstrated via resonant photoexcitation using magnetic second harmonic generation (MSHG) [2]. These studies reveal that the associated spin dynamics arise from the photoinduced non-equilibrium carrier distribution. While it is known that the optical excitation at low temperature, 10 K for instance, could dynamically enhance or quench the ferromagnetic order by tuning the exchange coupling between the localized  $4f$  spins in EuO [3], in this contribution we show the presence of magnetic ordering even at temperatures around and higher than the Curie Temperature ( $T_C = 69$  K), using optical pump-probe spectroscopy. We observe two distinct types of ultrafast processes related to the magnetic order that show different relaxation rates. Our results provide clear evidence of short-range magnetic order above  $T_C$ , originating from the so-called exciton magnetic polarons.

[1] M. Matsubara *et al.*, Phys. Rev. B **81**, 214447 (2010).

[2] M. Matsubara *et al.*, Nat. Commun. **6**, 6724 (2015).

[3] M. Matsubara *et al.*, Phys. Rev. B **86**, 195127 (2012).



# Photoinduced phase transitions in one-dimensional Mott insulators

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Applying optical pulses has becoming a key tool to weaken or strengthen order in strongly correlated electron systems. In this way even new phases can be established, being absent in the ground state. In this context  $\eta$ -pairing, which theoretically has been proposed by C. N. Yang for the Hubbard model long time ago [1], attracted renewed attention, because it has been suggested that pumping Mott insulators enhances  $\eta$ -pairing correlations at both zero [2] and finite [3] temperatures.

For this reason, in this talk, we thoroughly study the nonequilibrium dynamics of pumped Mott insulators by density matrix time-evolution techniques based on (infinite) matrix-product states [4]. The purpose is to prove photoinduced phase transitions numerically. We show that in the time-dependent photoemission spectra of the driven Hubbard model an extra band appears above the Fermi energy after pulse irradiation for optimal pump parameters, indicating an insulator-to-metal transition triggered by the formation of  $\eta$ -pairs. It may be noted that the developed numerical technique can be readily applied to other one-dimensional models driven out of equilibrium by optical pumping, such as the effective Falicov-Kimball model, the perhaps minimal theoretical model describing excitonic insulators [5].

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[1] C. N. Yang, Phys. Rev. Lett. **63**, 2144 (1989).

[2] T. Kaneko *et al.*, Phys. Rev. Lett. **122**, 077002 (2019).

[3] S. Ejima *et al.*, Phys. Rev. Res. **2**, 032008(R) (2020).

[4] S. Ejima, F. Lange and H. Fehske, Phys. Rev. Res. **4**, L012012 (2022).

[5] S. Ejima, F. Lange and H. Fehske, to be published.

## **Volatile and non-volatile insulator-to-metal transition in narrow gap Mott insulator GaMo<sub>4</sub>S<sub>8</sub>**

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Mott insulators are a class of strongly correlated materials with nonlinear optical and electric response, that can be used for innovative micro and nanoelectronics applications, such as neuromorphic circuits. The Insulator to Metal Transition (IMT) in these compounds can be induced by temperature, pressure, electric field, doping or light. We focus on the IMT triggered by electric field in the narrow gap Mott insulators GaMo<sub>4</sub>S<sub>8</sub> crystals.

The recent results I will present were obtained using the Nanoprobe, a combination of 4 Scanning Tunneling Microscopes (STM) and a high-resolution Scanning Electron Microscope (SEM) under Ultra High Vacuum (UHV). Four-point probe measurements were performed, we find the resistivity of 38Ω.cm in agreement with the literature [1]. High contact resistance will be highlighted. I will discuss the two types of transitions that we observed, volatile and non-volatile. We study the volatile transition at variable interelectrode distances, 3 to 200 microns. We find an intrinsic threshold voltage in agreement with literature and the corresponding electric field independent of the interelectrode distance. Additionally, a non-volatile transition was observed, in which a conductive filament is created between the electrodes.

[1] H. Koussir *et al* 2022 *J. Phys.: Conf. Ser.* **2164** 012046

# Dynamical quantum phase transition in a mesoscopic superconducting system

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We investigate the dynamics for a correlated quantum dot sandwiched between the metallic and superconducting leads driven by a quantum quench. The response to two types of quenches is examined. The first one is performed in the coupling between the quantum dot and the superconducting lead, while the other one is associated with a change in position of the orbital energy level. In particular, we study the interplay between the proximity induced electron pairing with Coulomb correlations and discuss the time-dependent charge occupancy, on-dot pair correlation, transient currents and evolution of the subgap quasiparticles.

Furthermore, we study the singlet-doublet dynamical phase transition upon traversing the phase boundaries between these ground states. The analysis of the Loschmidt echo and non-analytic features in the return rate reveals signatures of dynamical quantum phase transitions periodically occurring at critical times. We also show that observed phase transitions are accompanied with the corresponding local extrema in the pairing correlation function.

# Critical slowing down of fermionic quasiparticles in YbRh<sub>2</sub>Si<sub>2</sub> by terahertz time-domain spectroscopy

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A universal phenomenon in phase transitions is critical slowing down (CSD) – systems, after an initial perturbation, take an exceptionally long time to return to equilibrium. It is universally observed in the dynamics of bosonic excitations, like order-parameter collective modes. But it is not generally expected to occur for fermionic excitations because of the half-integer nature of the fermionic spin. Observation of CSD in fermionic excitations or quasiparticles would therefore be of fundamental significance. In heavy-fermion (HF) materials, the fermionic quasiparticles are composite objects, quantum super-positions of itinerant and localized electron states, which may disintegrate near a quantum phase transition.

Terahertz time-domain spectroscopy (THz-TDS) has recently been developed into a powerful tool for probing the HF quasiparticle dynamics [1-3]. HF materials respond to an incident single-cycle THz pulse by a time-delayed echo pulse whose delay time and intensity bear detailed and background-free information about the Kondo temperature and the quasiparticle weight, respectively.

Here, we observe fermionic CSD in HF compound YbRh<sub>2</sub>Si<sub>2</sub> by THz-TDS. We see that near the quantum phase transition in YbRh<sub>2</sub>Si<sub>2</sub>, the build-up of spectral weight towards the Kondo temperature  $T_{K^*}=25$  K is followed by a logarithmic rise of the quasiparticle excitation rate on the heavy-Fermi-liquid side below 10 K. A critical two-band HF liquid theory shows that this is indicative of fermionic CSD, the softening of the HF quasiparticle dispersion. This CSD also proves the breakdown of HF quasiparticles near the quantum phase transition. We can extract the critical exponent of the fermionic quasiparticle breakdown which sets the stage for classification of fermionic quantum phase transitions analogous to thermodynamic phase transitions [4].

[1] C. Wetli, S. Pal, J. Kroha, K. Kliemt, C. Krellner, O. Stockert, M. Fiebig, Nat. Phys. **14**, 1103 (2018).

[2] S. Pal, C. Wetli, F. Zamani, O. Stockert, H. von Löhneysen, M. Fiebig, J. Kroha, Phys. Rev. Lett. **122**, 096401 (2019).

[3] C.-J. Yang, S. Pal, F. Zamani, K. Kliemt, C. Krellner, O. Stockert, H. von Löhneysen, J. Kroha, M. Fiebig, Phys. Rev. Research **2**, 033296 (2020).

[4] C.-J. Yang, K. Kliemt, C. Krellner, J. Kroha, M. Fiebig, S. Pal, preprint.

# Pressure-induced BEC-BCS crossover in a doped spin liquid candidate

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Quantum spin liquid (QSL) is an exotic state possibly having quantum entanglement and fractionalization in excitations. Further intriguing is superconductivity that possibly emerges by doping QSL. In this presentation, I briefly review the present status of the QSL research on an organic triangular-lattice compound and present our recent experimental studies on the superconductivity in a 11% hole doped QSL candidate.

At ambient pressure, the  $^{13}\text{C}$  NMR measurements suggest spin-singlet nodal pairing. The superfluid density evaluated by the penetration depth measurements is considerably suppressed to the level of the doped-hole density, indicating that the substantial part of the spectral weight is incoherent [1]. The transport and Nernst effect measurements suggest that the superconductivity at ambient pressure is a BEC-like condensate from a non-Fermi liquid and is driven to a BCS condensate from a Fermi liquid by pressure, which reduces the Coulombic interactions among electrons [2]. I also present the thermoelectric signature of quantum criticality and its possible relevance to superconductivity [3] as well as the variation of the electronic state under uniaxial distortion of the triangular lattice [4].

The present work is a collaboration with Y. Suzuki, K. Wakamatsu, Y. Ueno, J. Ibuka, H. Oike, T. Fujii, K. Miyagawa and H. Taniguchi.

[1] K. Wakamatsu *et al.*, arXiv: 2205.03682.

[2] Y. Suzuki *et al.*, Phys. Rev. X **12**, 011016 (2022).

[3] K. Wakamatsu *et al.*, arXiv: 2201.10714

[4] H. Oike *et al.*, arXiv: 2202.06032

# Electrodynamics at the Mott transition: the disappearance of Landau's quasiparticles

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The low-energy properties of correlated metals can be understood in terms of long-lived quasiparticles with all complex interactions included in Fermi-liquid parameters, such as the effective mass  $m^*$ . The great success and wide applicability of Landau's ideas cannot hide the fact that the celebrated quasiparticle concept breaks down when approaching and crossing the Mott transition or when the metal turns bad at elevated temperatures. Here we investigate the spectral and temperature-dependent complex electrodynamic response  $\sigma_1(\omega, T) + i\sigma_2(\omega, T)$  of molecular quantum materials as the influence of electronic interactions is varied [1].

We have chosen the quantum-spin-liquid candidate  $\kappa$ -(BEDT-TTF)<sub>2</sub>Cu<sub>2</sub>(CN)<sub>3</sub> [2] as suitable model system because its effective correlation strength  $U/W$  can be easily varied by pressure or partial chemical substitution. While for a strongly-correlated Mott insulator the excitation spectrum is completely gapped, additional absorption occurs when entering the coexistence regime that appears at the first-order Mott transition below the critical endpoint [3]. Electronic phases of correlated metal and insulator are spatially separated: filling fraction and interaction strength vary concomitantly.

Beyond the percolation threshold, on the metallic side, we reveal persistent Fermi-liquid behavior with  $T^2$  and  $\omega^2$  dependences of the optical scattering rate  $\gamma(\omega, T)$ , along with a puzzling elastic contribution to relaxation. The strong increase of the resistivity beyond the Ioffe-Regel-Mott limit  $\rho \gg \rho_{\text{IRM}}$  is accompanied by a displaced Drude peak in  $\sigma_1(\omega)$ . Our results, supported by a theoretical model for the optical response, demonstrate the emergence of a bad metal from resilient quasiparticles that are subject to dynamical localization and dissolve near the Mott transition [4].

[1] M. Dressel and S. Tomić, *Adv. Phys.* **69**, 1 (2020).

[2] B. Miksch *et al.*, *Science* **372**, 276 (2021)

[3] A. Pustogow *et al.*, *Nat. Mater.* **17**, 773 (2018); *npj Quantum Mater.* **6**, 9 (2021).

[4] A. Pustogow *et al.*, *Nat. Commun.* **12**, 1571 (2021).

# Charge disproportionation and “Hund’s insulating” behavior in different transition metal oxides by DFT+DMFT

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Several materials such as the rare earth nickelates  $RNiO_3$  or the alkaline earth ferrate  $CaFeO_3$  exhibit a metal-insulator transition (MIT) involving a charge-disproportionation of the transition metal cation, resulting in inequivalent crystallographic sites with different nominal cation valence. The MIT coincides with a structural transition involving a “breathing”, i.e. an expansion or contraction, of the oxygen octahedra surrounding the inequivalent cation sites.

Calculations for purely electronic multiband Hubbard models indicate that a charge-disproportionated insulating phase can be stabilized if the Hund’s coupling is relatively strong and the Hubbard interaction is strongly screened [1,2,3]. Nevertheless, coupling to structural degrees of freedom is crucial to stabilize the insulating phase for realistic parameters [1,3,4].

We explore the coupling between charge disproportionation, MIT, and structural distortions using density functional theory in combination with dynamical mean-field theory (DFT+DMFT) for  $RNiO_3$ ,  $CaFeO_3$ , and  $SrCrO_3$ , which map to effective two-orbital, five-orbital, and three-orbital models, respectively. We discuss the relevance of a small or negative charge transfer energy, by comparing a description using an effective  $d$ -only basis with a more extended picture including also the oxygen  $p$  states for the case of  $CaFeO_3$ . This allows us to quantify the occupation in terms of “ligand-holes” and to assess the equivalence of the two different pictures.

This presentation results from collaborations with Maximilian Merkel, Alberto Carta (ETH Zurich), Alexander Hampel, Antoine Georges (Flatiron Institute), and Oleg Peil (Materials Center Leoben).

[1] A. Subedi, O. E. Peil, and A. Georges., Phys. Rev. B **91**, 075128 (2015).

[2] A. Isidori *et al.*, Phys. Rev. Lett. **122**, 186401 (2019).

[3] M. E. Merkel and C. Ederer, Phys. Rev. B **104**, 165135 (2021).

[4] O. E. Peil, A. Hampel, C. Ederer, and A. Georges., Phys. Rev. B **99**, 245127 (2019).

## ***Nickelates: A Tale of Two Stories***

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This talk will involve two stories; a) metal-insulator transition in BiNiO<sub>3</sub>, and b) superconductivity in infinite-layer nickelates (RENiO<sub>2</sub>, RE=Nd/La).

In the first story, using ab initio electronic structure and slave rotor theory calculations, we demonstrate [1,2] that *hybridization-switching induced Mott transition* happens in BiNiO<sub>3</sub>. We show that these systems exhibit a breathing phonon driven Bi to oxygen hybridization-wave instability which conspires with strong correlations on Ni site to induce a Mott insulator. In contrast to ABO<sub>3</sub> perovskites with passive A-site cations, these Mott insulators with active A-site orbitals like Bi are shown to undergo a pressure induced insulator to metal transition accompanied by a colossal volume collapse due to ligand hybridization switching.

In the second story, we explore superconductivity in NdNiO<sub>2</sub> and LaNiO<sub>2</sub> employing a first-principles derived low-energy model Hamiltonian, consisting of two orbitals: Ni  $x^2 - y^2$ , and an axial orbital. The *axial* orbital is constructed out of Nd/La  $d$ , Ni  $3z^2 - r^2$  and Ni  $s$  characters. Calculation of the superconducting pairing symmetry and pairing eigenvalue of the spin-fluctuation mediated pairing interaction underlines the crucial role of inter-orbital Hubbard interaction in superconductivity, which turns out to be orbital-selective. The *axial* orbital brings in materials dependence in the problem, making NdNiO<sub>2</sub> different from LaNiO<sub>2</sub>, thereby controlling the inter-orbital Hubbard interaction assisted superconductivity.[3,4]

\*This work is supported by the Department of Science and Technology, India.

[1] Atanu Paul, Anamitra Mukherjee, Indra Dasgupta, Arun Paramakanti, and Tanusri Saha-Dasgupta, Phys. Rev. Lett. **122**, 016404 (2019).

[2] Atanu Paul, Anamitra Mukherjee, Indra Dasgupta, and Tanusri Saha-Dasgupta, Phys. Rev. Res, **2**, 013333 (2020).

[3] Priyo Adhikary, Subhadeep Bandyopadhyay, Tanmoy Das, Indra Dasgupta, and Tanusri Saha-Dasgupta, Phys. Rev. B **102**, 100501(R) (2020).

[4] Subhadeep Bandyopadhyay, Priyo Adhikary, Tanmoy Das, Indra Dasgupta, and Tanusri Saha-Dasgupta, Phys. Rev. B **102**, 220502(R) (2020)



## Magnetically induced metal-insulated transition in $\text{Pb}_2\text{CaOsO}_6$

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Khalyavin,<sup>5</sup> Pascal Manuel,<sup>5</sup> Claire A. Murray,<sup>9</sup> Christian Donnerer,<sup>10</sup> James G. Vale,<sup>10</sup>  
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The double perovskite  $\text{Pb}_2\text{CaOsO}_6$  undergoes a transition from showing metallic conductivity at high temperatures, to being insulating at low temperatures [1]. This metal-insulator transition happens simultaneously with the onset of antiferromagnetic order, suggesting that the transition is spin-driven, and could be a rare example of a so-called Slater transition. In the sister compound  $\text{Pb}_2\text{ZnOsO}_6$ , neither magnetic order nor a transition to an insulating state are observed.

In this talk, I will present our work on understanding the metal-insulator transition in  $\text{Pb}_2\text{CaOsO}_6$  and its absence in  $\text{Pb}_2\text{ZnOsO}_6$ . Using neutron- and x-ray diffraction we have determined the structure of these materials. This shows that  $\text{Pb}_2\text{ZnOsO}_6$  is geometrically frustrated, while  $\text{Pb}_2\text{CaOsO}_6$  is heavily distorted, lifting the frustration. The distortion in  $\text{Pb}_2\text{CaOsO}_6$  is antiferroelectric; a rarity in metals. We have used neutron diffraction and muon spin rotation to pin down the magnetic structure, and conclude with resonant inelastic scattering to help understand the electronic structure.

[1] H. Jacobsen *et al.*, Phys. Rev. B **102**, 214409 (2020).

# Orbital imaging of the spin state transition in LaCoO<sub>3</sub>

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The gradual transition from a non-magnetic insulator at low temperatures to a paramagnetic semiconductor at high temperatures in LaCoO<sub>3</sub> is a fascinating phenomenon and continues to spark highly sophisticated and state-of-the-art investigations [1-6]. A key ingredient for a quantitative understanding is to know the Co 3d charge density and its temperature dependence. The general idea is that, at low temperatures, the Co<sup>3+</sup> ions are in a nonmagnetic low-spin state with the  $t_{2g}^6 e_g^0$  configuration. At high temperatures, the  $t_{2g}$  electrons get partially promoted into the  $e_g$  to form magnetic Co ions with the high-spin  $t_{2g}^4 e_g^2$  configuration [2,6]. This  $t_{2g}$  vs.  $e_g$  aspect is also of high relevance for the field of battery and catalysis research [7-9] where Co oxides are popular materials.

Here we have investigated the Co 3d orbital occupation across the spin state transition using a modified variant of the recently developed x-ray-based *orbital-imaging* method [10-12]. The images collected allow for a direct determination of the amount of the Co  $t_{2g}$  and  $e_g$  holes. We find that, at the lowest temperatures, the low-spin state with the nominally  $t_{2g}^6 e_g^0$  electron configuration *does* have holes in the  $t_{2g}$  subshell which we attribute to the presence of spin-orbit interaction. The hole amount, however, sets limits to the minimum energy gap between the lattice-frozen low-spin and high-spin states. At high temperatures, we find that the high-spin state occupation is about *half* (!) of the value reported in the most recent literature [6]. Implications for the modeling of the spin-state transition process are discussed.

- [1] D. Louca and J. L. Sarrao, Phys. Rev. Lett. **91**, 155501 (2003)
- [2] M.W. Haverkort *et al.*, Phys. Rev. Lett. **97**, 176405 (2006).
- [3] J. Kunes and V. Krapek, Phys. Rev. Lett. **106**, 256401 (2011).
- [4] P. Augustinsky, V. Krapek, and J. Kunes, Phys. Rev. Lett. **110**, 267204 (2013).
- [5] M. Karolak *et al.*, Phys. Rev. Lett. **115**, 046401 (2015).
- [6] K. Tomiyasu *et al.*, Phys. Rev. Lett. **119**, 196402 (2017).
- [7] M. S. Whittingham, Chemical Reviews **104**, 4271 (2004).
- [8] J. Suntivich *et al.*, Science **334**, 1383 (2011).
- [9] J. Zhou *et al.*, Nature Commun. **11**, 1984 (2020).
- [10] H. Yavaş *et al.*, Nature Physics **15**, 559 (2019).
- [11] B. Leedahl *et al.*, Nature Commun. **10**, 5447 (2019).
- [12] A. Amorese *et al.*, Phys. Rev. X **11**, 011002 (2021).

## Single thermodynamic transition at 2 K in superconducting UTe<sub>2</sub> single crystals

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UTe<sub>2</sub> is a recently discovered contender for multicomponent topological superconductivity. The presence of two superconducting transitions, however, remains a matter of contention. In this talk, I will first present a brief overview of key experimental results on the superconducting state of UTe<sub>2</sub>. I will then discuss recent developments in sample synthesis combined with thermodynamic measurements that shed light on the role of disorder and magnetic fluctuations in UTe<sub>2</sub>. Our results reveal that single crystals exhibiting a single bulk superconducting transition temperature at 2 K also show reduced residual specific heat values and enhanced residual resistance ratios. I will also discuss the role of spatial inhomogeneity in samples with an apparent split transition. At the end of the talk, I will highlight some of the pressing outstanding open questions regarding the superconducting order parameter of UTe<sub>2</sub>.

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# NMR study of magnetic and superconducting properties on UTe<sub>2</sub> under pressure

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Recently discovered U-based superconductor UTe<sub>2</sub> is the leading candidate for the spin-triplet superconductor, and many experiments support this scenario [2-5]. In addition to the interesting superconducting (SC) features of UTe<sub>2</sub> at ambient pressure, UTe<sub>2</sub> shows a more complicated and fascinating phase diagram under pressure. Specific-heat measurements [6] revealed two SC phases at zero fields (SC1 and SC2). The  $H_{c2}$  behavior of these two SC phases is completely different, indicating the SC-multi-phases due to the spin and orbital degrees of freedom.

To investigate the magnetic and SC properties of UTe<sub>2</sub> under pressure, we performed the NMR measurements under pressure. The typical heavy-fermion (HF) behavior and superconductivity were destroyed by pressure above 1.7 GPa [7]. Our measurements suggest the importance of the HF state for the superconductivity of UTe<sub>2</sub>. In addition, we performed the NMR measurements at low temperatures at 1.2 GPa. We will discuss the possible SC states based on our NMR results.

[1] S. Ran *et al.*, *Science* **365**, 684 (2019).

[2] G. Nakamine *et al.*, *J. Phys. Soc. Jpn.* **88**, 113703 (2019).

[3] G. Nakamine *et al.*, *Phys. Rev. B* **103**, L100503 (2021).

[4] K. Ishihara *et al.*, arXiv:2105.13721 (2021).

[5] H. Fujibayashi *et al.*, *J. Phys. Soc. Jpn.* **91**, 043705 (2022).

[6] D. Braithwaite *et al.*, *Comm. Phys.* **2**, 147 (2019).

[7] K. Kinjo *et al.*, arXiv: 2203. 12934 (2022).

## High pressure properties of UTe<sub>2</sub>

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We present the extraordinary high-pressure properties of the recently discovered paramagnetic heavy-fermion superconductor UTe<sub>2</sub>, which is a strong candidate for spin-triplet superconductivity [1-3]. Superconductivity vanishes near the critical pressure  $p_c \approx 1.5$  GPa at a first order-like transition to a probable antiferromagnetically ordered state [4-6]. Antiferromagnetic ordering is suggested from the observation of several transitions in the magnetoresistance above  $p_c$  [7], as well as a well-defined critical field corresponding to the suppression of magnetic order for all directions of applied field. We discuss the anisotropy of the electrical resistivity under pressure, which shows distinct differences dependent on the current direction. Remarkably, the magnetic anisotropy changes with pressure, and this has strong feedback on  $H_{c2}$ . We present the anisotropy of the superconducting upper critical field  $H_{c2}$  [8]. While the metamagnetic transition, which limits the upper critical field for field applied along the  $b$  axis, decreases from 35 T at zero pressure to zero near  $p_c$ , field induced superconductivity occurs near  $p_c$  for field along the  $c$  axis. [9] This reinforcement of superconductivity coincides with a strong enhancement of the effective mass. Under pressure a transition between two superconducting phases occurs in zero field [4]. When pressure is combined with a field applied along the  $a$  axis, multiple superconducting phases occur, which require a state for the spin-triplet superconducting order parameter more complex than an equal spin pairing [10]. These experiments show the potential of high pressure to tune the magnetic and superconducting properties and unravel the complex correlations between them.

[1] S. Ran et al. Science **365**, 684 (2019).

[2] D. Aoki, et al. J. Phys. Soc. Jpn. **88**, 043702 (2019).

[3] D. Aoki et al., J. Phys.: Condens. Matter **34**. 243002 (2022).

[4] D. Braithwaite, et al, Commun. Phys. **2** (2019).

[5] S. Thomas, et al. Sci. Adv. **6** : eabc8709 (2020).

[6] S. Ran, et al., Phys. Rev. B **101**, 140503(R) (2020).

[7] M. Vališka, et al., Phys. Rev. B **104**, 214507 (2021).

[8] G. Knebel, et al., J. Phys. Soc. Jpn., **89**, 053707 (2020).

[9] D. Aoki, J. Phys. Soc. Jpn **90**, 074705 (2021).

[10] D. Aoki, J. Phys. Soc. Jpn. **89**, 053705 (2020).

## Magnetic excitation spectrum of the unconventional superconductor UTe<sub>2</sub>

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The discovery of the heavy fermion superconductor UTe<sub>2</sub> ( $T_{SC} \approx 1.6$  K) has triggered a wealth of research owing to the possible triplet and chiral nature of the superconductivity, the observation of multiple superconducting phases under magnetic field and pressure, as well as the proximity to a magnetic instability. The spin dynamics of UTe<sub>2</sub> was investigated by inelastic neutron scattering on a single crystal sample. In the normal state, the presence of incommensurate spin fluctuations peaked at the wave-vector  $\mathbf{k}_1=(0, 0.57, 0)$  is confirmed. The associated quasielastic response is characterized by a relaxation rate  $\Gamma(\mathbf{k}_1) \approx 2.5$  meV. These fluctuations saturate below 15 K in possible relation with anomalies observed in bulk and NMR measurements. The low dimensional nature of the fluctuations is evidenced by the absence of correlations along the c-axis of the orthorhombic structure, where the signal has the characteristic signature of in-phase fluctuations of the two uranium atoms of the primitive unit cell. This peculiarity can be related to the spin ladder structure of UTe<sub>2</sub> with these two uranium atoms forming its rungs. A feedback effect of superconductivity on the magnetic excitation spectrum manifests through the development below  $T_{SC}$  of an inelastic mode at  $\Omega \approx 1$  meV for the wave-vector  $\mathbf{k}_1$ . The high ratio  $\Omega/k_B T_{SC} \approx 7.2$  and the large damping of this mode contrast with the most common behaviour found for the resonance peak in heavy fermion superconductors.

[1] W. Knafo *et al.*, Phys. Rev. B **104**, L100409 (2021).

[2] S. Raymond *et al.*, J. Phys. Soc. Japan **90**, 113706 (2021).

## Recent development in the spin-triplet superconductor UTe<sub>2</sub>

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Recently discovered spin-triplet superconductivity in UTe<sub>2</sub> shows several hallmarks, viz, ultra-high and anisotropic  $H_{c2}$  beyond the Pauli limit, miniscule Knight shift through the superconducting transition, reentrant superconducting phase above 40 T, topologically nontrivial with chiral in-gap surface states, broken time reversal symmetry in Kerr rotation, etc [1-3]. However, the superconducting state in UTe<sub>2</sub> has, for the most part, not displayed the exquisite sensitivity to disorder that is expected in the spin-triplet superconductors.

In this talk we will review the differences in superconducting properties in samples grown under different conditions and our ongoing attempts to control them. Studying electrical and thermal transport, along with heat capacity and elemental analysis on these different samples, we will discuss how the different measures of cleanliness correlate with the superconducting properties, shedding light on the emerging picture of superconductivity in UTe<sub>2</sub>.

Finally, we will discuss inelastic neutron scattering in the normal and superconducting states. We measured low-energy magnetic excitations that have a peak intensity at 4 meV, follow the Brillouin zone edges near  $b$ -axis, obey the paramagnetic structural symmetry, and track the temperature evolution of the heavy fermion bulk magnetic susceptibility. These results indicate that the imaginary part of the dynamic susceptibility follows the behavior of interband correlations in a hybridized Kondo lattice, and their presence does not necessarily suggest the dominance of ferromagnetic or antiferromagnetic correlations [4].

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- [1] S. Ran, C. Eckberg, S. R. Saha, J. Paglione, and N. P. Butch *et al.*, *Science* 365, 684 (2019).
- [2] I.M. Hayes, D.S. Wei, S.R. Saha, N.P. Butch, A. Kapitulnik, J. Paglione, *et al.*, *Science* 373, 797 (2021).
- [3] L. Jiao, S. Howard, S. Ran, N. P. Butch, and V. Madhavan, *et al.*, *Nature* 579, 523 (2020).
- [4] N.P. Butch, S. Ran, S. R. Saha, J. Paglione, *et al.*, *npj Quantum Materials* 7, 39 (2022).

## NMR studies of local magnetism in UTe<sub>2</sub> under pressure

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Recently, the candidate triplet superconductor UTe<sub>2</sub> (Fig. 1) has attracted increasing attention in which - unlike other U-based ferromagnetic superconductors (such as UCoGe, UGe<sub>2</sub>, and URhGe) [1] - superconductivity does not appear to coexist with magnetic order. Consequently, a prime interest is to understand the relation between the underlying magnetism and superconductivity, which has been intensively explored by various spectroscopic means, including inelastic neutron scattering [2,3], muon spin relaxation [4], and nuclear magnetic resonance (NMR) [5]. Upon applying hydrostatic pressure ( $P$ ), macroscopic and thermodynamic experiments have found multiple superconducting transitions, which are in close proximity to magnetic order above a critical pressure of 1.3-1.5 GPa [6-9]. Microscopically, however, the nature of these electronic phases under  $P$  is poorly understood, and their local magnetic properties remain to be fully elucidated.

In this talk, we will present our <sup>125</sup>Te NMR results in high-quality single crystals of UTe<sub>2</sub> to discuss local magnetism and spin dynamics under  $P$ . UTe<sub>2</sub> has two crystallographically nonequivalent Te sites: dubbed Te(1) and Te(2) in Fig. 1. At  $P = 1.8$  GPa we have measured nuclear spin-lattice relaxation rate,  $T_1^{-1}$ , and have found a notable site asymmetry developing upon cooling below 30 K (Fig. 2) [10]; For the Te(1) site,  $T_1^{-1}$  shows a clear divergence around 10 K, indicative of long-range magnetic ordering. By contrast, for the Te(2) site,  $T_1^{-1}$  only shows a very weak divergence, suggesting that strongly anisotropic spin fluctuations develop inside the unit cell. Spectral intensity and line shape change around the same temperature, at which a clear site asymmetry equally emerges. The observed contrasting temperature dependence at the two sites presumably suggests a magnetic ordering with a non-zero wave-vector ( $\mathbf{Q} \neq \mathbf{0}$ ). More systematic comparisons of such local magnetism at a wider  $P$  range will be discussed.

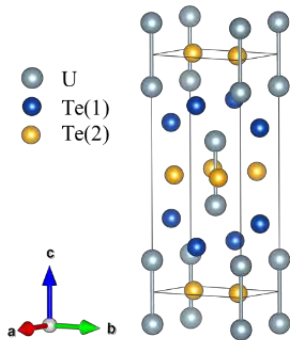


Figure 1: Crystal structure of UTe<sub>2</sub>

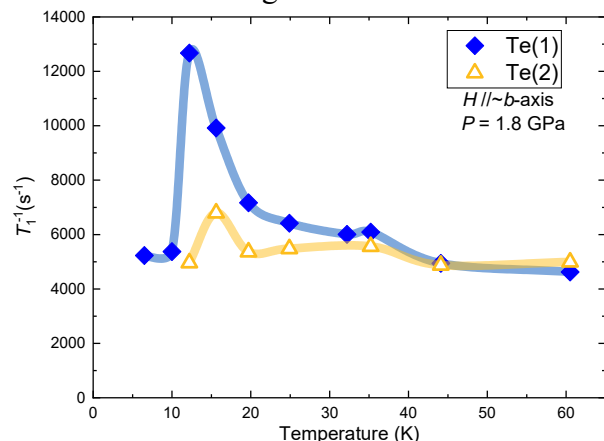


Figure 2: Spin-lattice relaxation rate vs temperature [10]

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[1] D. Aoki *et al.*, J. Phys. Soc. Jpn. **88**, 022001 (2019). [2] C. Duan C *et al.*, Phys. Rev. Lett. **125**, 237003 (2020). [3] W. Knafo C *et al.*, Phys. Rev. B **104**, L100409 (2021). [4] S. Sundar, Phys. Rev B **100**, 140502(R) (2019). [5] Y. Tokunaga *et al.* J. Phys. Soc. Jpn. **88** 073701 (2019), J. Phys. Soc. Jpn. **91**, 023707 (2022). [6] S. M. Thomas *et al.*, Sci. Adv., **6** (42), eabc8709 (2020). [7] D. Braithwaite *et al* *Comm. Phys.* **2**, 147 (2019). [8] D. Aoki *et al* J. Phys. Soc. Jpn. **89**, 053705 (2020) [9] D. Li *et al.*, J. Phys. Soc. Jpn. **90**, 073703 (2021). [10] R. Yamamoto *et al.*, APS March Meeting 2022, Q64-030943.



## Incoherent Transport and the Evolution of Power-Law Scaling of the Magnetoresistance in Cuprate Superconductors

The high-field normal-state magnetoresistance (MR) of cuprate superconductors can be used to define doping ( $p$ ) regimes within which distinct scaling behaviours are observed. Within the strange metal regime ( $p^* < p < p_{sc}$ ), a doping range characterized by a linear-in-temperature in-plane resistivity that persists to lowest temperatures, an unexpectedly large linear-in-field MR has been observed at high  $H$  and low  $T$  that exhibits signatures of incoherence: insensitivity to disorder, insensitivity to magnetic-field orientation and the adherence of quadrature ( $H/T$ ) scaling [1]. More extensive study [2] of Tl2201, Bi2201 and LSCO has revealed that the two anomalous linearities grow in tandem as optimal doping is approached from the overdoped end of the superconducting dome ( $p_{sc}$ ) and anticorrelates with the number of coherent carriers contributing the Hall carrier number [3]. Upon entry into the pseudogap regime ( $p < p^* \sim 0.19$ ), the growth of the  $H$ -linear MR persists but the  $H/T$  scaling rapidly cedes to a new power-law scaling behaviour:  $H/T^2$  scaling. Finally, coincident with the loss of superconductivity at  $p > p_{sc}$  is an abrupt return to (non-power-law) Kohler scaling, indicating that conventional metallic behaviour is finally restored in non-superconducting compositions.

1. Ayres, Berben et al. *Nature* **595**, 661-666 (2021)
2. Berben, Ayres et al. (under review)
3. Putzke et al. *Nature Physics* **17**, 8260831 (2021)

# Charge orders and strange metal in cuprate superconductors

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Charge orders and charge fluctuations have been ubiquitously observed in the phase diagram of Cuprate superconductors. We will review the experimental status of these various observations, differentiating the under-doped region and the optimally-doped and over-doped ones. Various theories have been advanced to explain the presence of these orders and their implication for our understanding of the pseudo-gap, from the idea of “vestigial order” to the one of “fluctuating Pair Density Wave (PDW)”. We will discuss these theoretical approaches in direct comparison with experiments. We will then introduce a proposal of “fractionalization of a PDW” in order to explain the pseudo-gap state. We will show that this idea produces a strong phenomenology, especially ARPES experiments, and giving a clue for the puzzling transport properties recently reported in the optimally doped and over-doped regions. We will then focus on the strange metal phase of those compounds and make a proposal for electric transport in this phase.

# Hidden magnetic texture in the pseudogap phase of high-Tc $\text{YBa}_2\text{Cu}_3\text{O}_{6.6}$

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Despite decades of intense researches, the enigmatic pseudo-gap (PG) phase of superconducting cuprates remains an unsolved mystery. In the last 15 years, condensed matter physicists discovered that this phase hosts symmetry breaking states as an intra-unit cell (or  $q=0$ ) magnetism, interpreted in terms of loop current patterns [1], preserving lattice translation (LT) and breaking time-reversal and parity symmetries, followed, upon cooling, by an additional incipient charge density wave [2] breaking the LT symmetry. However, none of these states can (alone) account for the partial gapping of the Fermi surface.

Our recent polarized neutron diffraction measurements in two different underdoped  $\text{YBa}_2\text{Cu}_3\text{O}_{6.6}$  single crystals [3] reveal a novel hidden LT-breaking magnetism that may be crucial to elucidate the PG puzzle. This short-range magnetism (typical correlations over 5-6 unit cells), carried by the  $\text{CuO}_2$  layers, settles in at the PG onset temperature. Distinct from the  $q=0$  magnetism, its planar propagation wave vector is  $(\pi,0)\equiv(0,\pi)$ , yielding a  $(2\times 2)$  quadrupling of the magnetic unit cell ( $q=1/2$  magnetism). It further displays a strong out-of-plane anisotropy of the associated magnetic moments, predominantly pointing perpendicular to the  $\text{CuO}_2$  planes

We discovered that the  $q=0$  and  $q=1/2$  magnetisms could be embedded within a single complex and highly spread-out chiral magnetic texture. This phase could correspond to the smallest possible domain of LC supercell breaking LT, recently proposed to account for the PG opening [4]. The existence of such broad entities reveals an unexpected aspect of the PG physics that may modify our understanding of that state of matter.

[1] P. Bourges, D. Bounoua, Y. Sidis, C.R. Phys **22**, 1 (2021).

[2] B. Keimer *et al.*, Nature **518**, 179 (2015).

[3] D. Bounoua *et al.*, [arXiv:2111.00525v1](https://arxiv.org/abs/2111.00525v1) (under review in Phys. Rev. X)

[4] C.M. Varma, Phys. Rev. B, **99**, 224516 (2019).

## Mimicking cuprates with silver and fluorine

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We combine density functional theory, exact diagonalization in small clusters and different spectroscopies (neutrons, XPS, RIXS, optics) to elucidate the electronic structure of silver fluorides and their degree of similarity with cuprates[1,2]. We find that  $\text{AgF}_2$  is a charge-transfer insulator with strong analogies with parent cuprates but also some important differences. In particular, a strong buckling of  $\text{AgF}_2$  planes substantially reduces the superexchange constant  $J$  to nearly 70% of a typical cuprate value and disfavors metallization. This “buckling problem” can be greatly diminished or solved by epitaxial engineering[3] of flat silver fluoride analogues in appropriate substrates. To estimate the maximum superconducting  $T_c$  attainable by doping, we first study systematically a strong correlation previously found in monolayer cuprates between  $T_c$  and  $J$  confirming its validity. Extrapolating to fluorides we reach the conclusion that if doping is achieved, the superconducting  $T_c$  in monolayers can reach nearly 200K.

[1] J. Gawraczyński, et al. PNAS **116**, 1495 (2019).

[2] N. Bachar, K. Koterak, J. Gawraczyński, W. Trzcinski, J. Paszula, R. Piombo, P. Barone, Z. Mazej, G. Ghiringhelli, A. Nag, K.-J. Zhou, J. Lorenzana, D. van der Marel, and W. Grochala, Charge Transfer and dd Excitations in  $\text{AgF}_2$ , arXiv:2105.08862 (2021).

[3] A. Grzelak, et al. Phys. Rev. Mater. **4**, 084405 (2020).

# Unconventional and high- $T_c$ superconductivity from Fermi surface fluctuations in strongly correlated metals

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In quantum materials, electrons that have strong correlations tend to localize, leading to quantum spins as the building blocks for low-energy physics. When these electrons coexist with more weakly-correlated conduction electrons, multiple channels of effective interactions develop and compete. The competition creates quantum fluctuations having a large spectral weight, with the associated entropies reaching significant fractions of  $(R \ln 2)$  per electron. Advancing a framework to understand how the fluctuating local moments influence unconventional superconductivity is both pressing and challenging. Here we report our recent work [1] along this direction in the exemplary setting of heavy-fermion metals, where the quantum fluctuations manifest in the form of Kondo destruction and large-to-small Fermi-surface fluctuations [2]. We demonstrate unconventional superconductivity developing from Fermi surface fluctuations in the Anderson lattice model. For quantum criticality of both the Kondo-destruction type and the spin-density-wave type (SDW<sub>r</sub>, where the subscript “r” stands for the strong renormalization of the underlying quasiparticles and for which the quantum fluctuations above a nonzero but small cutoff scale  $E_{cr}$  are of the Kondo-destruction type [3]), the superconducting transition temperature is found to be exceptionally high relative to the effective Fermi temperature, reaching several percent of the bare Kondo scale [1].

Our results provide a natural understanding of the enigmatic superconductivity in a host of heavy-fermion metals. Moreover, the qualitative physics underlying our findings and their implications for the formation of unconventional superconductivity apply to a variety of highly correlated metals with strong Fermi surface fluctuations.

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[1] H. Hu, et al., arXiv:2109.13224 (2021).

[2] S. Paschen & Q. Si, Nat. Rev. Phys. 3, 9 (2021); S. Kirchner et al, Rev. Mod. Phys. 92, 011002 (2020); Q. Si et al, Nature 413, 804 (2001).

[3] L. Chen, H. Hu et al., in preparation (2022).

# Current pulses, critical currents, and cuprates: a novel means of exploring the ground state

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In the nearly-four decades following the discovery of the high-T<sub>c</sub> superconducting cuprates, researchers have toyed with the vast playground of unique phases and behaviours that manifest [1-3], however the puzzle of the normal-state ground-state lying beneath the superconducting dome has yet to be pieced together. Amusingly, in order to understand the origins of superconductivity, one must first destroy it. In weak superconductors, this is achieved using magnetic fields that exceed the superconductor's (upper) critical field, yet with upper critical fields reaching an excess of 100 T [4], magnetic fields alone do not suffice in the (optimally-doped) cuprates at the lowest temperatures.

Here, we use a novel approach combining intense current pulses to achieve high current densities and strong static magnetic fields in order to suppress superconductivity in La<sub>2-x</sub>Sr<sub>x</sub>CuO<sub>4</sub> thin films at temperatures far below the zero-field transition temperature. Using fields of up to 30 T and current densities of 10<sup>10</sup> Am<sup>-3</sup>, we demonstrate that in a sample with nominal T<sub>c</sub> = 20 K the superconducting state is almost completely removed at temperatures as low as 1.3 K without signs of self-heating. The success of this technique provides a new route for exploring the low temperature phase diagram of optimally-doped cuprates.

\* This work was supported by the ERC under the European Union's Horizon 2020 research and innovation programme (Grant Agreement no. 835279-Catch-22).

- [1] R. A. Cooper *et al.*, *Science*, **323**, 603, (2009)
- [2] N. Doiron-Leyraud *et al.*, *Nat. Commun.*, **8**, 2044, (2017)
- [3] J. Ayres *et al.*, *Nature*, 595, 661-666, (2021)
- [4] G. Grissonnanche *et al.*, *Nat. Commun.*, **5**, 3280, (2014)

**"Electron Spin Resonance in SCES materials and the SCES 2020/21 conference:  
Two hard tasks in my carrier"**

P.G. Pagliuso – IFGW/Unicamp – Brazil.

Electron Spin Resonance (ESR) was the main technique of my PhD work and I have used this technique during that time to study doped single-crystals of many intermetallic materials (including Heavy-Fermions) grown in the USA mostly by Zach Fisk and John Sarrao. This motivated my PhD Thesis Adviser Prof. Carlos Rettori to recommend to me a Post-Doc at LANL on Materials Synthesis and Characterization, supervised by John Sarrao.

I arrived there in May 1999, just after the first experiments that discovered superconductivity under pressure in CeRhIn<sub>5</sub>. I spent nearly three very exciting years there that only increased my interest in SCES materials.

Now, 21 years later, our group has an independent and fully equipped Materials Synthesis and Characterization laboratory at Unicamp – Campinas – Brazil (with a 4th Generation Synchrotron lab just around the corner) and it has helped the SCES critical mass to increase, spreading talented young researchers working in SCES all around Brazil and abroad.

However, we still have complicated issues regarding ESR on SCES that we do not quite understand that I would like to share with you in this talk.

It is a complicated challenge that we will do our best to overcome, as we did to keep the SCES community connected during the pandemic until the realization of SCES2020/21 Brazil online!

# New materials platform for two-dimensional magnetism and strong correlation studies: van der Waals magnets

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The modern history of magnetism is full of great advances in our knowledge of strong correlation. A list of materials that have been used is long and rich, but most of them are three-dimensional. It is not because materials with lower dimensions are less interesting but because such examples are relatively rare in nature. Not surprisingly, there have been consistent efforts to overcome this natural limit regarding two-dimensional (2D) magnetism: one notable example is thin films grown by a pulsed laser deposition technique. Although one should acknowledge thin films' important contributions to the 2D magnetism and correlation studies, however, better access to naturally occurring materials would be more beneficial in these challenging, otherwise exciting endeavors.

Against this backdrop, in 2016, several van der Waals magnets were reportedly exfoliated down to monolayer [1]: many new opportunities these materials might offer were immediately discussed, too [2]. We have since witnessed enormous sea changes in the research landscape of van der Waals magnets. The initial report of 2D Ising magnetism on monolayer antiferromagnetic FePS<sub>3</sub> [3] was followed by similar reports on ferromagnetic Cr<sub>2</sub>Ge<sub>2</sub>Te<sub>6</sub> [4] and CrI<sub>3</sub> [5]. In this talk, I will give an overview of the field [6] with several more recent highlights, including entangled magnetic exciton [7] and giant modulation of optical nonlinearity [8]. Finally, I will end my talk with a personal view of how the field might develop in the future.

[1] Cheng-Tai Kuo et al., *Scientific Reports* 6, 20904 (2016).

[2] Je-Geun Park, *J. Phys. Condens. Matter* 28, 301001 (2016).

[3] Jae-Ung Lee et al., *Nano Lett.* 16, 7433 (2016).

[4] Cheng Gong et al., *Nature*, 546, 265 (2017).

[5] Bevin Huang et al., *Nature*, 546, 270 (2017).

[6] Kenneth S. Burch, David Mandrus, and Je-Geun Park, *Nature* 563, 47 (2018).

[7] Soonmin Kang et al., *Nature* 583, 785 (2020).

[8] Jun-Yi Shan et al., *Nature* 600, 235 (2021).



## Entropy engineering and tunable magnetic order in the spinel high entropy oxide

Alannah Hallas

High entropy oxides (HEOs) are a new class of disordered materials that exhibit great promise for a range of applications due to their enhanced structural stability. The “entropy” in an HEO originates from the random mixture of five or more metal ions sharing a single crystal lattice. However, the actual degree of configurational disorder, its role in stabilizing the HEO phase, and its effect on other physical properties such as magnetism all remain open questions. To shed light on these questions, we have selected the spinel HEO  $(\text{Mn,Fe,Cr,Co,Ni})_{3-x}\text{Ga}_x\text{O}_4$  as our model system. Our study makes use of experimental probes with sensitivities that extend over many orders of magnitude in length scale, which is important for characterizing the true degree of randomness. We show that while site selectivity has an overall suppressing effect on the configurational entropy, over a certain range of compositions, Ga substitution yields a striking increase to the configurational entropy and may confer additional stabilization. Spinel oxides can be tuned seamlessly from the low entropy to the high entropy regime, making this an ideal platform for entropy engineering.

# Weyl-Kondo semimetals: $\text{Ce}_3\text{Bi}_4\text{Pd}_3$ and beyond

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Gapless topology driven by strong correlations is an emerging field of great interest. The rich landscape of strongly correlated metals [1] in conjunction with nontrivial topology is expected to be fertile ground for breeding novel, robust topological quantum phases, with potential for topological quantum devices. I will report on the recent discovery of one such material, the heavy fermion compound  $\text{Ce}_3\text{Bi}_4\text{Pd}_3$  [2]. It exhibits giant signatures of electronic topology [2,3], which are attributed to Weyl nodes pinned to the immediate vicinity of the Fermi level, giving rise to quasiparticles with ultraslow velocity [2-4]. In this system, genuine topology control can be achieved by magnetic field tuning, leading to the annihilation of Weyl nodes at moderate fields [5,6]. I will also discuss design strategies [7-9] for further correlation-driven topological metals, and point to new candidate materials.

\*Financial support has been provided by the Austrian Science Fund (FWF projects I2535-N27, W1243-N16, I4047-N27, and I5868-N/FOR 5249 "QUAST").

- [1] S. Paschen and Q. Si, *Nat. Rev. Phys.* **3**, 9 (2021).
- [2] S. Dzsaber, L. Prochaska, A. Sidorenko, G. Eguchi, R. Svagera, M. Waas, A. Prokofiev, Q. Si, and S. Paschen, *Phys. Rev. Lett.* **118**, 246601 (2017).
- [3] S. Dzsaber, X. Yan, M. Taupin, G. Eguchi, A. Prokofiev, T. Shiroka, P. Blaha, O. Rubel, S. E. Grefe, H.-H. Lai, Q. Si, and S. Paschen, *PNAS* **118**, e2013386118 (2021).
- [4] H.-H. Lai, S. E. Grefe, S. Paschen, and Q. Si, *PNAS* **115**, 93 (2018).
- [5] S. Dzsaber, D.A. Zocco, A. McCollam, F. Weickert, R. McDonald, M. Taupin, X. Yan, A. Prokofiev, L.M.K. Tang, B. Vlaar, L. E. Winter, M. Jaime, Q. Si, and S. Paschen, arXiv:1906.01182.
- [6] S. E. Grefe, H.-H. Lai, S. Paschen, and Q. Si, arXiv:2012.15841.
- [7] W. T. Fuhrman, A. Sidorenko, J. Hänel, H. Winkler, A. Prokofiev, J. A. Rodriguez-Rivera, Y. Qiu, P. Blaha, Q. Si, C. L. Broholm, and S. Paschen, *Sci. Adv.* **7/21**, eabf9134 (2021).
- [8] L. Chen, C. Setty, H. Hu, M. G. Vergniory, S. E. Grefe, L. Fischer, X. Yan, G. Eguchi, A. Prokofiev, S. Paschen, J. Cano, and Q. Si, arXiv:2107.10837.
- [9] H. Hu, L. Chen, Ch. Setty, S. E. Grefe, A. Prokofiev, S. Kirchner, S. Paschen, J. Cano, and Q. Si, arXiv:2110.06182.

# Search for new europium-based intermetallic 122 materials with non-trivial topological properties

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Today, more and more Eu-based compounds come into focus of magnetic topological non-trivial materials. The first examples were thin films of EuS on Bi<sub>2</sub>Se<sub>3</sub> [1]. In recent studies, the material EuCd<sub>2</sub>As<sub>2</sub> has attracted a lot of attention due to emergence of a variety of topological phases and magnetic phenomena [2,3]. Recently, a spin fluctuation induced Weyl semimetal state in the paramagnetic phase of EuCd<sub>2</sub>As<sub>2</sub> [2] and its tunability by pressure [4] was discovered. Furthermore, the similar material EuCd<sub>2</sub>P<sub>2</sub> has been explored due to its strong colossal magnetoresistance effect [5].

In this work, we present the single crystal growth and characterization of the system EuT<sub>2</sub>P<sub>2</sub>, with T = Cd, Zn, Mn crystallizing in the same trigonal structure (P-3m1) in order to search for similar effects in these materials. Single crystals were grown using a high-temperature Sn-flux technique. The physical properties of the compounds are explored via magnetization, electrical transport, heat capacity, and angle-resolved photoemission spectroscopy measurements.

[1] Katmis et al., Nature 533, 513 (2016).

[2] Ma et al., Science Adv. 5, eaaw4718 (2019).

[3] Jo et al., Phys. Rev. B 101, 140402(R) (2020).

[4] Gati et al., Phys. Rev. B 104, 155124 (2021).

[5] Wang et al., Adv.Mater., 33, 2005755 (2021).

# Quantum critical point in the high-pressure structure of CeSb<sub>2</sub>

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Ce-based heavy fermion compounds exhibit a variety of exotic states brought about by strong electronic correlations. Their properties are often susceptible to pressure-tuning, which can stabilise new phases and push materials through quantum phase transitions.

CeSb<sub>2</sub> at ambient pressure displays a series of complex magnetic phases and is thought to adopt a ferromagnetic ground state, a rare case in Ce systems which invites further study [1]. Magnetic transitions have been known to depend only weakly on applied pressure up to about 20 kbar, where material properties change abruptly [2]. Using high-pressure powder X-ray diffraction, we have recently demonstrated that this abrupt change can be attributed to a structural transition, and we have resolved the high pressure crystal structure [3]. Here, we focus on the low-temperature properties in the new high-pressure structure.

We have accessed the high-pressure structure of CeSb<sub>2</sub> using both piston-cylinder and anvil pressure cells at mK temperatures. Our resistivity and AC heat capacity data reveal two new phase transition anomalies which move to lower temperatures with increasing pressure. The temperature dependence of the resistivity above the ordering temperature is unusually steep, suggesting a low coherence temperature and very high effective masses. In the pressure region where the transitions extrapolate to zero temperature, we observe non-Fermi liquid behaviour, suggesting the presence of a quantum critical point. We will show data on the temperature-, field- and pressure-dependence of the resistivity in the vicinity of the quantum critical point, and we will discuss our findings in the context of recent experimental and theoretical results in other heavy fermion compounds.

[1] S. L. Bud'ko, P. C. Canfield, C. H. Mielke, and A. H. Lacerda, *Anisotropic Magnetic Properties of Light Rare-Earth Diantimonides*, Phys. Rev. B 57, 13624 (1998).

[2] T. Kagayama, Y. Uwatoko, S. L. Bud'ko, and P. C. Canfield, *Pressure-Induced Collapse of Ferromagnetism in CeSb<sub>2</sub>*, Physica B: Condensed Matter 359–361, 320 (2005).

[3] C. K. de Podesta *et al.*, this conference (2022).

# Chemical tuning effects on the extreme magnetoresistance of Dirac nodal arc semimetals

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PtSn<sub>4</sub> is a novel topological semimetal and hosts Dirac arcs in its momentum space such that the conduction and valence band touch along extended lines rather than at a fixed point [1]. One of the dominating electronic properties of this material is its ultrahigh “extreme” magnetoresistance (XMR) at low temperature, which onsets at 30 K [2]. This XMR has been linked to the unique energy dispersion and gapless band crossings, which impart topological character to the electronic structure of PtSn<sub>4</sub>. Hence, the XMR can be inextricably linked to the topology, as in WTe<sub>2</sub>, NbP, and others [1,2]. Another characteristic property of PtSn<sub>4</sub> is its high Residual resistivity ratio (RRR), which shows low defect density in as-grown crystals. This low defect density influences carrier mobility and can partly affect the XMR. In this talk, I will address the chemical and electronic properties related to the topology of the band structure of PtSn<sub>4</sub> and explain what happens when we perturb the system via chemical substitutions. The new material design involves the partial replacement of Pt in PtSn<sub>4</sub> with Au/Ir/Pd and characterizing the structural modifications and the effects on the XMR and RRR. This interplay between the electronic, chemical, and topological properties can provide us with the much-needed playground to find and investigate Dirac nodal arc-based topological semimetals. Ultimately, it will also help us understand the origin of XMR and whether it is related to the topology or low-defect density in the material.

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[1] Y. Wu *et al.*, Nat. Phys. **12**, 667 (2016).

[2] E. Mun *et al.*, Phys. Rev. B **85**, 035135 (2012).

# Field-induced quantum critical behavior in topological antiferromagnet $\text{CePtAl}_4\text{Ge}_2$

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Ce-based Kondo metals exhibit exotic quantum phenomena, such as quantum criticality, unconventional superconductivity, and topological magnetism, due to an intricate balance between Kondo effects and RKKY (Ruderman-Kittel-Kasuya-Yosida) interaction. When the magnetic frustration effects are present in the Kondo lattice, novel quantum phases such as the spin-liquid phase, topological spin texture, etc., have been suggested [1-3].  $\text{CePtAl}_4\text{Ge}_2$  exhibits an antiferromagnetic state below 2.3 K in which the size of ordered moments modulates with an ordering wave vector  $\mathbf{k} = (1.39, 0, 0.09)$  [4]. Single-crystal neutron diffraction experiments have been recently performed and revealed that the magnetic structure of  $\text{CePtAl}_4\text{Ge}_2$  is of multi- $\mathbf{k}$  structure in which symmetry-equivalent three arms of  $\mathbf{k} = (1.39, 0, 0.09)$  are superposed. Theoretical calculation of the topological numbers on singular points in the multi- $\mathbf{k}$  spin structure shows non-trivial hedgehog numbers, indicating that a three-dimensional topological spin texture is realized in this frustrated Kondo lattice. When subjected to a magnetic field applied along the [010] direction ( $H \parallel [010]$ ), the magnetic structure undergoes a phase transition at the critical field ( $H^* = 10$  kOe) from the multi- $\mathbf{k}$  to single- $\mathbf{k}$  phase while the ordering wave vector  $\mathbf{k}$  remains the same. At  $H^*$ , the temperature-coefficient of electrical resistivity and magnetic entropy exhibit the maximum value, suggesting that the field-induced topological transition from the hedgehog state to a non-topological single- $\mathbf{k}$  state is correlated with the quantum critical behavior. In this presentation, we will discuss the possible origin of the topological magnetic structure and the relationship between the topological transition and quantum criticality.

[1] P. Coleman and A. H. Nevidomskyy, *Journal of Low Temperature Physics* **161**, 182 (2010).

[2] Q. Si, J. H. Pixley, E. Nica, S. J. Yamamoto, P. Goswami, R. Yu, and S. Kirchner, *Journal of the Physical Society of Japan* **83**, 061005 (2014).

[3] T. Kurumaji *et al.*, *Science* **365**, 914 (2019).

[4] S. Shin *et al.*, *Physical Review B* **101**, 224421 (2020).

## Pressure tuned quantum phase transition in $\text{Fe}(\text{Ga}_{1-x}\text{Ge}_x)_3$

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Recent work reporting a ferromagnetic quantum critical point (FM-QCP) and associated strange metal behaviour in the heavy fermion system  $\text{CeRh}_6\text{Ge}_4$  [1] has brought renewed interest to the topic of quantum phase transitions in weak itinerant ferromagnets. In this talk I will present evidence of ferromagnetic quantum criticality in the d-electron material  $\text{Fe}(\text{Ga}_{1-x}\text{Ge}_x)_3$ .

$\text{FeGa}_3$  is a diamagnetic semiconductor, proposed to be a Kondo insulator [2], that becomes metallic with a small amount of germanium doping ( $x=0.002$ ). A weak ferromagnetic moment develops at a critical doping  $x_c=0.042$ . In the vicinity of the critical doping, heat capacity and resistivity show non-Fermi liquid behaviour [3], suggesting a FM-QCP in  $\text{Fe}(\text{Ga}_{1-x}\text{Ge}_x)_3$ . Theory predicts that a ferromagnetic phase transition generally turns first order as the Curie temperature is suppressed [4], but, so far, there are no signs that the FM-QCP is avoided in  $\text{Fe}(\text{Ga}_{1-x}\text{Ge}_x)_3$ .

To investigate the behaviour of  $\text{Fe}(\text{Ga}_{1-x}\text{Ge}_x)_3$  as the quantum phase transition is approached, I measured the temperature dependence of the resistivity as the Curie temperature is suppressed with hydrostatic pressure in  $\text{Fe}(\text{Ga}_{0.93}\text{Ge}_{0.07})_3$ . There is no evidence from these measurements that the phase transition becomes first order. However, disorder effects can suppress a first order phase transition [5], allowing the ferromagnetic transition to remain second order. Since the effects of disorder in  $\text{Fe}(\text{Ga}_{1-x}\text{Ge}_x)_3$  are unknown, I also measured the temperature dependence of resistivity at various germanium concentrations, at ambient pressure. In this talk I will present the resistivity data as a function of doping and pressure, which reveal strange metal behaviour over an extended region of the phase diagram.

\*This work is supported by the Program Committee.

[1] B. Shen et al., *Nature* 579, 51 (2020)

[2] Y. Zhang et al., *Proc. Natl. Acad. Sci* 115, 13 (2018)

[3] K. Umeo et al., *Phys. Rev. B* 86, 14 (2012)

[4] T.R. Kirkpatrick et al., *Phys. Rev. B* 85, 13 (2012)

[5] D. Belitz et al., *Phys. Rev.* 86, 23 (1999)

# Mesoscale Quantum Phase Transitions in LiHoF<sub>4</sub>

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The perhaps best understood experimental realization of a quantum phase transition may be observed in the dipolar Ising ferromagnet LiHoF<sub>4</sub> [1-3]. By applying a magnetic field perpendicular to the easy axis, the ferromagnetic phase transition is suppressed down to zero temperature at the quantum critical point at  $B_c \approx 5.1$  T. We report an investigation of the easy-axis AC susceptibility of LiHoF<sub>4</sub> as a function of the magnetic field direction relative to the hard magnetic axis, deriving the evolution of the magnetic-phase-diagram as a function of field orientation. When tilting the magnetic field away from the hard axis, present-day theory predicts a crossover from the ferromagnetic state in zero field to a field polarized state, as the longitudinal field component breaks the Ising symmetry. In contrast, we find that a line of well-defined phase transitions emerges from the QCP under perfectly transverse field, which connects the quantum critical point in transverse field ( $\Phi = 0^\circ$ ) with the coercive field in longitudinal field ( $\Phi = 90^\circ$ ). Our observations are in excellent quantitative agreement with a self-consistent model taking into account the non-Kramers nature of the Ho ions, the effects of hyperfine coupling and the presence of magnetic domains. We show that a continuous suppression of magnetic domains, resulting in quantum phase transitions purely involving magnetic domains, provides an intuitive explanation for the evolution of the phase diagram of LiHoF<sub>4</sub> as a function of field orientation.

[1] Bitko et al., Physical Review Letters **77**, 940-943 (1996).

[2] Rønnow et al., Science **308**, 389-392 (2005).

[3] Chakraborty et al., Phys. Rev. B **70**, 144411 (2004).



# Dynamics of the critical phonon modes in quantum paraelectric SrTiO<sub>3</sub>

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We report our recently performed triple-axis inelastic neutron scattering experiments on single-crystal SrTiO<sub>3</sub> at 37 mK. These are the first measurements deep into the enigmatic quantum polar acoustic state in the vicinity of the ferroelectric QCP. Measurements are taken at and around  $\mathbf{q} = 0$  in multiple directions in reciprocal space. In addition, we explore how the pressure affects the phonon mode in SrTiO<sub>3</sub> up to 5.0 kbar around 2 K. Our observations shed light on the coupling of the soft optical mode with the acoustic phonons, and its response to external pressure [1]. We believe this could help us understand the importance of anharmonic lattice dynamics and unusual thermal transport in SrTiO<sub>3</sub>.

The proximity of SrTiO<sub>3</sub> to a quantum critical point [2] and the evolution of the underlying modes when being tuned with even modest applied pressure has become a promising new branch of the study of quantum critical phenomena. The critical point here is associated with a soft optical phonon mode responsible for the ferroelectric instability through a continuous displacive transition. Our recent dielectric measurements under pressure [1,3] expose the formation of a ‘quantum polar-acoustic state’ below 2 K.

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[1] M. J. Coak, *et al.*, Phys. Rev. B **100**, 214111 (2019).

[2] S. E. Rowley, *et al.*, Nat. Phys., **10**(5), 367–372 (2014).

[3] M. J. Coak, *et al.*, PNAS **117**, 12707 (2020).

# Two channel Kondo physics in one dimension: algebraic hastatic order and remnants of quantum criticality

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The two-channel Kondo lattice likely hosts a rich array of phases, including magnetic orders, composite pair superconductivity and non-Fermi liquids, as well as *hastatic order*, a channel-symmetry breaking heavy Fermi liquid that has been predicted to have a spinorial order parameter[1,2]. We revisit its one-dimensional phase diagram using density matrix renormalization group. In contrast to previous work[3], we find algebraic hastatic orders generically for sufficiently strong coupling[4]. We show that these are heavy Tomonaga-Luttinger liquids with nonanalyticities at Fermi wave-vectors that are well-described by incommensurate hastatic density waves. Intriguingly, we find a recently predicted additional order parameter[2], not present at large-N that arises from RKKY mediated interference between hastatic spinors, and indications of increasingly strong residual repulsive interactions at strong coupling, suggesting that these hastatic orders might be non-Fermi liquids in higher dimensions.

\*This work is supported by the Program Committee.

[1] P. Chandra, P. Coleman, and R. Flint, *Nature* **493**, 621 (2013).

[2] M. Kornjača and R. Flint, arXiv:2012.08511 [cond- mat.str-el] (2020).

[3] T. Schauerte, D. L. Cox, R. M. Noack, P. G. J. van Dongen, and C. D. Batista, *Phys. Rev. Lett.* **94**, 147201 (2005).

[4] M. Kornjača and R. Flint arXiv:2203.07367 [cond- mat.str-el] (2022).

# Quantum criticality on a compressible lattice

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As an example of quantum criticality on a compressible lattice we study the Lorentz invariant  $\phi^4$  theory with an  $N$ -component field  $\phi$ , where strain couples to the square of the order parameter. In three spatial dimensions this coupling as well as the self-interaction of the  $\phi$  field are both marginal on the tree-level. We compute the one-loop renormalization group equations treating the  $\phi$  field as well as the phonons on the same footing. We find that the velocities of the  $\phi$  field as well as of the phonons are renormalized yielding an effective dynamical exponent  $z > 1$ . The renormalization group flow is found to depend on the number of components  $N$ . Whereas we find run-away flow for  $N < 4$  a new fixed-point emerges for  $N \geq 4$ . We discuss the relation to known results for classical criticality. Our findings are directly relevant to insulating quantum critical antiferromagnets.

# Emergent Magnetic and Electronic Phases in Pressure-Tuned van der Waals Antiferromagnets

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We report discovery of new metallic and magnetic phases in the van-der-Waals antiferromagnets MPS<sub>3</sub>, where M = Transition Metal, form an ideal playground for tuning both low-dimensional magnetic and electronic properties[1-4]. These are layered honeycomb antiferromagnetic Mott insulators, long studied as near-ideal 2D magnetic systems with a rich variety of magnetic and electric properties across the family.

We will present magnetic, structural and electrical transport results and compare the behaviour of Fe-, V-, Mn- and NiPS<sub>3</sub> as we tune them towards 3D structures – and Mott transitions from insulator to metal. I will show recent results on record high-pressure neutron scattering, which has unveiled an enigmatic form of short-range magnetic order in metallic FePS<sub>3</sub>.

We have mapped out the full phase diagram - a first in this crucial family of materials. We observe multiple transitions and new states, and an overall increase in dimensionality and associated changes in behaviour.

[1] G. Ouvrard et al., *Mat. Res. Bull.*, 1985, 20, 1181.

[2] C.R.S. Haines et al., *Phys. Rev. Lett.* 2018, 121, 266801.

[3] M.J. Coak et al., *J.Phys.:Cond. Mat.* 2019, 32, 124003.

[4] M.J. Coak et al., *Phys. Rev. X*, 11, 011024 (2021)

# Uniaxial pressure effects, magnon excitations and the emerging anisotropic nature of short-range order in CrI<sub>3</sub>

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CrI<sub>3</sub> is a quasi-2D semiconducting van der Waals ferromagnet which evolves long-range order down to the single-layer limit. Engineering the critical temperature to achieve room temperature applications is one of the critical next steps on the path to technological application. Hence, quantitative determination of uniaxial pressure effects, of magnetic anisotropy and of magnetic correlations are crucial to further exploit this material. Here, we report high-resolution capacitance dilatometry data, ferromagnetic resonance in a broad frequency regime of 30 - 330 GHz and in magnetic fields up to 18 T, and determine the short-range correlation lengths above T<sub>C</sub> [1-3]. Our data prove significant magnetoelastic coupling and provide quantitative values of the uniaxial pressure effects on long-range magnetic order derived from thermodynamic relations. Modelling the magnon branches by means of a domain-based ferromagnetic resonance model provides the microscopic parameters describing the magnetic excitations in the two-dimensional ferromagnet. Our data reveal the anisotropy gap of  $\Delta = 80$  GHz at 2 K which remarkably remains finite at T<sub>C</sub> and vanishes only above T<sub>Δ</sub> ~ 80 K, i.e. for T > 1.3 T<sub>C</sub>. In addition, we detect short-range magnetic correlations up to at least 160 K. Notably, the nature of the short-range correlations changes at T<sub>Δ</sub>, confirming the importance of spin-orbit coupling for the evolution of long-range ferromagnetism which develops from magnetically anisotropic short-range order. In addition, our analysis of the isothermal macroscopic magnetisation yields the number of correlated spins, which allows us to estimate the temperature dependence of the in-plane magnetic correlation length  $\xi_{\text{ab}}$ .

[1] J. Arneth et al., Phys. Rev. B 105, L060404 (2022).

[2] A. Ghosh et al., Phys. Rev. B 105, L081104 (2022).

[3] M. Jonak et al., arxiv.

# Spontaneous and strain induced metallic phase due to modified interlayer stacking in $1T\text{-TaS}_2$

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Tantalum disulphide ( $1T\text{-TaS}_2$ ) is a layered material which hosts an insulating commensurate charge density wave (CCDW) at temperatures below  $\sim 165\text{K}$ . Recent investigations of  $1T\text{-TaS}_2$  have revealed the existence of a metastable metallic phase accessible from this CCDW phase by applying a laser- or current pulse [1,2]. Here, we present Scanning Tunnelling Microscopy and Spectroscopy (STM/STS) measurements on  $1T\text{-TaS}_2$  surfaces not exposed to such pulses which show the same metallic electronic structure and topographic features as the pulse induced phase over distances of hundreds of *nanometres*. By analysing the CDW lattice shift across domain walls separating the normal and metallic phase, we provide evidence of a change in top layer stacking in this metallic phase. This finding agrees with recent theoretical and experimental works [3,4] which indicate a strong influence of the interlayer stacking on the electronic structure of the material.

Using angle resolved photoelectron spectroscopy (ARPES), we demonstrate that a correlated-metal phase can be stabilized from the insulating CCDW phase over hundreds of *micrometres* by the application of uniaxial strain to the sample [5]. The nascent quasi-particle peak at the Fermi level indicates that the system hosts Mott correlations, which is further confirmed by advanced electronic structure calculations performed for a non-equilibrium bulk stacking order of the material [6].

Our work highlights  $1T\text{-TaS}_2$  as a versatile and promising platform for the manipulation of Mott correlations through interlayer coupling and strain as a potential tuning parameter.

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[1] Stojchevska, L. *et al.*, *Science* **344**, 177 (2014).

[2] Vaskivskiy, I. *et al.*, *Nat. Commun.* **7**, 1 (2016).

[3] Ritschel, T. *et al.*, *Phys. Rev. B* **98**, 195134 (2018).

[4] Wu, Z. *et al.*, *Phys. Rev. B* **105**, 035109 (2022).

[5] Nicholson, C. *et al.*, arXiv, **2204.05598** (2022).

[6] Petocchi, F. *et al.*, arXiv, **2202.01285** (2022).

# Emergent phenomena in structurally engineered square-lattice iridates

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Spin-orbit coupling (SOC) is a key ingredient of nontrivial band topology in weakly interacting materials. On the other hand, the impact of SOC in strongly correlated systems often manifests in magnetic anisotropy. *5d* transition metal oxides offers unique opportunities to explore the SOC-correlation interplay since they have a similar energy scale. A prominent example is the square-lattice iridates which are surprisingly similar to weakly spin-orbit-coupled high- $T_c$  cuprates. To understand this intriguing SOC-correlation interplay, it is necessary to obtain model systems and tune the interactions by structural engineering in dimensionality, symmetry, strain, etc. In this talk, I will discuss our recent work on pseudospin-half square lattices realized in artificial perovskite superlattices as well as the Ruddlesden-Popper phases. By implementing different structural designs, we demonstrated control of the antiferromagnetic fluctuations in virtual of the hidden  $SU(2)$  symmetry and archived giant magnetic responses probed by resonant x-ray scattering. Transport signatures of the Slater-Mott crossover regime was also identified. Strain and gating were also applied to tune the properties. The results showcase the rich emergent behaviors and functional properties beyond the analogy with cuprates.

## Optical Properties of Superconducting $\text{Nd}_{0.8}\text{Sr}_{0.2}\text{NiO}_2$ Nickelate

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The intensive search for alternative non-cuprate high-transition-temperature ( $T_c$ ) superconductor has taken a positive turn recently with the discovery of superconductivity in Nickelates by Li et al. [1]. Indeed, this discovery is expected to be the basis for disentangling the puzzle behind the physics of high  $T_c$  in oxides. In the unsolved quest for the physical conditions necessary for inducing superconductivity, we report an optical study of a  $\text{Nd}_{0.8}\text{Sr}_{0.2}\text{NiO}_2$  film measured using synchrotron THz and IR/VIS/UV absolute reflectance spectroscopy, at temperatures above and below the critical  $T_c \sim 13$  K [2]. In the normal state, the film is described by the Drude model for metallic transport, from which the scattering time just above  $T_c$  is determined. The observed Mid-IR absorption indicates the presence of strong electronic correlation effect in the  $\text{NiO}_2$  plane similarly to cuprates. Below  $T_c$ , the formation of a superconducting energy gap ( $2\Delta$ ) at  $\sim 3.2$  meV is extracted using a fitting algorithm based on the Mattis-Bardeen model. These results together with an estimation of the scattering time are consistent with the superconductive film being in the dirty limit. Finally, a zero-temperature value of 490 nm is extracted for the London penetration depth, which is in accordance with the type-II superconductive nature.

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

[2] <https://arxiv.org/abs/2203.16986>



# Kondo anisotropy in URu<sub>2</sub>Si<sub>2</sub>

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The Kondo lattice physics is generally based on local and isotropic antiferromagnetic Kondo interaction between conduction and f-localized electrons. In certain circumstances, however, a momentum-dependent Anderson hybridization or a nonlocal Kondo coupling can give rise to the formation of heavy quasiparticles with a strong  $k$ -dependence. As a consequence, the Kondo pseudogap opening in the Kondo coherent regime can be strongly anisotropic in  $k$ -space with important consequences for the subsequent phases.

We present here, thanks to polarized electronic Raman scattering studies, the signature of the development of a coherent Kondo pseudogap predominantly in a single channel that highlights strong anisotropy in the Kondo physics in URu<sub>2</sub>Si<sub>2</sub> [1]. A calculation of the Raman vertices demonstrates that the strongest Raman vertex does, indeed, develop within this  $E_g$  channel for interband transitions and reaches a maximum along the diagonals of the Brillouin zone, implying a  $d$ -wave-like geometry for the Kondo pseudogap.

We will also discuss the magnetic field dependence of the Kondo physics in URu<sub>2</sub>Si<sub>2</sub> and clarify the Uranium f-electrons state thanks to Raman scattering studies under very high magnetic field up to 30 T.

[1] J. Buhot *et al.*, Phys. Rev. B **101**, 245103 (2020).

## Orbitally Selective Enhanced Spin-Orbit Coupling in Itinerant Actinides

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We investigate the effect of many-body correlations in anisotropic metallic materials which have strong spin-orbit coupling. We show that the spin-orbit coupling can be significantly enhanced for systems that are highly hybridized and are on the verge of a magnetic instability [1,2]. Furthermore, we show that the enhancement is extremely anisotropic and may lead to giant magnetic anisotropies in paramagnetic states. Such giant magnetic anisotropies have been observed in compounds such as URu<sub>2</sub>Si<sub>2</sub> and have been investigated in magnetically ordered phases [3]. Here, we show that the enhancement is also present in materials in which time-reversal symmetry is unbroken. We use the Under-screened Anderson Lattice Model that was proposed to describe the uranium and plutonium compounds [4]. By using a rotationally invariant approximation, we show that Coulomb interactions induce off-diagonal correlations which enhance the components of the spin-orbit coupling and results in extreme magnetic anisotropies.

[1] P.S. Riseborough et al., J. Phys., Cond. Mat. 32, 4455601 (2020).

[2] Xiao Yuan et al., Electron. Struct. 3, 024009 (2021).

[3] M. Werwinski et al., Phys. Rev. B, 90, 064430 (2014).

[4] C. Thomas, et al., Phys. Rev. B, 83, 014415 (2011).

# Quantum-well states at the surface of the heavy fermion URu<sub>2</sub>Si<sub>2</sub>

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Electrons can form a two-dimensional electron gas at metal surfaces. Lateral confinement, for example between surface steps, then leads to quantum well states. Electronic correlations considerably modify the band structure of some metals, leading to heavy fermions, unconventional superconductivity, and other new ordered phases. However, it remains open if correlated quantum well states can be formed at their surface. The heavy fermion metal URu<sub>2</sub>Si<sub>2</sub> shows a bulk electronic band structure with correlated heavy electron bands that become superconducting below 1.5 K. Here we study atomically flat terraces on surfaces of URu<sub>2</sub>Si<sub>2</sub> using millikelvin scanning tunneling spectroscopy. We find two-dimensional heavy fermions (2DHF) that obey the electron-in-a-box quantization with an effective mass 17 times the free electron mass. The lifetimes of the quantum well states are tens of picoseconds for energies of few meV, showing their correlated nature. We model the connection between surface and bulk states and show that the surface superconducting density of states is strongly affected by the 2DHF. Our results provide a route to realize quantized correlated electrons.

# Hidden-orders of uranium compounds

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Hidden order is often discussed in a strongly correlated electron systems. Among them, URu<sub>2</sub>Si<sub>2</sub> is known as a typical hidden-ordered material [1]. Such hidden-ordered states show few structural distortions and no magnetic response, so that the order should be explained as electronic multipole origin. As discussed for URu<sub>2</sub>Si<sub>2</sub> [1], the space group #139 (*I4/mmm*,  $D_{4h}^{17}$ ) has 8 IIa type maximal non-isomorphic subgroups, 4 of which are non-symmorphic and any atoms U, Ru, and Si are not necessarily moved. The screw or glide remain atoms in crystallographic equivalent positions, instead of the body centered translation (1/2, 1/2, 1/2). Each subgroup corresponds anti ferro electric multipole ordering. Most promising subgroups is #126 (*P4/nnc*,  $D_{4h}^4$ ) [2].

Interestingly, superconductors UTe<sub>2</sub> and UGe<sub>2</sub>, which belongs to symmorphic space group, #71 (*Immm*,  $D_{2h}^{25}$ ) and #65 (*Cmmm*,  $D_{2h}^{19}$ ), respectively, can also belong to the non-symmorphic subgroup, #48 (*Pnnn*,  $D_{2h}^2$ ), and #50 (*Pban*,  $D_{2h}^4$ ), respectively. In these cases, any atoms are not necessarily moved. It means, anti-ferro electric quadrupole ordering states can be found in both compounds. It should be emphasized that the atomic space group is unchanged, but the symmetry of electronic states only is lowered.

Recently, it is reported that URhSn (#189 (*P-62m*,  $D_{3h}^3$ )) undergoes the hidden-order transition at 54 K [2]. 3-fold rotational symmetry remains atoms in crystallographic equivalent positions, in this case. But the local symmetry of U, “2mm”, lowers to “2..”, in UTe<sub>2</sub>, UGe<sub>2</sub>, and URhSn.

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[1] H. Harima *et al.*, J. Phys. Soc. Jpn. **79**, 033705 (2010), and references therein.

[2] S. Kambe *et al.*, JPS Conf. Proc. **30**, 011035 (2020).

[3] Y. Shimizu *et al.*, Phys. Rev. B **102**, 134411 (2020).

# Crystal-field ground state wave function of UGa<sub>2</sub> probed with Resonant & Non-resonant Inelastic X-ray Scattering

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A central aspect in actinide research is the question of the  $5f$  occupancy: in uranium intermetallics, the  $5f$  states are usually believed to be itinerant, with band structure approaches providing successful descriptions. UGa<sub>2</sub> is a hexagonal intermetallic compound that orders ferromagnetically at 125 K, with moments of about 3  $\mu_B$  along [100] [1, 2, 3]. For this binary, however, the magnitude of the magnetic moments indicates a more localized nature of the  $5f$  electrons. DFT-based studies significantly underestimate the moments [4, 5] and the importance of correlation effects have recently been theoretically taken into consideration [6]. Spectroscopic investigations also show remarkable evidence for a localized character of the  $5f$  electrons [7, 8, 9].

In such scenario, the influence of crystal-field effects becomes relevant. Here we apply state-of-the-art high resolution Resonant Inelastic Scattering (RIXS) at the U M<sub>5</sub> edge and directional dependent Non-Resonant Inelastic X-ray Scattering (NIXS) at the U O<sub>4,5</sub> edge at large momentum transfers  $|q|$ . The comparison with full multiple calculations (Quany code [10]) shows the compatibility of the M-edge RIXS spectra with the multiplets of the U $5f^2$  configuration. Also the comparison of the isotropic high- $|q|$  NIXS data with full multiplet calculations shows that the symmetry of UGa<sub>2</sub> originates from the two electron system of U $5f^2$ . Both, the RIXS as well as NIXS spectra exhibit a strong directional dependence that is well described with the assumption of  $\Gamma_1$  or  $\Gamma_6$  symmetries for the ground state of the crystal-field split  $^3H_4$  multiplet, thus ruling four out of six possible states.

[1] A. Andreev *et al.*, Sov. Phys. JETP **48**, 1187 (1987).

[2] A. C. Lawson *et al.*, J. Magn. Magn. Mater. **50**, 83 (1985).

[3] R. Ballou *et al.*, J. Phys. Colloques **43**, CZ-279 (1982).

[4] M. Diviš *et al.*, Phys. Rev. B **53**, 9658 (1996).

[5] B. Chatterjee *et al.*, MRS Adv. **5**, 2639 (2020).

[6] B. Chatterjee *et al.*, Phys. Rev. B **103**, 205146 (2021).

[7] S. Fujimori *et al.*, J. Phys. Soc. Jpn. **85**, 062001 (2016).

[8] S. Fujimori *et al.*, Phys. Rev. B **99**, 035109 (2019).

[9] A. V. Kolomiets *et al.*, Phys. Rev. B **104**, 045119 (2021).

[10] M.W. Haverkort *et al.*, Phys. Rev. B **85**, 165113 (2012)

# Alloying-driven transition between ferromagnetism and antiferromagnetism in UTGe compounds: $\text{UCo}_{1-x}\text{Ir}_x\text{Ge}$

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We have conducted the study of the magnetic properties of an isostructural solid solution of the superconducting itinerant  $5f$ -electron ferromagnet  $\text{UCoGe}$  ( $T_C = 2.7$  K) with antiferromagnet  $\text{UIrGe}$  ( $T_N = 16.5$  K). The study includes magnetization, AC susceptibility, specific heat, and electrical resistivity measurements of a series of  $\text{UCo}_{1-x}\text{Ir}_x\text{Ge}$  compounds in polycrystalline and single crystalline forms. The results show that the weak ferromagnetism and superconductivity of parent  $\text{UCoGe}$  are already suppressed by very low Ir substitution for Co ( $x = 0.02$ ). Similarly, the rapid decrease in Néel temperature and the critical field of the metamagnetic transition both vanishing just above  $x = 0.8$  with decreasing Ir concentration is pointing to the gradual suppression of the antiferromagnetic state of  $\text{UIrGe}$ . The mid-range of the  $T$ - $x$  phase diagram  $0.02 \leq x \leq 0.8$  is made of correlated paramagnetic phase showing very broad bumps in temperature dependencies of  $b$ -axis magnetization and specific heat developing with increasing  $x$ . Above  $x = 0.24$ , the wide symmetrical peak also appears in the  $c$ -axis magnetization curve reflecting the reinforcement of antiferromagnetic correlations which may eventually lead to frozen incoherent spin configurations at low temperatures. The detected electrical resistivity anomalies support the presence of antiferromagnetic correlations in this concentration range as well.

Compared to the  $\text{UCo}_{1-x}\text{Ir}_x\text{Ge}$  system, the  $\text{URh}_{1-x}\text{Ir}_x\text{Ge}$   $T$ - $x$  phase diagram shows the discontinuous transition from ferromagnetic to antiferromagnetic phase without the existence of the correlated paramagnetic phase between them. The striking difference is preliminarily ascribed to either the instability of tiny U moment in the weak itinerant ferromagnet  $\text{UCoGe}$  or to the rather stable U moment in  $\text{URhGe}$  formed by much less delocalized  $5f$ -electrons assisted by weakly varying lattice parameters of  $\text{URh}_{1-x}\text{Ir}_x\text{Ge}$  compounds.

# Unconventional properties of unconventional superconductors: the concept of superconducting fitness

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The apparently contradicting responses of complex superconductors to different experimental probes poses fundamental difficulties that hinder our understanding of the full potential of these materials. In this context, the concept of superconducting fitness introduces two measures that quantify the unusual effects of external symmetry breaking fields and allows us to engineer the normal state electronic structure towards the optimization and stabilization of desirable superconducting phases [1,2]. This concept was applied to several families of materials, including ruthenates [3-5] and doped topological insulators [6,7]. For the former, the concept of superconducting fitness allowed us to identify a possible mechanism for the stabilisation of a chiral d-wave superconducting state. For the latter, the concept of superconducting fitness is associated with a generalization of Anderson's theorem, which explains the remarkable robustness of some unconventional superconductors in presence of impurities. The superconducting fitness measures were most recently associated with the presence of odd-frequency correlations, anomalous Hall effect in chiral superconductors, opening of high-energy gaps in nonunitary superconductors, Bogoliubov Fermi surfaces in even-parity time-reversal symmetry-breaking superconductors, and photon-induced supercurrents in anapole superconductors. The ubiquity of the fitness measures in theories associated with unusual responses in complex superconducting states reflects their importance and versatility.

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[1] Aline Ramires and Manfred Sigrist, *Phys. Rev. B* **94**, 104501 (2016).

[2] Aline Ramires, Daniel F. Agterberg and Manfred Sigrist, *Phys. Rev. B* **98**, 024501 (2018).

[3] Han Gyeol Suh, Henri Menke, P. M. R. Brydon, Carsten Timm, Aline Ramires and Daniel F. Agterberg, *Phys. Rev. Research* **2**, 032023(R) (2020).

[4] Aline Ramires, *J. Phys.: Conf. Ser.* **2164**, 012002 (2022).

[5] Sophie Beck, Alexander Hampel, Manuel Zingl, Carsten Timm, and Aline Ramires *Phys. Rev. Research* **4**, 023060 (2022)

[6] Lionel Andersen\*, Aline Ramires\*, Zhiwei Wang, Thomas Lorenz, Yoichi Ando *Science Advances* **6**, eaaY6502 (2020).

[7] Bastian Zinkl and Aline Ramires, arXiv.2201.05045, under review in *Phys. Rev. B* (2022).

# Superconductivity in Magic-angle Graphene Family

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The discovery of correlated states and superconductivity in magic-angle twisted bilayer graphene (MATBG) established a new platform to explore interaction-driven and topological phenomena. However, while multitudes of correlated phases have been observed in moiré systems, robust superconductivity has been the least common of all, only found in MATBG and more recently in magic-angle twisted trilayer graphene (MATTG). Here, we report the experimental realization of superconducting magic-angle twisted 4-layer and 5-layer graphene, hence establishing alternating-twist magic-angle multilayer graphene as a robust family of moiré superconductors. This discovery suggests that the flat bands shared by the members play a central role in the superconductivity. Moreover, our measurements in parallel magnetic fields, in particular the investigation of Pauli limit violation and spontaneous rotational symmetry breaking (nematicity), reveal a clear distinction between the MATBG and other structures with more than two layers, consistent with the discrepancy in their orbital response to the magnetic field. Our results expand the emergent family of moiré superconductors, providing new insight with potential implications for the design of novel superconducting materials platforms.



# ***Accuracy of moiré Wannier function models for twist bilayer graphene***

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Recent experimental observations of correlated phases in magic-angle twisted bilayer graphene (MATBG) strongly indicate the enhanced importance of electronic correlations in this flat band system [1, 2]. Twist in graphene layers in MATBG results in the formation of moiré patterns with length scales much larger than the atomic distance between carbon atoms in individual layers. It is often believed that most of the crucial physical properties occur at the moiré length scale. Thus a natural first step towards treating correlations is to construct a tight-binding model based on Wannier functions localized on the effective moiré lattice. However, the construction of such a model for twisted bilayer graphene is under debate due to the topological character of the energy bands [3]. We discuss the accuracy of such Wannier descriptions for the widely-used Bistritzer and MacDonald model for a range of twist-angles and values of relaxations. Our study provides a starting point for investigating interaction effects in MATBG.

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[1] Y. Cao et. al., Nature 556, 80 (2018); Y. Cao et. al., Nature 556, 536 (2018).

[2] X. Lu et. al, Nature 574, 653 (2019).

[3] Z. Song et. al., Phys. Rev. B 103, 205412 (2021).

# Direct evidence for Cooper pairing without a spectral gap in a disordered superconductor above $T_c$

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The idea that preformed Cooper pairs could exist in a superconductor at temperatures higher than its zero-resistance critical temperature ( $T_c$ ) has been explored for unconventional, interfacial and disordered superconductors, but direct experimental evidence is lacking. In this talk, I will present how we use scanning tunneling noise spectroscopy to show that preformed Cooper pairs exist up to temperatures much higher than  $T_c$  in the disordered superconductor titanium nitride (TiN). This is done by observing an enhancement in the shot noise that is equivalent to the change of the effective charge from one to two electron charges. We further show that the spectroscopic gap fills up rather than closes with increasing temperature. Our results [1] demonstrate the existence of a state above  $T_c$  that, much like an ordinary metal, has no (pseudo)gap but carries charge through paired electrons.

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[1] K.M. Bastiaans *et al.*, *Science* **374**, 608-611 (2021).

# Non-Fermi liquids and quantum criticality in multipolar Kondo Systems

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We discuss emergent non-Fermi liquid behaviors in multipolar Kondo systems, where conduction electrons interact with the local moments carrying higher-rank multipolar moments such as quadrupolar and octupolar moments. We first show that unexpected non-Fermi liquid states arise in the single impurity multipolar Kondo system using the renormalization group and conformal field theory. Next, we study the competition between the Kondo and RKKY interactions in the Bose-Fermi Kondo systems, where the RKKY interaction between multipolar moments is represented by a bosonic degree of freedom. We present the renormalization group solution of this problem and describe the quantum critical behaviors. We also discuss possible superconducting states arising from the multipolar Kondo interactions. We compare the theoretical results with existing experimental data on various f-electron systems such as  $\text{Pr}(\text{Ti},\text{V})_2\text{Al}_{20}$ ,  $\text{YbRu}_2\text{Ge}_2$ , and  $\text{Ce}_3\text{Pd}_{20}\text{Si}_6$ .

\*This work is supported by the NSERC of Canada and the Centre for Quantum Materials at the University of Toronto

- [1] A. S. Patri and Y. B. Kim, "Critical theory of non-Fermi liquid fixed point in multipolar Kondo problem", *Phys. Rev. X* **10**, 041021 (2021).
- [2] A. S. Patri, I. Khait, and Y. B. Kim, "Emergent non-Fermi-liquid phenomena in multipolar quantum impurity systems", *Phys. Rev. Research* **2**, 013257 (2020).
- [3] D. J. Schultz, A. S. Patri and Y. B. Kim, "Rise and Fall of Non-Fermi Liquid Fixed Points in Multipolar Kondo Problems", *Phys. Rev. Research* **3**, 013189 (2021).
- [4] D. J. Schultz, A. S. Patri and Y. B. Kim, "Non-Trivial Fixed Points and Truncated SU(4) Kondo Models in a Quasi-Quartet Multipolar Quantum Impurity Problem", *Phys. Rev. B* **104**, 125144 (2021).
- [5] A. S. Patri and Y. B. Kim, "Unconventional Superconductivity arising from multipolar Kondo interactions", *SciPost Physics* **12**, 057 (2022).

# Quadrupolar Kondo Effect and Generalized Doniach Phase Diagram for Non-Kramers Ions: Praseodymium Heavy Fermion Materials

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The paradigmatic Doniach phase diagram describes the competition between the long-range magnetic order and Kondo screening observed in many heavy fermion materials. Compounds with non-Kramers ions, notably U and Pr, pose an apparent challenge in that their ground state may not have a local dipole magnetic moment. In the  $\text{PrT}_2\text{Al}_{20}$  ( $T=\text{V, Ti}$ ) family of compounds in particular, the  $\text{Pr}^{3+}$  ion has an  $f^2$  configuration with a non-magnetic non-Kramers doublet as the lowest crystal-field state [1]. Nevertheless, this  $\Gamma_3$  doublet carries a quadrupolar moment [2], which is screened by conduction electrons with a  $\mathbf{k}$ -dependent hybridization function that results from projecting onto quadrupolar orbitals [2, 3]. The resulting Kondo effect is two-channel in nature, originating from the Kramers spin degeneracy of the conduction electrons.

We use a combination of *ab initio* density functional theory (DFT) calculations with dynamical mean-field theory (DMFT) to construct and solve a realistic periodic Anderson model, focusing on  $\text{PrV}_2\text{Al}_{20}$  for concreteness. The  $\mathbf{k}$ -dependent hybridization function and two-channel nature of the Kondo effect are essential features, which we capture both at the level of mean-field theory and the non-crossing approximation (NCA). Allowing for the interaction between the quadrupolar moments on nearby Pr ions, we obtain a long-range quadrupolar order which competes with the two-channel Kondo (over)screening, resulting in a generalized Doniach picture. Since the quadrupolar moments do not contribute to the Curie–Weiss susceptibility, we further find that inclusion of the first excited crystal-electric-field (CEF) multiplet, a spin triplet, is crucial in order to correctly reproduce the experimentally observed magnetic response [1].

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[1] A. Sakai and S. Nakatsuji, *J. Phys. Soc. Jpn.* **80**, 063701 (2011).

[2] For review, see: T. Onimaru and H. Kusunose, *J. Phys. Soc. Jpn.* **85**, 082002 (2016).

[3] G. Zhang, J. S. Van Dyke and R. Flint, *Phys. Rev. B* **98**, 235143 (2018).

## Two-channel Kondo problem in non-Kramers doublet systems

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There has been considerable interest in two-channel Kondo problem as focused on feasibility of quadrupole Kondo effect in the non-Kramers  $\Gamma_3$  doublet of cubic  $4f^2$  systems [1,2]. When the local quadrupole of the  $\Gamma_3$  doublet could interact with two equivalent conduction bands, it is expected that an anomalous metallic state concomitant with so-called non-Fermi liquid (NFL) behavior manifests itself. Among the Pr-based cubic compounds with the  $4f^2$  configuration,  $\text{PrT}_2\text{Zn}_{20}$  ( $T = \text{Rh, Ir}$ ) and  $\text{PrT}_2\text{Al}_{20}$  ( $T = \text{Ti, V}$ ) with the  $\Gamma_3$  doublet ground state exhibit coexistence of quadrupole order and superconducting states [3-5]. For  $\text{PrIr}_2\text{Zn}_{20}$ , upon applying nonhydrostatic pressure above 6.3 GP, the antiferroquadrupole order and the superconductivity simultaneously vanish [6]. Suppose the cubic symmetry is indispensable for them, on-site quadrupole fluctuations play a role for the superconductivity. On the other hand, above the quadrupole ordering temperatures, the NFL behaviors were observed, which indicates formation of the quadrupole Kondo lattice [7,8]. In the Pr diluted system  $\text{Y}(\text{Pr})\text{Ir}_2\text{Zn}_{20}$ , we observed single-site NFL behaviors such as the electrical resistivity of  $\Delta\rho \propto \sqrt{T}$  and the specific heat of  $C/T \propto -\log T$  [9]. The elastic constant  $(C_{11} - C_{12})/2$  shows softening on cooling with logarithmic variation [10]. Moreover, the quadrupolar Grüneisen ratio obtained from thermal expansion measurements shows  $-\log T$  dependence [11]. These anomalous NFL behaviors are consistent with the scenario of the quadrupole Kondo effect.

- [1] P. Nozières and A. Blandin, *J. Physique* **41**, 193 (1980).
- [2] D. L. Cox and A. Zawadowski, *Adv. Phys.* **47**, 599 (1998).
- [3] T. Onimaru *et al.*, *Phys. Rev. Lett.* **106**, 177001 (2011).
- [4] A. Sakai *et al.*, *J. Phys. Soc. Jpn.* **81**, 083702 (2012).
- [5] T. Onimaru and H. Kusunose, *J. Phys. Soc. Jpn.* **85**, 082002 (2016).
- [6] K. Umeo, T. Onimaru *et al.*, *Phys. Rev. B* **102**, 094505 (2020)
- [7] A. Tsuruta and K. Miyake, *J. Phys. Soc. Jpn.* **84**, 114714 (2015).
- [8] T. Onimaru *et al.*, *Phys. Rev. B* **94**, 075134 (2016).
- [9] Y. Yamane, T. Onimaru *et al.*, *Phys. Rev. Lett.* **121**, 077206 (2018).
- [10] T. Yanagisawa, T. Onimaru *et al.*, *Phys. Rev. Lett.* **123**, 067201 (2019).
- [11] A. Wörl, M. Garst, Y. Yamane, S. Bachus, T. Onimaru, and P. Gegenwart, arXiv:2205.01347.

# Symmetrized quadrupolar expansivity as sensitive probe of the quadrupolar Kondo effect: diluted $\text{PrIr}_2\text{Zn}_{20}$

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The quadrupolar Kondo effect provides a route to fascinating entangled quantum states with inherent non-Fermi liquid behavior and residual entropy. We focus on highly diluted cubic Kondo metal  $\text{Y}_{1-x}\text{Pr}_x\text{Ir}_2\text{Zn}_{20}$  ( $x \approx 0.04$ ) with non-Kramers  $\Gamma_3$  doublet ground state, which displays generic signatures of the single-ion quadrupolar Kondo effect in electrical transport, specific heat and the temperature dependence of the elastic constants [1,2].

Our novel experimental approach establishes the symmetrized quadrupolar thermal expansion and magnetostriction, derived by combination of various linear expansivities, as highly sensitive and, so far, overlooked probes to directly deduce the quadrupolar Kondo effect. In particular, the quadrupolar Grüneisen ratio which quantifies the adiabatic elastocaloric effect, displays a characteristic  $H^2/T^2$  divergence [3].

Probing strain effects in quantum materials, is currently a topic of significant general relevance. The approach of symmetrized quadrupolar expansivity and quadrupolar Grüneisen parameter measurements is not only a novel powerful approach to characterize critical behavior arising from quadrupole moments but could also be a highly suitable means to examine nematic fluctuations in cuprates and iron-based superconductors.

- [1] Y. Yamane, T. Onimaru, K. Wakiya, K.T. Matsumoto, K. Umeo, T. Takabatake, *Phys. Rev. Lett.* **121**, 077206 (2018).
- [2] T. Yanagisawa, H. Hidaka, H. Amitsuka, S. Zherlitsyn, J. Wosnitza, Y. Yamane, T. Onimaru, *Phys. Rev. Lett.* **123**, 067201 (2019).
- [3] A. Wörl, M. Garst, Y. Yamane, S. Bachus, T. Onimaru, P. Gegenwart, to be published.

# Equilibration time in many-body quantum systems

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A major open question in studies of nonequilibrium quantum dynamics is how long it takes for an isolated many-body quantum system to reach equilibrium. We show that there is not a single answer for this question. The equilibration time depends not only on the model and the initial state, but also on the quantity and the dynamical features considered. We discuss a recent NMR experiment, where we measured a new entropy -- the correlation Rényi entropy -- and showed that it keeps growing even after the evolution of the entanglement entropy has already saturated [1]. We also discuss the case of chaotic models, where the equilibration time can scale either exponentially or polynomially with system size depending on whether dynamical manifestations of spectral correlations in the form of the correlation hole ("ramp") are taken into account or not [2].

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[1] M. Niknam *et al.*, Phys. Rev. Lett. **127**, 080401 (2021).

[2] T. Lezama *et al.*, Phys. Rev. B **104**, 085117 (2021).

# Higgs spectroscopy of superconductors

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In conventional time-resolved pump-probe experiments on superconductors one measures the relaxation of an optical probe after the excitation by an ultra-short laser pulse. With the recent development of THz laser technology it is now possible to excite or quench collective excitation, such phonons or the superconducting condensate. In the past we have predicted characteristic Higgs oscillations after a quantum quench in superconductors that allows investigating the ground state directly that, indeed, has been confirmed experimentally for an s-wave superconductor. Furthermore, several predictions have been made for a 2-band superconductor in which two Higgs oscillations interact.

During the last few years we have developed a classification scheme that allows to characterize Higgs oscillations of all possible symmetries [1]. Using polarized light in different directions, we predict that it is possible to map out the underlying gap symmetry of the superconducting ground state. We compare our analytical calculations with full (numerically exact) methods to get further insights into the nature of the Higgs mode. An alternative to a quench by THz laser is to measure the resonant third-harmonic generation (THG) signal; we have developed a theory for both cases [2-4]. As an example, we have applied our theory to *d*-wave high- $T_c$  superconductors: two Higgs modes are predicted. This, and other predictions, have been recently confirmed by experiment by the MPI Stuttgart and TU Dresden groups [5-10].

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- [1] L. Schwarz, D. Manske *et al.*, Nat. Commun. **11**, 287 (2020).
- [2] L.Schwarz and D. Manske, Phys. Rev. B 101, 184519 (2020).
- [3]. L. Schwarz, R. Haenel, and D. Manske, Phys. Rev. B 104, 174508 (2021).
- [4]. R. Haenel, P. Froese, D. Manske, and L. Schwarz, Phys. Rev. B 104, 134504 (2021).
- [5]. H.Chu, S. Kaiser, D. Manske et al., Nat. Commun. 11, 1793 (2020).
- [6]. H.Chu, S. Kaiser, D. Manske et al., arXiv:2109.09971, submitted to Nature Materials (2021).
- [7]. M.-J. Kim, S. Kaiser, D. Manske et al., submitted to Nature Photonics (2021).
- [8]. M. Puviani, L. Schwarz, X.-X. Zhang, S. Kaiser, and D. Manske, Phys. Rev. B 101, 220507 (2020).
- [9]. L.Schwarz, B. Fauseweh, and D. Manske, Phys. Rev. B 101, 224510 (2020).
- [10]. M. Puviani, R. Hackl, D. Manske et al., Phys. Rev. Lett. 127, 197001 (2021).



# Emergent dynamical phases in periodically driven BCS systems

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We study the out-of-equilibrium dynamics of a BCS system subject to a periodic drive in the absence and presence of dissipation. The phase diagram is surprisingly rich, with four dynamical phases involving first and second-order type transitions. For excitation frequency above the gap, we show the existence of a new collective mode, dubbed Rabi-Higgs [1] which turns into a gapless regime following a second-order phase transition. In the presence of dissipation, the Rabi-Higgs mode becomes a transient effect and interesting steady-states with strong nonlinearities can be observed [2]. On the other hand, for subgap excitations, we demonstrate that the combined effect of drive and many-body interactions results in emerging parametric resonances [3]. In particular, Arnold's tongues arise when the driving frequency matches  $2\Delta_0/n$ , with  $n$  being a natural number and  $\Delta_0$  the equilibrium gap parameter. Inside Arnold's tongues, we find a commensurate time-crystal condensate that retains the  $U(1)$  symmetry breaking of the parent superconducting phase. Outside the tongues, the synchronized collective Higgs mode found in quench protocols [4] is stabilized without the need for a strong perturbation. We show the parametric resonances are quite robust and do not need long coherence times to be observed. Our results are directly relevant to cold-atom and condensed-matter systems and may have applications in parametric amplification, frequency converters, and sensing.

[1] H. P. Ojeda Collado *et al.*, Phys. Rev. B **98**, 214519 (2018).

[2] H. P. Ojeda Collado *et al.*, Phys. Rev. B **101**, 054502 (2020).

[3] H. P. Ojeda Collado *et al.*, Phys. Rev. Research **3**, L042023 (2021).

[4] H. P. Ojeda Collado *et al.*, Phys. Rev. B **99**, 174509 (2019).

# Exchange scaling of ultrafast angular momentum transfer in 4f antiferromagnets

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Among the ternary silicides,  $\text{LnRh}_2\text{Si}_2$  ( $\text{Ln} = \text{Ce-Nd}, \text{Sm-Yb}$ ), different lanthanides lead to a drastic change of magnetic properties. All compounds order antiferromagnetically but their Néel temperatures vary over a wide temperature range between 70 mK ( $\text{YbRh}_2\text{Si}_2$  [1]) and 107 K ( $\text{GdRh}_2\text{Si}_2$  [2]). Recently new interest emerged because of surface states presenting interesting magnetic properties [3-5].

We obtained platelet-shaped single crystals in this series from indium flux applying a modified Bridgman method up to 1550°C [2]. The magnetic ground state of the crystals was characterized using magnetization, specific-heat and electrical transport measurements. In addition, we studied the ultrafast magnetization dynamics and systematically varied the 4f occupation, thereby altering the magnitude of the RKKY coupling energy [6]. We find that the rate of direct transfer between opposing magnetic moments is directly determined by this coupling. Given the high sensitivity of RKKY to the conduction electrons, our results offer a useful approach for fine tuning the speed of magnetic devices.

Work in collaboration with: S.-E. Lee, D. Zahn, V. Borisov, D. Thonig, A. Ernst, C. Schüßler-Langeheine, N. Pontius, U. Staub, O. Eriksson

[1] O. Trovarelli *et al.*, Phys. Rev. Lett. **85**, 626 (2000).

[2] K. Kliemt, *et al.*, Cryst. Res. Technol. **55**, 1900116 (2020).

[3] S. Schulz *et al.*, npj Quantum Materials **4**, 26 (2019).

[4] G. Poelchen *et al.*, npj Quantum Materials **5**, 70 (2020).

[5] D. Usachov *et al.*, PRL **124**, 237202 (2020).

[6] Y.W. Windsor, *et al.*, Nat. Mater. (2022). <https://doi.org/10.1038/s41563-022-01206-4>

# Non-chiral bosonization of strongly inhomogeneous Luttinger liquids driven out of equilibrium

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Non-chiral bosonization (NCBT) is a modification of the standard Fermi-Bose correspondence in one spatial dimension, done (in the first instance) to reproduce exactly the correlation functions of otherwise free fermions in presence of strong inhomogeneities. This modified correspondence has been shown to reproduce the most singular parts of the correlation functions exactly when (forward-scattering) mutual interactions between fermions are included and the system is in equilibrium [1,2,3,4,5,6,7,8].

The present work extends the above ideas to systems that are driven out of equilibrium by an application of bias between right and left movers [9]. We show that an appropriate version NCBT reproduces exactly the one-particle Green functions of this system under bias when mutual interaction between fermions is absent.

Lastly, we indicate the method to be used to obtain the correlation functions when mutual interactions are present.

- [1] Joy Prakash Das and Girish S. Setlur. "**The one step fermionic ladder.**" *Physica E: Low-dimensional Systems and Nanostructures* 94 (2017): 216-230.
- [2] Joy Prakash Das and Girish S. Setlur. "**Ponderous impurities in a Luttinger liquid.**" *Euro Physics Letters* 123.2 (2018): 27002.
- [3] Joy Prakash Das and Girish S. Setlur. "**The Quantum Steeplechase**" *International Journal of Modern Physics A* 33.29 (2018): 1850174.
- [4] Joy Prakash Das, Chandramouli Chowdhury and Girish S. Setlur. "**Non-chiral bosonization of strongly inhomogeneous Luttinger liquids.**" *Theoretical and Mathematical Physics, Springer* 199.2 (2019): 302-329.
- [5] Joy Prakash Das and Girish S. Setlur. "**Transport properties of a Luttinger liquid with a cluster of impurities.**" *Physica E: Low-dimensional Systems and Nanostructures* 110 (2019): 39-48.
- [6] Joy Prakash Das and Girish S. Setlur. "**Conductance of inhomogeneous Luttinger liquids with an infinite bandwidth.**" *Physics Letters A* 383.25 (2019): 3149-3161.
- [7] Joy Prakash Das, Chandramouli Chowdhury and Girish S. Setlur. "**Friedel oscillations and dynamical density of states of an inhomogeneous Luttinger liquid.**" *Physica Scripta* 95 075710 (2020).
- [8] Nikhil Danny Babu, Joy Prakash Das and Girish S. Setlur. "**Density Density Correlation Function of Strongly Inhomogeneous Luttinger Liquids.**" *Physica Scripta* 95 115206 (2020).
- [9] Nikhil Danny Babu and Girish S. Setlur. "**Non-Markovian transients in transport across chiral quantum wires using space-time non-equilibrium Green functions.**" *2022 J. Phys.: Condens. Matter* 34 125602.

# Planckian Metal at a Doping-Induced Quantum Critical Point

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We numerically study a model of interacting spin-1/2 electrons with random exchange coupling on a fully connected lattice [1]. This model hosts a quantum critical point separating two distinct metallic phases as a function of doping: a Fermi liquid phase with a large Fermi surface volume and a low-doping phase with local moments ordering into a spin-glass. We show that this quantum critical point has non-Fermi liquid properties characterized by T-linear Planckian behavior,  $\omega/T$  scaling and slow spin dynamics of the Sachdev-Ye-Kitaev (SYK) type. The  $\omega/T$  scaling function associated with the electronic self-energy is found to have an intrinsic particle-hole asymmetry, a hallmark of a *skewed non-Fermi liquid*.

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[1] Ph. Dumitrescu, N. Wentzell, A. Georges, O. Parcollet, Phys. Rev. B **105**, L180404 (2022).

[2] P. Cha, N. Wentzell, O. Parcollet, A. Georges, E-A Kim, PNAS August 4, 117 (31) 18341-18346 (2020).

# Quasiparticle metamorphosis in a doped random t-J model: a many-body localization perspective

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Doped Mott insulators, especially the t-J model, are the starting point for the study of a variety of fractionalization phenomena and emergent excitations in strongly correlated systems such as quantum spin liquids and the cuprate superconductors. Although the exact many-body states are typically very complex and highly entangled, they can sometimes be approximated as local excitations – quasiparticles – with some well-defined quantum numbers associated with local conserved quantities. Owing to their additive property, identifying the parameter regimes where quasiparticles are good approximations to the low-lying many-body states can greatly simplify our understanding of these systems. For example, the anomalously large thermal Hall conductivity seen in underdoped cuprates and Kitaev materials suggests the existence of fractionalized fermions, but it is not fully understood if these quasiparticles can be stable in the presence of magnetic order that these systems exhibit.

Here we report our study [1] of the metamorphosis of quasiparticles – magnons and Jordan-Wigner fermions to Landau quasiparticles - upon increasing the hole doping in an SYK-like disordered t-J model. We identify the quasiparticle fractionalization and metamorphosis with a localization transition in the many-body Hilbert space, where bad quasiparticles are fully (many-body) delocalized. This approach, based on a scaling treatment of the quasiparticle support size in the many-body Hilbert space, was originally proposed [2] in the context of Landau quasiparticle lifetimes in disordered interacting quantum dots, and was recently generalized by two of us [3] to disorder-free quantum spin systems.

We find that away from critical doping, some stable quasiparticles are always present. In the magnetically ordered underdoped phase, apart from the spin-1 magnons, (natural excitations of a magnetic state), a very different emergent quasiparticle – essentially a Jordan-Wigner (JW) fermion – is also shown to be stable, but Landau quasiparticles are not. We believe these JW excitations likely play a significant role in determining some of the properties of underdoped cuprates such as an anomalously large thermal Hall conductivity even in the presence of collinear magnetic order, reminiscent of the Kitaev materials. In the overdoped regime, we find that Landau quasiparticles are stable but magnons and JW fermions are not. At a certain critical hole doping, we find the none of the quasiparticles is stable, which is the expectation for a strange metal phase.

The JW quasiparticles we found are inherently nonlocal in the microscopic (spinful fermion) degrees of freedom, and their emergence would not be easy to capture using other contemporary local numerical approaches such as those based on the dynamical mean-field theory. Our analysis requires the evaluation of a large number of excited states, for which we have used the the FEAST exact diagonalization technique.

[1] Aman Kumar, Subir Sachdev and Vikram Tripathi, arXiv:2112.01760.

[2] B. L. Altshuler *et al.*, , Phys. Rev. Lett. **78**, 2803 (1997).

[3] Aman Kumar and Vikram Tripathi, Phys. Rev. B **102**, 100401(R) (2020).

# The fate of the spin polaron in the 1D $t$ - $J$ model

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We study the intrinsic origin of the well-established differences in the motion of a single hole in the 1D and 2D antiferromagnet. To this end, we consider a 1D  $t$ - $J$  model, perform the slave fermion transformation to the holon-magnon basis, and solve the obtained model in a numerically exact manner [1].

We explicitly show that the spin polaron quasiparticle, which is well-known from the studies of a single hole in the 2D antiferromagnet, is destroyed in the 1D  $t$ - $J$  model by the magnon-magnon interactions. Nevertheless, we observe surprising similarities between the spectra obtained with and without magnon-magnon interactions, indicating that some of the key features of the spin polaron physics are still preserved in 1D. Connecting the obtained results to our previous works [2, 3], we show an intuitive picture explaining the role of the magnon-magnon interactions in the 1D and 2D  $t$ - $J$  model.

[1] P. Wrzosek *et al.*, arXiv:2203.01846 (2022).

[2] K. Bieniasz, P. Wrzosek, A. M. Oleś and K. Wohlfeld, *SciPost Phys.* **7**, 066 (2019).

[3] P. Wrzosek and K. Wohlfeld, *Phys. Rev. B* **103**, 035113 (2021).

## ***Charge transport in pinned, gapless charge density waves***

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Gapped, pinned charge density waves are charge insulators. Charge density wave states in strongly-correlated materials are often gapless. Using effective field theory methods [1], I will show how this gives rise to a nonzero electric dc conductivity. Remarkably, the leading contribution is independent from the strength of disorder in the system. I will comment on the potential relevance of this mechanism to strange metallic transport in cuprate high T<sub>c</sub> superconductors.

[1] Luca V. Delacrétaz, Blaise Goutéraux and Vaios Ziogas, Phys.Rev.Lett. 128 (2022) 14, 141601.

# Information-theoretic measures of superconductivity in a two-dimensional doped Mott insulator

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Quantum information can be used to advance our understanding of phases of matter in many-body quantum systems. We use tools of quantum information to characterize the entanglement-related properties of unconventional superconductivity in a doped Mott insulator. We study the two-dimensional Hubbard model with cluster dynamical mean-field theory to show how key measures of correlations -local entropy, thermodynamic entropy and total mutual information- detect the superconducting phase obtained upon doping the Mott insulating phase. We find that the behavior of the difference in the local entropy between the normal and superconducting states follows that of the potential energy. In the superconducting state thermodynamic entropy is strongly suppressed near the Mott insulator, whereas the total mutual information is amplified and shows a peak versus doping.

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# Automatic differentiation applied to excitations with projected entangled-pair states

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While the low-lying charge excitations of the Hubbard model at half filling can be studied using quantum Monte Carlo (QMC) techniques without a negative sign problem, the accuracy of the results, such as the charge gap, can be difficult to control, especially in the large interaction  $U/t$  limit. We show how a new method based on tensor networks produces accurate results for a wide range of  $U/t$  and compare these to new and existing QMC data. This method provides a competitive alternative with a broad range of applications.

The excitation ansatz for tensor networks is a powerful tool for simulating the low-lying quasiparticle excitations above ground states of strongly correlated quantum many-body systems. Recently, the two-dimensional tensor network class of infinite projected entangled-pair states gained new ground state optimization methods based on automatic differentiation, which are at the same time highly accurate and simple to implement.

Naturally, the question arises whether these new ideas can also be used to optimize the excitation ansatz, which has recently been implemented in two dimensions as well. In this talk, based on our recent paper [1], we describe a straightforward way to reimplement the framework for excitations using automatic differentiation, and demonstrate its performance for the Hubbard model at half filling.

[1] B. Ponsioen, F. Assaad, and P. Corboz, SciPost Physics 12, 006 (2022).

# Electric Quadrupolar Response in the Magnetic Phases of UNi<sub>4</sub>B

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UNi<sub>4</sub>B (*Cmcm*,  $D_{2h}^{17}$ , No. 63) shows antiferromagnetic order with a vortex-type magnetic structure below  $T_N \approx 20.4$  K in the pseudo-honeycomb plane [1]. This compound is now attracting renewed attention because current-induced magnetization in a metallic system, *i.e.*, a new cross-correlation phenomenon based on recent advances in the theory of augmented multipoles [2], has experimentally been demonstrated [3].

In the present study, the ultrasound technique, which can sensitively detect electric multipolar degrees of freedom, is combined with the advanced high-magnetic-field generation equipment at the HLD and Tohoku Univ. We studied the electric quadrupolar susceptibility derived from the multipolar degrees of freedom in both paramagnetic and the vortex magnetic state of UNi<sub>4</sub>B by means of ultrasonic measurements. We have succeeded in identifying the electric quadrupoles that maintain their degrees of freedom without ordering at the center of a magnetic-vortex arrangement [4].

Furthermore, we traced magnetic field-temperature phase diagrams up to 30 T and observed a highly anisotropic elastic response within the honeycomb layer. Strong correlations have been observed between the magnetic-field-induced phases and the electric quadrupole response in magnetic field. We conclude that the electric quadrupoles play an important role in the vortex-like magnetic structure of this system and contribute to the spin-reorientation process.

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[1] S. A. M. Mentink *et al.*, Phys. Rev. Lett. **73**, 1031 (1994).

[2] S. Hayami *et al.*, Phys. Rev. B **98**, 165110 (2019).

[3] H. Saito *et al.*, J. Phys. Soc. Jpn. **87**, 033702 (2018).

[4] T. Yanagisawa *et al.*, Phys. Rev. Lett. **126**, 157201 (2021).

## Hyperfine interactions at ultra-low temperatures: their role in PrOs<sub>4</sub>Sb<sub>12</sub>

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Many strongly correlated electron systems develop ordered phases at low temperatures that can be well understood in terms of an electronic order parameter. At ultra-low temperatures, however, the hyperfine interaction between nuclei and electrons becomes increasingly important, and we have to consider how this affects ordered phases and phase transitions close to zero temperature.

PrOs<sub>4</sub>Sb<sub>12</sub> is a superconductor below 1.85 K and 2.2 T, and develops antiferroquadrupolar (AFQ) order in magnetic fields between ~4 T and 14 T. The hyperfine constant of Pr is relatively large at 52 mK and the Pr crystal electric field levels are closely involved in both the superconducting and AFQ phase. This combination of properties makes PrOs<sub>4</sub>Sb<sub>12</sub> an ideal material to study the effects of the hyperfine interaction on ordered phases [1].

I will describe magnetic susceptibility experiments performed at the London Low Temperature Laboratory to study the phase diagram of PrOs<sub>4</sub>Sb<sub>12</sub>. We found that the phase boundaries in PrOs<sub>4</sub>Sb<sub>12</sub> continuously develop down to temperatures as low as a few mK and that the hyperfine interaction in this material suppresses superconductivity and enhances AFQ order.

We explain our results in terms of a ground state composed of hybrid nuclear-electronic states. That is, the low temperature Pr energy levels can no longer be considered as purely electronic entities, but must be described in terms of both electron and nuclear quantum numbers. Thus, hybrid nuclear-electronic order develops with novel low energy excitations.

\*This work was supported by the European Microkelvin Platform, EU's H2020 project under grant agreement no. 824109 and HFML-RU/NWO-I, member(s) of the European Magnetic Field Laboratory (EMFL).

[1] A. McCollam *et al.*, Physical Review B, **88**, 075102 (2013).

# Field-space anisotropy of magnetic phases and excitations in cubic Ce<sup>3+</sup> compounds

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Cubic *f*-electron compounds commonly exhibit highly anisotropic magnetic phase diagrams consisting of multiple long-range ordered phases. Field-driven metamagnetic transitions between them may depend not only on the magnitude, but also on the direction of the applied magnetic field. Examples of such behavior are plentiful among rare-earth borides, such as  $RB_6$  or  $RB_{12}$  ( $R$  = rare earth). In our recent works, we used torque magnetometry and neutron scattering to measure anisotropic field-angular phase diagrams of La-doped cerium hexaborides,  $Ce_{1-x}La_xB_6$  [1,2] and  $Ce_3Pd_{20}Si_6$  [3]. We propose a simple qualitative model for the field-space anisotropy that considers a pair of localized Ce<sup>3+</sup> ions in a cubic crystal electric field, coupled by a single nearest-neighbor exchange interaction. The field-directional anisotropy in these compounds is also pronounced in the magnetic excitation spectrum, investigated with inelastic neutron scattering (INS). Our work demonstrates that the rotating-field technique at fixed momentum can complement conventional INS measurements of the dispersion at a constant field and holds great promise for identifying the symmetry of multipolar order parameters and the details of intermultipolar interactions that stabilize hidden-order phases in rare-earth compounds.

- [1] D. S. Inosov, S. Avdoshenko, P. Y. Portnichenko, E. S. Choi, A. Schneidewind, J.-M. Mignot, M. Nikolo, *Phys. Rev. B* **103** (2021), 214415.
- [2] P. Y. Portnichenko, A. Akbari, S. E. Nikitin, A. S. Cameron, A. V. Dukhnenko, V. B. Filipov, N. Yu. Shitsevalova, P. Čermák, I. Radelytskyi, A. Schneidewind, J. Ollivier, A. Podlesnyak, Z. Huesges, J. Xu, A. Ivanov, Y. Sidis, S. Petit, J.-M. Mignot, P. Thalmeier, D. S. Inosov, *Phys. Rev. X* **10** (2020), 021010.
- [3] F. Mazza, P. Y. Portnichenko, X. Yan, P. Steffens, M. Boehm, E. S. Choi, M. Nikolo, A. Prokofiev, S. Paschen, and D. S. Inosov, *Metamultipolar phase transitions in the field-angular magnetic phase diagram of  $Ce_3Pd_{20}Si_6$*  (2022, to be published).

## Multipole polaron in the devil's staircase of CeSb

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An electron-boson coupling, that leads to a quasiparticle (QP) of an electron combined with a local bosonic field, can cause interesting properties of condensed matter. One of the most famous QPs is the polaron by electron-phonon coupling but such a QP state can be realized by coupling to other bosonic modes. Despite a number of investigations, however, only three types of electron–boson coupling have been experimentally identified so far: electron-phonon (or polaron), electron–magnon (or magnetic polaron) [1] and electron–plasmon (or plasmaron) couplings [2].

Here, we found a new type of electron–boson coupling which leads to a unique QP state, ‘multipole polaron’, by investigating a rare-earth intermetallic compound CeSb [3]. This new coupling mediates between the itinerant electrons and the bosonic field constituted by the crystal-electric-field (CEF) excitations of the localized  $4f$  states. As evidence for it, we present laser angle-resolved photoemission spectroscopy [4] revealing band renormalization via the coupling of the mobile electron with the CEF excitation. This low-energy feature corresponds to a quadrupole CEF excitation ( $J_z = \pm 2$ ) in the  $J$  multiplets of the  $4f$  orbitals, possessing the ‘multipole’ freedom.

[1] J. Schäfer *et al.*, Phys. Rev. Lett. **92**, 097205 (2004).

[2] A. Bostwick *et al.*, Science **328**, 999 (2010).

[3] Y. Arai *et al.*, Nat Matter. *in press*.

[4] K. Kuroda, Y. Arai *et al.*, Nat. Commun. **11**, 2888 (2020).

# Hidden order, magnetic excitations and multipolar exchange striction in neptunium dioxide

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Localized f-shells in lanthanide and actinide compounds may give rise not only to conventional dipole magnetic moments, but also to higher rank multipole ones [1]. Coupled by inter-site exchange interactions, these moments form a vast space of competing order parameters. Exhibiting no dipole moments, high-rank multipolar ordered states are not seen by neutron diffraction. Hence, they are often named "hidden-order" (HO) phases.

We evaluate the ground-state order and magnetic excitations for a prototypical HO system, neptunium dioxide  $\text{NpO}_2$ , from an ab initio low-energy Hamiltonian [2]. Our approach to derive this Hamiltonian is based on the density-functional+dynamical mean-field theory (DFT+DMFT) in conjunction with a quasi-atomic approximation to local correlations on the actinide  $5f$  shell. Starting from the high-temperature paramagnetic state described within DFT+DMFT, we compute all relevant inter-site (superexchange) exchange interactions by a many-body ab initio force theorem [3]. Superexchange interactions between the lowest crystal field quadruplet of  $\text{Np}^{4+}$  ions are shown to induce a primary noncollinear order of rank-5 (triakontadipolar) magnetic moments. A secondary order of quadrupoles preserves the cubic symmetry of  $\text{NpO}_2$ . The calculated on-site exchange splitting and magnetic excitation spectrum of the  $\text{NpO}_2$  HO phase agree well with experiment. Our study also reveals an unconventional multipolar exchange striction mechanism behind the anomalous volume contraction of the  $\text{NpO}_2$  HO phase.

\*This work is supported by the Program Committee.

[1] P. Santini *et al.*, Rev. Mod. Phys. **81**, 807 (2009).

[2] L. V. Pourovskii and S. Khmelevskiy, PNAS **118**, e2025317118 (2021).

[3] L. V. Pourovskii, Phys. Rev. B **94**, 115117 (2016).

# From spin ices to quadrupolar ices: the enigmatic case of the magnetic pyrochlore $Tb_2Ti_2O_7$

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In geometrically frustrated magnetism, the very nature of the ground state of the  $Tb_2M_2O_7$  pyrochlore where M is a transition metal element has remained a longstanding conundrum despite extended studies. The most enigmatic case arises in  $Tb_2Ti_2O_7$  where no conventional spin-ice or long-range magnetic order is stabilized, even at very low temperatures. Quantum fluctuations are suspected of being at the origin of such an exotic quantum phase.

In this compound, magneto-elastic couplings are strong, in particular in the form of hybridizations between  $Tb^{3+}$  crystal-field and phonon modes [1]. This so-called vibronic process affects the electronic ground state and involves quadrupolar degrees of freedom. We present here new results of THz spectroscopy on two  $Tb_{2+x}Ti_{2-x}O_{7+y}$  samples, with different stoichiometry, implying that one is in a spin liquid state and the second one in a quadrupolar ordered phase [2]. Interestingly, our measurements relate the magnitude of the vibronic process to the ground state of the sample. Symmetry analysis suggests that, similarly to spin ices, quadrupolar degrees of freedom may order following an "ice rule". On the other hand, vibronic coupling favors "all in / all out" correlations between the quadrupoles, which compete with the quadrupolar long-range order, destabilizing it, for slightly different stoichiometry [3].

This remarkable result shows that, to understand the ground state of  $Tb_2Ti_2O_7$ , it is necessary to go beyond the interactions between magnetic dipoles in the multipolar expansion. Moreover, quadrupolar correlations of different origins may compete, thus generalizing the concept of frustration to quadrupolar degrees of freedom.

[1] E. Constable *et al.*, Phys. Rev. B **95**, 020415(R) (2017)

[2] T. Taniguchi *et al.*, Phys. Rev. B **87**, 060408(R) (2013)

[3] Y. Alexanian, *et al.*, to be published

# Optical Spectroscopy of 2-Dimensional van der Waals Antiferromagnets

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Magnetism in low dimensional systems is an interesting topic for the fundamental physics, and atomically thin 2-dimensional (2D) van der Waals magnetic materials are promising candidates for novel spintronic devices. Antiferromagnetic 2D materials are particularly interesting both for fundamental physics and also for antiferromagnetism-based spintronic devices. On the other hand, it is difficult to probe the magnetism in these materials because traditional research tools such as neutron scattering cannot be employed due to the very small sample volume. Optical spectroscopy is becoming increasingly important for the study of antiferromagnetic 2-dimensional materials. Raman spectroscopy, for example, has been established as an invaluable tool to probe the magnetic transition in antiferromagnetic van der Waals materials as it has been found that the magnetic ordering sometimes correlates with the changes in the Raman spectrum [1]. Furthermore, recent spectroscopic studies revealed a novel coherent state in some of these materials stabilized by the antiferromagnetic ordering [2]. In this presentation, I will review recent achievements in the study of antiferromagnetism in 2 dimensions using optical spectroscopy, focusing on the transition metal phosphorus trichalcogenide family  $\text{TMPX}_3$  (TM=Fe, Mn, Ni, *etc.*; X=S, Se).

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[1] K. Kim, J.-U. Lee, H. Cheong, *Nanotechnology* **30**, 452001 (2019).

[2] S. Kang, *et al.*, *Nature* **583**, 785 (2020).



# Observation of the Rashba-driven anomalous Hall effect in an antiferromagnetic metal

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Diverse mechanisms yield the anomalous Hall effect (AHE) and these mechanisms are often intertwined, challenging efforts to elucidate this fundamental physics [1]. Here we report the observation of an unconventional AHE in a new type of antiferromagnetic system. In particular, we find that AgCrSe<sub>2</sub>—a layered, non-centrosymmetric, antiferromagnetic crystal [2]—exhibits an anomalous Hall resistivity of up to 3  $\mu\Omega$  cm at 2 K. Systematic temperature and angular dependent Hall measurements reveal that the observed AHE is an intrinsic behavior. Through complementary experimental investigations and first-principles calculations, we demonstrate that the Rashba-like spin-orbit coupling allowed by the non-centrosymmetric crystalline structure is the key driver for the observed anomalous Hall response. Furthermore, we report the observation of a rather pronounced plateau feature in the Hall resistivity as a function of the angle between the applied field and the crystalline *c*-axis. The plateau feature suggests possible existence of topological protected state.

[1] N. Nagaosa, J. Sinova, S. Onoda, A. H. MacDonald, and N. P. Ong, Rev. Mod. Phys. 82, 1539 (2010).

[2] M. Baenitz, et al., Phys. Rev. B 104, 134410 (2021)

## Large topological Hall effect from fluctuating skyrmion textures

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A contribution to the Hall effect arises when charge carriers traverse a static magnetic texture with finite topological winding and the spin of the electron follows the spin texture adiabatically. This so-called topological Hall effect is a key characteristic of the Skyrmion lattice found in cubic chiral magnets such as MnSi or Fe<sub>1-x</sub>Co<sub>x</sub>Si [1]. The observation of a topological Hall signal in MnSi under high pressures [2], and the identification of fluctuating Skyrmion textures in the paramagnetic state of MnSi under small magnetic fields [3] raises the question for direct evidence if fluctuating Skyrmion textures can generate a topological Hall effect. Combining transport, ac susceptibility and specific heat measurements with neutron resonance spin-echo spectroscopy, we report the observation of a topological Hall effect in Mn<sub>1-x</sub>Fe<sub>x</sub>Si in a regime of fluctuating Skyrmion textures without static order down to 50mK.

[1] A. Neubauer *et al.*, Phys. Rev. Lett. **102**, 186602 (2009).

[2] R. Ritz *et al.*, Nature 497, 231 (2013); R. Ritz *et al.*, Phys. Rev. B **87**, 134424 (2013).

[3] J. Kindervater *et al.*, Phys. Rev. X **9**, 041059 (2019).

# Scattering from magnetic monopoles and antiferromagnetic domain manipulation in a frustrated pyrochlore iridate

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Magnetically frustrated systems provide fertile ground for complex behaviour, including unconventional ground states with emergent symmetries, topological properties, and exotic excitations. A canonical example is the emergence of magnetic-charge-carrying quasiparticles in spin-ice compounds [1–3].

Despite extensive work, a reliable experimental indicator of the density of these magnetic monopoles is yet to be found. Using measurements on single crystals of  $\text{Ho}_2\text{Ir}_2\text{O}_7$  combined with dipolar Monte Carlo simulations, we show that the isothermal magnetoresistance is highly sensitive to the monopole density. Moreover, we uncover an unexpected and strong coupling between the monopoles on the holmium sublattice and the antiferromagnetically ordered domains of iridium ions [4].

These results pave the way towards a quantitative experimental measure of monopole density and demonstrate the ability to control antiferromagnetic domain walls using a uniform external magnetic field, a key goal in the design of next-generation spintronic devices.

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\*This work is supported by the Program Committee.

[1] M. J. Harris *et al.*, *Phys. Rev. Lett.* **79**, 2554 (1997).

[2] S. T. Bramwell *et al.*, *Science* **294**, 1495 (2001).

[3] C. Castelnovo *et al.*, *Nature* **451**, 42 (2008).

[4] M. J. Pearce *et al.*, *Nat. Commun.* **13**, 444 (2022).

## New fragmented state in pyrochlore ruthenate $\text{Ho}_2\text{Ru}_2\text{O}_7$

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The apparent fragmentation [1, 2] of magnetic moments in spin ice systems into coexisting longitudinal, transverse and harmonic parts is a direct consequence of emergent electromagnetism in these systems, and the associated Helmholtz decomposition. At the microscopic level, moments of fixed length act as elements of this emergent lattice field from which topological defects - magnetic monopoles [3] - can be excited. By construction, the leftover is the sum of the (divergence-free) transverse and harmonic parts. The most prominent example of magnetic fragmentation is the monopole crystal phase observed in the pyrochlore iridates  $\text{Ho}_2\text{Ir}_2\text{O}_7$  [4] and  $\text{Dy}_2\text{Ir}_2\text{O}_7$  [5], in which the longitudinal (monopole) field constitutes an antiferromagnet with long range order. The transverse part remains disordered, with dipolar correlations.

In this talk we present evidence of a new fragmented state in  $\text{Ho}_2\text{Ru}_2\text{O}_7$ . Contrary to the previous results in Refs [6, 7], we find that the Ru orders following a  $\Gamma_5$  representation, which corresponds to an AF ordering in the plane perpendicular to the  $\langle 111 \rangle$  direction. We perform specific heat, neutron diffraction and magnetic measurements to show that the transition on the holmium sublattice at 1.5 K results in a new type of fragmentation, where a harmonic and a transverse term coexist giving a ferromagnetic state with residual entropy at low temperature. It is analog to the kagome ice state stabilized in conventional spin ice under a [111] field. We show how self consistent interactions between Ho-Ho ions mediated by the Ru ions could stabilise the required ferromagnetic state. Finally, we show the existence of unconventional slow dynamics below 1.5 K, using a.c. susceptibility data measured down to 1 mHz.

- [1] M. E. Brooks-Bartlett et al., *Physical Review X* **2014**, *4*, 011007.
- [2] E. Lhotel, L. D. C. Jaubert, P. C. W. Holdsworth, *Journal of Low Temperature Physics* **2020**, *201*, 710–737.
- [3] C. Castelnovo, R. Moessner, S. L. Sondhi, *Nature* **2008**, *451*, 42–45.
- [4] E. Lefrançois et al., *Nature Communications* **2017**, *8*, 209.
- [5] V. Cathelin et al., *Physical Review Research* **2020**, *2*, 032073.
- [6] C. Wiebe et al., *Physical Review Letters* **2004**, *93*, 076403.
- [7] J. S. Gardner et al., *Journal of Physics: Condensed Matter* **2005**, *17*, 7089–7095.

# Magnetic particles and strings in iron langasites

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The dimensionality and symmetry properties of the order parameter determine the topology of defects in order states of matter. The diversity and complexity of topological defects grow with the number of dimensions of the order parameter space, with a prominent example being the A-phase of superfluid  $^3\text{He}$ . Three-dimensional order parameter spaces can be realized in non-collinear antiferromagnets with triangle-based spin lattices showing the 120-degree ordering of spins described by an  $\text{SO}(3)$  matrix [1]. An eminent candidate is the frustrated and chiral Fe-based langasite,  $\text{Ba}_3\text{TaFe}_3\text{Si}_{24}\text{O}_{14}$ . Geometric frustration and competing exchange interactions in this material make spins non-collinear at the scale of one unit cell, whereas Dzyaloshinskii-Moriya interactions give rise to large-scale modulations of the spin orders and stabilize unconventional topological defects.

The iron langasite spin lattice is built of triangles formed by antiferromagnetically coupled  $\text{Fe}^{3+}$  ions. This material shows a non-collinear 120-degree spin order in the triangles, modulated in a spiral with a period of 7 lattice constants and complex spin superstructures at the scale of 100 nm. We derive an effective model describing long-range magnetic modulations and find unusual two and three-dimensional defects: a coreless vortex and particle-like three-dimensional skyrmion. The skyrmion is similar to the Shankar monopole in  $^3\text{He-A}$  and hedgehog soliton in the Skyrme model of baryons. Compact magnetic particles that propagate in all three spatial directions can play an important role in antiferromagnetic spintronics.

[1] H. Kawamura and S. Miyashita, *J. Phys. Soc. Jpn.* **51**, 4138 (1984).

[2] M. Ramkrishnan *et al.*, *npj Quantum Mater.* **4**, 60 (2019).

[3] E. Barts and M. Mostovoy, *npj Quantum Mater.* **6**, 104 (2021).

# Electronic, superconducting and quantum critical signatures of iron-chalcogenides tuned by chemical and hydrostatic pressures

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Iron-based superconductors display a plethora of competing electronic phases and offer a unique platform to explore unconventional superconductivity [1]. The electronic structure originating mainly from Fe layers has a multi-band character stabilized by orbitally-dependent electronic correlations and band shifts. The magnetic moments are often strongly fluctuating and can provide the exchange for superconducting pairing.

The family of iron-chalcogenide superconductors displays electronic nematic orders and spin-density wave phases which are often intertwined and it makes it difficult to assess their relevance to superconductivity [2,3]. Tuning parameters, like applied and chemical pressure [4,5], are versatile tools to explore their relative importance. In this talk, I will present quantum oscillations studies on single crystals of  $\text{FeSe}_{1-x}\text{S}_x$  tuned via chemical and applied hydrostatic pressures using magnetotransport and tunnel diode oscillator experiments in high-magnetic fields [4,5,6]. I will discuss the evolution of the Fermi surfaces and the behavior of the quasiparticle effective masses across the nematic quantum critical points. I will also evaluate the unusual electronic and superconducting behavior inside the high-pressure phase where superconductivity is enhanced in  $\text{FeSe}_{1-x}\text{S}_x$  [7]. The role of the Fermi surfaces and electronic correlations on the superconductivity and the upper critical field in these multi-band iron-based superconductors will also be discussed.

\*This work was supported by the EPSRC, UK and the Oxford Centre for Applied Superconductivity.

[1] R. M. Fernandes, A. I. Coldea, *Nature* **601**, 35 (2022).

[2] A. I. Coldea, M. D. Watson, *Ann. Rev. Cond. Matt. Phys.*, **9**, 125 (2018).

[3] A. I. Coldea, *Frontiers in Phys.* **8**, 594500 (2021).

[4] A. I. Coldea et al., *npj Quantum Materials*, **4**, 2 (2019).

[5] P. Reiss et al, *Nature Physics*, **16**, 89 (2020).

[6] Pascal Reiss, et al., *Phys. Rev. Lett.* **127**, 246402 (2021).

[7] Z. Zajicek et al., in preparation (2022).

# Superconductivity in infinite-layer nickelates

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Finding unconventional superconductors in proximity to various strongly correlated electronic phases has been a recurring theme in materials as diverse as heavy fermion compounds, cuprates, pnictides, and twisted bilayer graphene. The recent discovery of superconductivity in layered nickelates [1] was motivated by looking for an analog of the cuprates. The synthesis of the nickelates is in and of itself interesting – it involves the removal of planes of oxygen from a 3D nickel oxide using soft chemistry techniques. We will introduce this new family of superconductors and our current understanding of their electronic and magnetic structure. Notable aspects are a doping-dependent superconducting dome [2], strong magnetic fluctuations [3], instabilities towards charge stripes [4], and a landscape of unusual normal state properties from which superconductivity emerges [5]. These features are strongly reminiscent of the cuprates, despite key differences in the electronic structure and the absence of a proximate correlated insulator.

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[1] D. F. Li *et al.*, *Nature* **572**, 624 (2019).

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

[3] H. Lu *et al.*, *Science* **373**, 213 (2021).

[4] M. Rossi *et al.*, arXiv: 2112.02484.

[5] K. Lee *et al.*, arXiv: 2203.02580.

## Hot Hydride Superconductivity above 550 K

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The search for room temperature superconductivity has accelerated dramatically in the last few years driven largely by theoretical predictions that first indicated alloying dense hydrogen with other elements could produce conventional phonon-mediated superconductivity at very high temperatures and at accessible pressures, and more recently, with the success of structure search methods that have identified specific candidates and pressure-temperature (P-T) conditions for synthesis. These theoretical advances have prompted improvements in experimental techniques to test these predictions. As a result, experimental studies of simple binary hydrides under pressure have yielded high critical superconducting transition temperatures ( $T_c$ ), of 260 K in LaH<sub>10</sub>, close to the commonly accepted threshold for room temperature, 293 K, at pressures near 180 GPa. We successfully synthesized a metallic La based superhydride from La metal and ammonia borane, NH<sub>3</sub>BH<sub>3</sub>, and find an initial multi-step transition with a  $T_c$  of 294 K for the highest onset, in line with previously reported work [1],[2]. When subjected to subsequent thermal excursions to higher temperatures that promoted a chemical reaction to a ternary or higher order system, the transition temperature was driven to higher temperatures. X-Ray structural data confirm the formation of a higher order hydride. Although the reaction does not appear to be complete, the onset temperature was pushed from 294 K to 556 K. The results provide evidence for hot superconductivity well above room temperature, in line with recent predictions for a higher order hydride under pressure [3].

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[1] Somayazulu, M. *et al.* Evidence for Superconductivity above 260 K in Lanthanum Superhydride at Megabar Pressures. *Physical Review Letters* **122** (2019).

[2] Drozdov, A. P. *et al.* Superconductivity at 250 K in lanthanum hydride under high pressures. *Nature* **569**, 528–531 (2019).

[3] Sun, Y., Lv, J., Xie, Y., Liu, H. & Ma, Y. Route to a Superconducting Phase above Room Temperature in Electron-Doped Hydride Compounds under High Pressure. *Physical Review Letters* **123** (2019)



# Pressure phase diagram of unidimensional iron based superconductors $\text{BaFe}_2\text{Se}_3$

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In the last years, superconductivity has been observed in iron based one dimensional compounds,  $\text{BaFe}_2\text{X}_3$  X=S,Se [1-3]. They have a centrosymmetric average space group (Cmcm and Pnma respectively) at room temperature, in which iron atoms form two distinct ladders along the b-axis. Below the Néel temperature (110 K and  $225\pm 30$  K respectively), the iron spins are arranged in squares of 4 ferromagnetically ordered spins, each block being coupled antiferromagnetically to its neighbours, revealing a underlying magnetic frustration [1]. However for both system the stacking of these magnetic ladders differs, resulting in different magnetic orders. Upon pressure, a metalization is observed and superconductivity develops below 14K above 10GPa. Our recent results [4-6] on the compounds  $\text{BaFe}_2\text{Se}_3$  revealed a different set of structural and magnetic properties from ambient pressure up to the superconducting critical pressure. Combining single crystal X-ray diffraction, Raman scattering, neutron diffraction and X-ray spectroscopy, we propose a vastly updated version of the pressure-temperature phase diagram. These results shed a new light on the possible origin of superconductivity common to both  $\text{BaFe}_2\text{X}_3$  X=S,Se, together with experimental evidence of multiferroicity at ambient pressure.

\*This work is supported by the ANR COCOM 20-CE30-0029 and CSC scholarship #201806830111

[1] H. Takahashi et al., *Nature Materials* **14**, 1008 (2015).

[2] J. Ying et al., *Physical Review B* **24**, 241109 (2017).

[3] J.M. Caron et al., *Physical Review B* **18**, 180409 (2011)

[4] W. Zheng, V. Balédent et al., *Physical Review B* **20**, 020101(R) (2020)

[5] M. J. Weseloh , V. Balédent et al., accepted in *Journal of Physics : Cond. Mat.* (2022)

[6] W. Zheng, V. Balédent et al. accepted in *Nature Com. Physics* (2022)

## Pressure tuning of the low-temperature states of CeRh<sub>2</sub>As<sub>2</sub>

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Heavy-fermion superconductor CeRh<sub>2</sub>As<sub>2</sub> ( $T_c \approx 0.3$  K) is a tetragonal Kondo lattice system lacking local inversion symmetry at Ce sites. The material stands out by having two superconducting states of even and odd parities [1]. Absence of the Pauli limit in the odd-parity state results in an extremely high upper critical field of  $\sim 15$  T [2]. The compound also hosts what is believed to be a quadrupole-density-wave (QDW) order below 0.4 K, manifesting as a periodic modulation of the quadrupolar moment of  $f$ -orbitals and coexisting with the superconductivity [3]. The relationship between the two orders has so far remained unclear.

We conducted a high-pressure electrical resistivity study of CeRh<sub>2</sub>As<sub>2</sub>, tracking the change of the low-temperature phase diagram while applying hydrostatic pressure and magnetic field. The QDW order is highly sensitive to lattice compression and gets fully suppressed with about 0.7 GPa. At the same time, the  $T_c$  of superconductivity reduces at a significantly slower rate of about -30 mK/GPa, suggesting no influence of QDW on superconductivity. We relate our observations to the change of the relevant energy scales, such as Kondo temperature, Rashba spin-orbit coupling, and interlayer hopping.

\*This work is supported by the Max Planck Society.

[1] S. Khim, J. Landaeta *et al.*, *Science* **373**, 1012 (2021).

[2] J. Landaeta *et al.*, *Phys. Rev. X*, to be published.

[3] D. Hafner *et al.*, *Phys. Rev X* **12**, 011023 (2022).

# Interplay between CDW and superconductivity of underdoped

## $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$

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It is well established that the charge order (CDW) is a universal phase in cuprate superconductors though the interplay between the CDW and the superconductivity is still unclear. It is associated with a Fermi surface reconstruction that takes place in the underdoped side of the phase diagram and leads to the sign change of the Hall coefficient ( $R_H$ ). This makes the Hall effect a perfect bulk probe to track the evolution of the CDW as the material is tuned across the phase diagram as a function of doping [1].

To get more insight into the relation between the CDW and the superconductivity, we have tuned these phases using hydrostatic pressure (up to 6 GPa), high magnetic fields (up to 60T) and disorder (both Zn-doped and electron irradiation). We have performed Hall effect and X-ray measurements in YBCO single crystals down to 1.5K for different doping. This combination of tunable parameters allows us to vary the relative strengths of these two ground states and thus reveal whether they compete or coexist in unison [2].

[1]. D. LeBoeuf et al, Phys. Rev. B **83**, 054506 (2011).

[2]. C. Putzke et al, Phys. Rev. L **120**, 117002 (2018).

# ***Evolution of magnetic stripes under uniaxial stress in $\text{La}_{1.885}\text{Ba}_{0.115}\text{CuO}_4$ studied by neutron scattering***

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We present the effect of uniaxial stress on the magnetic stripes in the cuprate system  $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$  with  $x = 0.115$ , previously found to have a stress-induced enhancement in the superconducting transition temperature [1]. By means of neutron scattering, we show that the static stripes are suppressed by stress, pointing towards a trade-off between superconductivity and static magnetism, in direct agreement with previously reported  $\mu\text{SR}$  measurements [1].

Additionally, we show that some of the reduced weight in the elastic channel appears to have moved to the inelastic channel. Moreover, a stress-induced momentum shift of the fluctuations towards the typical  $1/8$  value of commensurability is observed. These results impose a strong constraint on the theoretical interpretation of stress-enhanced superconductivity in cuprate systems.

[1] Z. Guguchia et al., Phys. Rev. Lett. **125**, 097005 (2020)

## Normal-state charge transport of $\text{YBa}_2\text{Cu}_3\text{O}_{6.67}$ under uniaxial stress

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The anomalous normal-state transport properties of the cuprate superconductors challenge the fundamental tenets of solid-state theory, and have thus become emblematic of related phenomena in a much larger class of strongly correlated electron systems. To provide a foundation for theoretical models, experimental research has sought to establish correspondences between macroscopic transport coefficients and atomic-scale correlation functions measured by spectroscopic probes under identical experimental conditions. This research avenue has been confounded by the gradual onset of electronic ordering phenomena and of the corresponding transport anomalies, caused by the two-dimensionality of the electron system in conjunction with competing instabilities and doping-induced disorder.

Here, we report measurements of normal-state resistivity and Hall coefficient of twin-free single crystals of the underdoped high-temperature superconductor  $\text{YBa}_2\text{Cu}_3\text{O}_{6.67}$  (doping level  $\sim 0.12$  holes per Cu ion) under uniaxial stress. We observe a remarkable correspondence between the differential stress responses of the transport coefficients and resonant x-ray diffraction features indicative of charge ordering, which parallels the phenomenology of classical charge-density-wave compounds. However, our observations imply that a Fermi surface reconstruction due to static charge order is not responsible for the most prominent transport anomalies including a sign reversal of the Hall coefficient and suggest that the interplay with nearly critical charge correlations is essential for anomalous transport in the underdoped cuprates. Our observations call for the development of theoretical methods to describe electronic transport in systems with nearly critical collective fluctuations [1].

[1] S. Nakata *et al.*, submitted.

## Fermi surface of heavy fermion ferromagnet CeRh<sub>6</sub>Ge<sub>4</sub>

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Ferromagnetic quantum critical point was recently revealed in heavy fermion ferromagnet CeRh<sub>6</sub>Ge<sub>4</sub>, where the Curie temperature can be continuously suppressed to zero under a moderate hydrostatic pressure [1]. Here we report the investigations on the fermi surface of CeRh<sub>6</sub>Ge<sub>4</sub> by quantum oscillations and DFT (density functional theory) calculations at ambient pressure. Fermi surfaces of CeRh<sub>6</sub>Ge<sub>4</sub> have been mapped with angle-dependent measurements of quantum oscillations, and the experimental results were compared with DFT calculations assuming Ce 4f electrons were either localized or itinerant. The similarity between the quantum oscillation frequencies and calculations with localized 4f electrons provides the evidence for the localized feature of Ce 4f electrons at ambient pressure, suggesting that localized ferromagnetism is a key factor for the occurrence of a ferromagnetic quantum critical point in CeRh<sub>6</sub>Ge<sub>4</sub> [2].

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[1] B. Shen *et al.*, Nature **579**, 51 (2020).

[2] A. Wang *et al.*, Science Bulletin **66**, 1389 (2021).

# Fermi surface and mass renormalization in the iron-based superconductor $\text{YFe}_2\text{Ge}_2$

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The iron-germanide superconductor  $\text{YFe}_2\text{Ge}_2$  [1-3] exhibits strong electronic correlations: its Sommerfeld ratio is enhanced by an order of magnitude over density functional theory (DFT) estimates [4, 5], the normal state resistivity  $\rho$  follows a  $T^{3/2}$  non-Fermi liquid (NFL) temperature dependence, photoemission spectroscopy has revealed renormalised energy bands [6], and it displays enhanced magnetic fluctuations [7]. Further interest in this material derives from theoretical proposals for the superconducting state, which include  $s_{\pm}$  or triplet pair wavefunctions [5] and from its striking similarities to some of the iron pnictide superconductors [1, 3, 8].

Here we present results of quantum oscillation measurements [4] in high-quality  $\text{YFe}_2\text{Ge}_2$  single crystals which resolve all four Fermi surface pockets expected from band structure calculations, including an electron pocket in the Brillouin zone corner and three hole pockets enveloping the centers of the top and bottom of the Brillouin zone. Our data highlight the key role of the electron pocket, which despite its small volume accounts for about half the total density of states. Carrier masses reach up to 20 times the bare electron mass and are among the highest ever observed in any iron-based material, accounting for the enhanced heat capacity Sommerfeld coefficient  $\approx 100$  mJ/molK<sup>2</sup>. Mass renormalization is uniform across reciprocal space, suggesting predominantly local correlations, as in the Hund's metal scenario.

[1] J. Chen *et al.*, Phys. Rev. Lett., **116**, 127001 (2016).

[2] J. Chen *et al.*, Phys. Rev. B, **99**, 020501(R) (2019).

[3] J. Chen *et al.*, Phys. Rev. Lett., **125**, 237002 (2020).

[4] J. Baglo *et al.*, arXiv:2104.11791 (2021)

[5] A. Subedi, Phys. Rev. B **89**, 024504 (2014); D. J. Singh, Phys. Rev. B **89**, 024505 (2014).

[6] D. F. Xu *et al.*, Phys. Rev. B **93**, 024506 (2016).

[7] H. Wo *et al.*, Phys. Rev. Lett. **122**, 217003 (2019).

[8] D. Guterding *et al.*, Phys. Rev. Lett. **118**, 017204 (2017).

# The Fermi surface of the ferromagnetic superconductor UCoGe under external magnetic fields.

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UCoGe is a heavy fermion system and one of the few known materials to display co-existence of ferromagnetism ( $T_{\text{Curie}} \approx 2.7$  K) and superconductivity ( $T_{\text{sc}} \approx 0.6$  K) at ambient pressure. Magnetic fluctuations originating from the uranium  $5f$  electrons are important for both superconductivity and magnetism in this material [1]. Understanding the relationship between the  $5f$  moments and the conduction electrons may therefore be key to understanding the unconventional superconductivity.

If an external magnetic field is applied along the magnetic easy-axis ( $c$ -axis), the magnetic fluctuations and the superconductivity are rapidly suppressed, and a number of transitions can be observed in resistivity and thermopower [2]. Some of these transitions are associated with Lifshitz transitions of the Fermi surface.

To gain further information about the nature of these field-induced transitions and the behaviour of the Fermi surface, we measured magnetic susceptibility in fields up to 30 T and temperatures down to 48 mK. The transitions all appear extremely distinctly in the susceptibility, and we have, moreover, been able to track the magnetic field dependence of multiple Fermi surface pockets via de Haas-van Alphen oscillations.

To support our experimental data, we carried out DFT calculations of the UCoGe bandstructure using the WIEN2k package [3], and extended these calculations to examine the effect of an external magnetic field.

I will present our magnetic susceptibility results and make an effort to couple them to our calculations to give insight into the co-evolution of the magnetization and the heavy electron Fermi surface in magnetic field.

\*This work is supported by the Nederlandse Organisatie voor Wetenschappelijk Onderzoek (NWO), HFML-RU/NWO member of the European Magnetic Field Laboratory (EMFL).

[1] K. Karube *et al.*, J. Phys. Soc. Jpn. **80**, 064711 (2011).

[2] G. Bastien *et al.*, Phys. Rev. Lett. **117**, 206401 (2016).

[3] P. Blaha *et al.*, J. Chem. Phys. **152**, 074101 (2020).



# Quantum oscillations in heavy-fermion ferromagnet $\text{YbNi}_4\text{P}_2$ over many Zeeman induced Lifshitz transitions

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$\text{YbNi}_4\text{P}_2$  is a heavy-fermion Kondo-lattice metal situated near a very rare ferromagnetic quantum critical point (FM QCP) [1]. Understanding the nature of this ferromagnetism requires knowledge of the Fermi surface; it has been speculated that this FM QCP is due to a quasi-1D Fermi surface [2]. At the same time, the strongly renormalised bandstructure is readily modified by relatively small magnetic fields, with nine Lifshitz transitions (abrupt topological changes in the Fermi surface) below 20 T due to Zeeman energy shifts [3].

Here we present quantum oscillations in resistivity and Hall effect of  $\text{YbNi}_4\text{P}_2$  up to 35T, including detailed rotation and mass studies. We present analysis over several of these Lifshitz transitions, observing frequency changes and appearances/disappearances using moving window FFT and Landau indexing. Notably, we observe large frequencies  $\sim 6$  kT indicative of large Fermi surfaces due to Kondo hybridisation gaps near the Fermi level, and large cyclotron masses  $\sim 7 m_0$  and  $\sim 12 m_0$  from the heavy fermions.

To work towards the zero field Fermi surface of  $\text{YbNi}_4\text{P}_2$ , we model the bandstructure of the non-heavy fermion reference compound  $\text{LuNi}_4\text{P}_2$  then extract the expected frequencies at a variety of rigid-band shifts. With these predictions we gain insight in to the shape of the Fermi surface observed, and the Lifshitz transitions it undergoes. Finally, we consider a few scenarios for Lifshitz transitions and, through the use of several toy models, how the measured frequencies should evolve a function of field.

\*This work is supported by the EPSRC (grant no. EP/L015544/1), and by HFML-RU, member of the European Magnetic Field Laboratory (EMFL).

[1] A. Steppke *et al.*, Science **339**, 6122:933-936 (2013).

[2] M. Brando *et al.*, Rev. Mod. Phys. **88**, 025006 (2016).

[3] H. Pfau *et al.*, Phys. Rev. Letters **119**, 126402 (2017).

# Heavy quasiparticles in CeRh<sub>2</sub>As<sub>2</sub>: Renormalized bands, Fermi surfaces, and electronic instabilities

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The heavy-fermion superconductor CeRh<sub>2</sub>As<sub>2</sub> exhibits a rich phase diagram at low temperatures. The observation of multi-phase superconductivity has been of particular interest [1]. The present contribution deals with the low-temperature normal state out of which the superconducting phases are forming. The central focus are the narrow quasiparticle bands and the electronic instabilities of the Fermi liquid state. We present calculations of the heavy quasiparticles in the heavy-fermion compound CeRh<sub>2</sub>As<sub>2</sub>. The narrow quasiparticle bands that are derived from the Ce-4f degrees of freedom are calculated by means of the Renormalized Band (RB) method. The RB scheme provides a framework for a realistic description of the coherent low-energy excitations in a Fermi liquid which combines material-specific ab-initio methods and phenomenological considerations in the spirit of the Landau theory of Fermi liquids. The central focus of the present study is the role played by the non-symmorphic lattice structure and the consequences of the Crystalline Electric Field (CEF) which removes the orbital degeneracy of the Ce 4f states. We conjecture that the quasi-quartet CEF ground state in combination with pronounced nesting features of the Fermi surface may give rise to a quadrupole density wave [2].

\*This work is supported by the ANR-DFG program Fermi-NESt.

[1] S. Khim et al., *Science* **373**, 1012 (2021).

[2] D. Hafner et al., *Phys. RevX* **12**, 011023 (2022)

## Extended Non-Fermi-Liquid Phases

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In a non-fermi-liquid the low-temperature electrical resistivity and heat capacity have leading temperature-dependences different from a fermi-liquid, while the magnitude of the residual electrical resistivity remains metallic. Such states are typically found above a quantum critical point where magnetic order is suppressed. As such, as the temperature is reduced to absolute zero, the non-fermi-liquid state shrinks to a point in phase space in any direction the the quantum phase transition is crossed.

This talk will focus on a small group of materials whose residual electrical resistivity remains metallic but where non-fermi-liquid behaviour occurs over a range of material parameters and is apparently unrelated to a quantum critical point.

Recent data will be presented on antiferromagnetic UAu<sub>2</sub> which is a non-fermi liquid over a range of applied magnetic fields from zero to several Tesla [1] and under pressure. Rather than being enhanced when the magnetic order is suppressed at high pressure, the non-fermi-liquid state weakens, showing that the magnetic order is key to sustaining the non-fermi-liquid state. Even more intriguingly at the critical pressure where magnetic order is suppressed, a T<sup>2</sup> resistivity is recovered. Possible origins of the non-fermi liquid behaviour will be described.

[1] Non-fermi liquid behaviour below the Neel temperature in the frustrated heavy Fermion magnet UAu<sub>2</sub>. Christopher D. O'Neill, Julian L Schmeh, Harry D. J. Keen, Luke Pritchard Cairns, Dmitry A Sokolov, Andreas Hermann, Didier Wermeille, Pascal Manuel, Frank Kruger and Andrew D. Huxley, Proceedings of the National Academy of Sciences of the United States of America, **118**, 49 (2021)

# Field control of fluctuation-driven modulated magnetism in the metallic ferromagnet PrPtAl

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Strong electronic particle-hole fluctuations in metals render ferromagnetic phase transitions first order and stabilize modulated magnetic phases at low temperatures. This phase reconstruction can be understood in terms of a fermionic quantum order-by-disorder (QOBD) mechanism: the Fermi surface deformations associated with the modulated order enlarge the phase space of electronic fluctuations, leading to a lowering of the free energy.

We will apply this theory to PrPtAl which shows helimagnetic order on the border of ferromagnetism below 5.5K [1]. This helical order is distorted due to a small magnetic anisotropy in the  $a$ - $b$  plane. As evidenced by magnetic resonant X-ray scattering [2], the modulated magnetism can be controlled by a small magnetic field along the harder  $b$  direction, resulting in a fan state that extends to zero temperature. Experimental evidence supporting the QOBD explanation is provided by the large increase of the  $T^2$  coefficient of the resistivity and the direct detection of enhanced magnetic fluctuations with inelastic neutron scattering, across the field range spanned by the fan state.

[1] G. Abdul-Jabbar *et al.*, Nature Physics **11**, 321 (2015).

[2] C. D. O'Neill *et al.*, Phys. Rev. Lett. **126**, 197203 (2021).

## T-linear resistivity from an isotropic Planckian scattering rate

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Perfectly  $T$ -linear resistivity is observed in a variety of strongly correlated metals close to a quantum critical point [1] and has been attributed to a scattering rate  $1/\tau$  of charge carriers that reaches the Planckian limit [2,3], with  $\hbar/\tau = \alpha k_B T$  where  $\alpha$  is of order unity. While this relationship is often inferred from simple estimates, a  $T$ -linear scattering rate has yet to be measured.

To directly access the Planckian scattering rate, we measured the angle-dependent magnetoresistance (ADMR) of Nd-LSCO at  $p = 0.24$ : a cuprate that demonstrates  $T$ -linear resistivity over a wide temperature range at the pseudogap critical point  $p^*$  [4]. The ADMR reveals a well-defined Fermi surface that precisely agrees with ARPES [5]. In addition, we extract a  $T$ -linear scattering rate that has the Planckian value, namely  $\alpha = 1.2 \pm 0.4$ . Remarkably, this inelastic scattering rate is isotropic.

Not only our findings [6] extend the validity of the semi-classical approach to explain the properties of the strange metal phase, but they also suggest that  $T$ -linear resistivity in strange metals is the direct consequence of a  $T$ -linear scattering rate, that reaches the Planckian bound for all directions of electron motion.

[1] J. Zaanen, *SciPost Phys.* 6, 061 (2019).

[2] J. A. N. Bruin et al., *Science* 339, 804 (2013)

[3] A. Legros et al., *Nat. Phys.* 15, 142 (2019)

[4] R. Daou et al., *Nat. Phys.* 5, 31 (2009).

[5] C. Matt et al., *Phys. Rev. B* 92, 134524 (2015)

[6] G. Grissonnanche et al., *Nature* 595, 667 (2021)

# Pseudogap Induced Electronic Anisotropy in Underdoped Cuprates

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Several underdoped cuprates in the pseudogap phase exhibit electronic anisotropy in their thermodynamic and transport properties that are not proportional to their crystalline anisotropies. This has led to the debate whether the pseudogap phase is close to an electronic nematic instability. I will argue that, unlike in the case of the iron-based systems [1], there is no experimental signature of large nematic correlations in the underdoped cuprates. Consequently, it is unlikely that the cuprates are near a nematic criticality. Instead, I will show that the extra electronic anisotropy can be understood as a response of the pseudogap itself to directional symmetry breaking perturbation. In particular, I will present a theory to explain the unusual electronic anisotropy in the dependence of the superconducting  $T_c$  to longitudinal strains along the two in-plane directions of  $\text{YBa}_2\text{Cu}_3\text{O}_y$  measured using ultrasound [2].

[1] Y. Gallais and I. Paul, *C. R. Phys.* **17**, 113 (2016).

[2] M. Frachet, D. J. Campbell, A. Missiaen, S. Benhabib, F. Laliberté, B. Borgnic, T. Loew, J. Porras, S. Nakata, B. Keimer, M. Le Tacon, C. Proust, I. Paul, and D. LeBoeuf, *Phys. Rev. B* **105**, 045110 (2022).

# Fermi to non-Fermi liquid crossover in intercalated $V_xVS_2$ with the NiAs-defect structure

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$MX_2$  layered transition metal dichalcogenides exhibit a large variety of interesting physical properties including charge density waves, superconductivity, or topological phases [1]. Some of them are serious candidates for applications in electronics as transistors and in optics as emitters and detectors. In a bulk form, the common way to tune their properties is the cationic intercalation in the van der Waals gap, with an effective charge transfer to the electronically active  $MX_2$  layer that can modify the electronic band structure.

Here we present the case of (self-)intercalated  $V_xVS_2$  with a strong interaction between intercalating and intercalated V cations. We focus on  $V_{1/4}VS_2$  (or  $V_5S_8$ ) and  $V_{1/2}VS_2$  (or  $V_3S_4$ ) with the so-called NiAs-defect structure, for which we have determined the magnetic susceptibility, specific heat, and resistivity at ambient and high pressure. We show that these compounds develop relatively strong electronic correlations when compared to other transition metal sulfides, which is in accordance with a high density of states at the Fermi level. Furthermore, their resistivity also exhibits non-Fermi liquid behavior, at high pressure for  $V_5S_8$  and at ambient pressure for  $V_3S_4$ . We will discuss the crossover from the Fermi to non-Fermi liquid phase in terms of Kondo physics and RKKY interactions.

[1] S. Manzeli, D. Ovchinnikov, D. Pasquier *et al.*, Nat. Rev. Mater. **2**, 17033 (2017).

# Topological superfluid $^3\text{He}$ under mesoscopic confinement: from quasi-2D chiral superfluid to pair density wave.

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Confinement of superfluid  $^3\text{He}$  in a nanofabricated cavity of height comparable to the superfluid coherence length is a powerful tool to modify the p-wave superfluid order parameter [1,2], which is experimentally determined by sensitive NMR techniques [3]. Surface scattering is tuned *in situ* by coating surfaces with a  $^4\text{He}$  film. In an 80 nm tall cavity, with specular surfaces, the quasi-2D chiral A-phase is stabilized at all pressures [4]. Studies at low pressure in a 200 nm tall cavity, show that the order parameter suppression and the spectrum of surface bound states are fragile with respect to details of quasiparticle scattering [2]. In taller cavities a striped spatially-modulated superfluid order, similar to an FFLO state, was predicted near the transition between A and B phases [5]. This pair density wave (PDW) arises because “hard” domain walls in  $^3\text{He}$ -B [6,7] are energetically stable under confinement in a slab [8]. Superfluid  $^3\text{He}$  was confined in a cavity of height 1.1  $\mu\text{m}$ , corresponding to around 10 coherence lengths at zero pressure. By stabilizing two spin-orbit configurations of the B phase [9], and studying the tipping angle dependence of the NMR frequency shift, we can determine different averages of the gap structure across the cavity. The results are inconsistent with the predicted one-dimensional “striped” PDW and suggest a two dimensional PDW [10]. Recent theoretical work indeed finds topologically stable, energetically metastable 2D PDW [13], the experimental observation of which may be attributable to the physics of nucleation of this phase.

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[1] L. V. Levitin *et al.*, Science **340**, 841 (2013)

[2] P. J. Heikkinen *et al.*, Nat. Commun. **12**, 1574 (2021)

[3] L. V. Levitin *et al.*, App. Phys. Lett. **91**, 262507 (2007)

[4] P. J. Heikkinen *et al.*, in preparation.

[5] A. B. Vorontsov and J. A. Sauls, Phys. Rev. Lett. **98**, 045301 (2007)

[6] M. Salomaa and G Volovik, Phys. Rev B **37**, 9298 (1988)

[7] M. Silveri *et al.* Phys. Rev. B **90**, 184513 (2014)

[8] A. B. Vorontsov and J. A. Sauls, J, Low Temp. Phys. **139**, 283 (2005)

[9] L. V. Levitin *et al.*, PRL **111**, 235304 (2013)

[10] L. V. Levitin *et al.*, PRL **122**, 085301 (2019)

[11] T Mizushima, D. Ishiura and T. Kawakami, private communications.



## Surface states evolution in half-Heusler systems Y(Pd,Pt)Bi

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The phase transition between trivial and topologically nontrivial insulators are well predicted and demonstrated in three dimensional systems [1]. One of the most tunable platforms to investigate such transition is the half-Heusler family [2,3]. It was predicted that the increase of spin-orbit coupling and/or lattice parameter in this family can tune the topology, however this transition was not unambiguously demonstrated yet [2,3]. In this work, using scanning tunneling microscopy/spectroscopy (STM/STS), we investigate the half-Heuslers Y(Pd,Pt)Bi, where the main tuning parameter between them is the spin-orbit coupling [4-6]. We were able to obtain flat (120) reconstructed YBi-terminated surfaces in both systems. Strikingly, there is a clear evolution of the local density of states upon going from Pd (trivial) to Pt (nontrivial), which microscopically shows the appearance of metallic surface states in YPtBi compounds. Using density functional theory calculations, we argue that these surface states are linked to the band inversion between the *s*-type twofold-degenerate  $\Gamma_6$  and the *p*-type fourfold-degenerate  $\Gamma_8$  bands going from the trivial insulator YPdBi to the nontrivial YPtBi. Our work demonstrates the feasibility of applying microscopic techniques to study such a versatile family of compounds.

\*This work is supported by FAPESP (Grants no. 2020/12283-0, 2018/11364-7, 2017/10581-1) and the Minister of Science and Higher Education of Poland (no. 818/STYP/14/2019).

- [1] S.-Y. Xu et al., Science 332, 560-564 (2011);
- [2] K. Manna et al., Nat. Rev. Mater. 3, 244-256 (2018);
- [3] T. Graf et al., Prog. Solid State Ch. 39, 1-50 (2011);
- [4] W. Al-Sawai et al., Phys. Rev. B 82, 125208 (2010);
- [5] S. Chadov et al., Nat. Mater. 9, 541-545 (2010);
- [6] H. Lin et al., Nat. Mater. 9, 546-549 (2010).

# Simulation of chiral topological phases in driven quantum dot arrays

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Recent experimental evidence on scalable quantum dot (QD) devices demonstrates a reproducible and controllable 12-quantum-dot device, which opens up the possibility of simulating 1D systems upon quantum dot chains.

In this talk it will be shown how to use quantum dot arrays as quantum simulators of one-dimensional topological insulators, using Floquet engineering. In particular, we illustrate our findings by implementing an extended SSH model, a canonical example of topological insulators in 1D, where long-range hopping is added.

We show that, with our driving protocol, all hopping amplitudes can be modified at will: while the undesired hopping processes, which destroy chiral symmetry, are simultaneously suppressed, the relevant ones are enhanced, what allows to imprint bond-order and preserve the key symmetries that provide for topological protection, thus realizing unconventional configurations that would be unreachable otherwise. We have discussed its implementation in a 12-QD array with two interacting electrons with opposite spin, and found correlation effects in their dynamics when configurations with different number of edge states are considered. The correlated electrons dynamics, which can be experimentally detected with QD charge detectors, allows to discriminate between different topological phases and importantly, it opens a new avenue for quantum state transfer protocols [1]. Finally, we discuss the feasibility of other low dimensional systems with non-trivial topology for the transfer of quantum information.

[1] B. Pérez-González et al., Phys. Rev. Lett., **123**, 126401 (2019).

# Josephson effects between the Kitaev ladder superconductors

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A topological Josephson junction consisting of two Kitaev chains exhibits a fractional Josephson effect with a  $4\pi$  periodicity in the current-phase relationship [1]. This is a promising experimental proof for the existence of Majorana zero modes (MZMs) at the edges of the Kitaev chains. Multi-terminal Josephson junctions of the Kitaev chains have been proposed to realize the braiding operation of MZMs for topological quantum computation [2]. Experimentally, however, conclusive evidence even for the existence of MZMs has not yet been obtained, let alone braiding operations.

In this study, we theoretically investigate the variety of the Josephson effects in systems with multiple Kitaev chains to find their potential applications other than topological quantum computation. Since the two-leg ladder system consisting of two Kitaev chains coupled by a transverse hopping  $t_{\perp}$  is known to exhibit a richer phase diagram than the chain [3], we focus here on the Josephson junction consisting of *two* two-leg Kitaev ladders. We consider the Josephson phase difference  $\theta$  between these two ladder systems as well as the phase difference  $\phi$  between the parallel chains in each ladder system.

The total energy of the junction at  $T = 0$  is calculated by a numerical diagonalization method as functions of  $\theta$ ,  $\phi$ , and  $t_{\perp}$ . We find that, by controlling  $t_{\perp}$  and  $\phi$ , the junction exhibits not only the fractional Josephson effect for the phase difference  $\theta$ , but also the usual 0-junction and even  $\pi$ -junction properties. We will also discuss the physics behind these various Josephson current-phase relationships.

[1] A. Yu. Kitaev, Phys. Usp. **44**, 131 (2001).

[2] J. Alicea, Y. Oreg, G. Refael, F. von Oppen, and M. P. A. Fisher, Nat. Phys. **7**, 412 (2011).

[3] A. Maiellaro, F. Romeo, and R. Citro, Euro. Phys. J. Special Topics **227**, 1397 (2018).

# **Intrinsic topological magnons in arrays of magnetic dipoles**

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We study a simple magnetic system composed of periodically modulated magnetic dipoles with an easy axis [1]. Upon adjusting the geometric modulation amplitude alone, chains and two-dimensional stacked chains exhibit a rich magnon spectrum where frequency gaps and magnon speeds are easily manipulable. The blend of anisotropy due to dipolar interactions between magnets and geometrical modulation induces a magnetic phase with fractional Zak number in infinite chains and end states in open one-dimensional systems. In two dimensions it gives rise to topological modes at the edges of stripes. Tuning the amplitude in two-dimensional lattices causes a band touching, which triggers the exchange of the Chern numbers of the volume bands and switches the sign of the thermal conductivity.

\*This work is supported by Fondecyt Grand No 1210083

[1] Paula Mellado. *Scientific Reports*, 12.1 (2022).

# Unconventional Transport Properties in the High-Pressure Phase of $\text{FeSe}_{0.89}\text{S}_{0.11}$

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The iron-based superconductors  $\text{Fe}(\text{Se},\text{S})$  are a material family where an isolated electronic nematic phase and its quantum critical point (QCP) can be accessed through a careful combination of hydrostatic and iso-electronic chemical pressure [1].

In this talk, I will present the results of our magnetotransport studies probing the normal-state and superconducting properties of  $\text{FeSe}_{0.89}\text{S}_{0.11}$  tuned by hydrostatic pressure. At a moderate pressure of  $\sim 0.6$  GPa, this system features an isolated nematic QCP, across which we uncover evidence for weakened superconductivity and finite electronic correlations on one hand, but also clear signs of a highly unconventional quantum Griffiths phase on the other [2,3]. Upon further increasing the pressure, we detect signatures of yet another QCP located around 4 GPa which features a strongly enhanced  $T_c$ , comparable to undoped  $\text{FeSe}$ . Beyond this second QCP, our transport study reveals that superconductivity is gradually lost and the system develops insulating-like behaviour. I will discuss the low- and high-pressure results in terms of a stochastic distribution of Sulfur atoms and an apparent tendency for orthorhombic lattice instabilities in this system.

[1] K. Matsuura *et al.*, Nat. Commun. **8**, 1143 (2017)

[2] P. Reiss *et al.*, Nat. Phys. **16**, 89 (2020).

[3] P. Reiss *et al.*, Phys. Rev. Lett. **127**, 246402 (2021)

[4] I. Paul and M. Garst., Phys. Rev. Lett. **118**, 227601 (2017)

# Investigating a putative nematic quantum critical point using high magnetic field elastoresistivity measurements

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Electronic material properties are closely linked to the symmetry properties of the underlying crystal lattice. For instance, ferroelectric materials break spatial inversion symmetry and ferromagnetic materials break time reversal symmetry. With strain, i.e., deformations of the crystal structure, we can break lattice symmetries and have large effects on the electronic behavior of materials. This coupling between the electronic behavior and strain can be probed with measurements of the elastoresistivity, i.e., the relation between strain a material experiences and the induced resistivity change. To lowest order the elastoresistivity tensor is a fourth rank tensor and it carries detailed information about the symmetry properties of the response.

In this talk, I will present high magnetic field elastoresistivity data [1, 2] on a prototypical electron doped iron pnictide superconductor,  $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ . This material is a likely candidate to host an electronic nematic quantum critical point and these high field elastoresistivity measurements allow us to follow the electronic nematic fluctuations below the zero-field superconducting transition in a field induced normal state. By measuring the elastoresistivity as a function of temperature and composition close to the quantum critical point, we investigate a key prediction of quantum criticality: power-law scaling of the associated susceptibility upon tuning toward the critical point. We find the elastoresistivity appears to obey power-law behavior as a function of composition, however, the temperature dependence for compositions close to the critical value cannot be described by a single power law. In this talk, I will discuss the implications of these findings.

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[1] J. C. Palmstrom *et al.*, Nat. Comm. **13**, 1011 (2022).

[2] J. A. W. Straquadine *et al.*, Phys. Rev. B **100**, 125147 (2019).

# Quasiparticle coherence in the nematic state of iron-based superconductors

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The microscopic mechanism of nematicity in iron-based superconductors is still unresolved. Most models consider either spin or orbital degrees as driving force but typically do not take electronic correlations into account. However, the interplay of Coulomb interactions and Hund's rule coupling leads to observable bad metallic behavior, orbital-dependent mass renormalizations and an overall suppression of quasiparticle coherence. We studied the influence of nematic order on the quasiparticle coherence in BaFe<sub>2</sub>As<sub>2</sub> using strain-dependent ARPES and compare them to our results on detwinned FeSe. Inside the nematic phase, we find an anisotropy of the spectral weight between the  $d_{xz}$  and the  $d_{yz}$  orbitals in the coherent quasiparticle peak and in the incoherent Hubbard band. We interpret our results in terms of a more coherent  $d_{xz}$  orbital compared to the  $d_{yz}$  orbital. Our study highlights the importance of electronic correlations for the description of nematicity in iron-based superconductors.

## LaFeSiO<sub>1-δ</sub>: a novel superconducting member of the Fe silicide family

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Since their discovery in 2008, iron-based superconducting pnictides (As, P...) and chalcogenides (Te, Se...) have become a well-established class of unconventional superconductors, spanning multiple structural families, with  $T_c$  up to 55 K in bulk materials [1]. This category of superconductors has recently been extended to a new subgroup of materials where pnictogen/chalcogen atoms are replaced by Si in LaFeSiH ( $T_c \sim 10$  K) and LaFeSiF<sub>x</sub> [2,3].

By using a topotactical approach, we were able to intercalate oxygen in intermetallic LaFeSi, resulting in the novel crystallogenide, LaFeSiO<sub>1-δ</sub>. Our study, based on complementary experimental probes, reveals that this crystallogenide is superconducting with a  $T_c \sim 10$  K [4].

Considering its strongly squeezed Fe-Si anion height, below 1 Å, this  $T_c$  is surprisingly high, challenging the quasi-universal relationship between structure and superconductivity in Fe-based compounds [5]. The unique crystal structure of this new compound has a strong impact on its electronic properties where the doping is absorbed in a non-rigid-band fashion, resulting in a distinct fermiology. Specifically, the electron pockets, usually observed around the M point in the prototypical Fermi surface of iron-based superconductors, are strongly suppressed, while the hole-like pockets at the  $\Gamma$  point are retained. This, in turn, is detrimental to the usual  $(\pi, \pi)$ -nesting. The lack of such nesting suggests a departure from the  $s_{\pm}$  pairing mechanism.

Furthermore, above  $T_c$ , resistivity shows a non-Fermi liquid behaviour, implying significant electronic correlations. This correlated behavior is also visible in NMR where anti-ferromagnetic fluctuations are observed at low temperatures.

### References:

- [1] H. Hosono, K Kuroki, *Physica C* 514, 399 (2015).
- [2] F. Bernardini *et al.*, *Phys. Rev. B* 97, 1462 (2018).
- [3] J.-B. Vaney *et al.*, *Nature Communications*. 13, 100504 (2022).
- [4] M. F. Hansen *et al.*, *npj Quantum Materials* - in review (2021).
- [5] C. H. Lee *et al.*, *Solid State Communications*, 152, 8 (2012)



# Quantum Monte Carlo Simulations of Iron-Selenide Superconductors with No Sign Problem

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Unlike parent compounds to iron pnictides, magnetic order is absent in the phase diagram of iron-selenide superconductors at ambient pressure[1]. We propose that proximity to *hidden* antiferromagnetic order across the isotropic  $d_+=dxz+idy z$  and  $d_-=dxz-idy z$  iron orbital, at the checkerboard wavevector  $\mathbf{Q}_{AF}=(\pi,\pi)$ , instead is what drives superconductivity in iron selenides. Inelastic neutron scattering studies of electron-doped FeSe intercalated by organic molecules are consistent with this proposal[2,3]. Specifically, Eliashberg theory that includes the exchange of such hidden spin excitations over nested Fermi surfaces predicts band shifts that result in strong electron Fermi surface pockets and faint hole Fermi surface pockets at the corner of the two-iron Brillouin zone[4]. Eliashberg theory also predicts an instability to S-wave Cooper pairs that alternate in sign between the strong electron Fermi surface pockets and the faint hole Fermi surface pockets[4].

Within determinant quantum Monte Carlo (DQMC) simulations, the  $d_+$  and  $d_-$  orbital degrees of freedom result in interactions mediated by hidden spin fluctuations that are time-reversal invariant. In turn, this results in DQMC simulations that are free of the sign problem[5]. We shall perform such DQMC simulations in order test for the prediction by Eliashberg theory of a Lifshitz transition to electron Fermi surface pockets at the corner of the two-iron Brillouin zone. The competition between hidden magnetic order, S-wave superconductivity, and D-wave superconductivity shall also be probed by DQMC.

- [1] J.P. Rodriguez, D.S. Inosov, and J. Zhao, “Editorial on Research Topic: High- $T_c$  Superconductivity in Electron-Doped Iron Selenide and Related Compounds”, submitted to *Frontiers in Physics*, arXiv:2204.03735 .
- [2] B. Pan ... J. Zhao, “Structure of Spin Excitations in Heavily Electron-Doped  $\text{Li}_{0.8}\text{Fe}_{0.2}\text{ODFeSe}$  Superconductors”, *Nat. Commun.* **8**, 123 (2017).
- [3] J.P. Rodriguez, “Spin Resonances in Iron-Selenide High- $T_c$  Superconductors by Proximity to a Hidden Spin Density Wave”, *Phys. Rev. B* **102**, 024521 (2020).
- [4] J.P. Rodriguez, “Superconductivity by Hidden Spin Fluctuations in Electron-Doped Iron Selenide”, *Phys. Rev. B* **103**, 184513 (2021).
- [5] E. Berg, M.A. Metlitski, and S. Sachdev, “Sign-Problem-Free Quantum Monte Carlo of the Onset of Antiferromagnetism in Metals”, *Science* **338**, 1606 (2012).

## RIXS characterization of the giant crystal field in CeRh<sub>3</sub>B<sub>2</sub>

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The so-called *giant* crystal-field compound CeRh<sub>3</sub>B<sub>2</sub> with its very short Ce-Ce distances (shorter than in  $\alpha$ -Ce) represents a long standing puzzle because it orders ferromagnetic at an exceptionally high temperature of  $T_C=116$  K with strongly reduced magnetic moments [1-5]. There have been suggestions that the expected *giant* crystalline electric field effect in CeRh<sub>3</sub>B<sub>2</sub> may lead to a breakdown of the *L-S-J* coupling scheme (see e.g. Ref. [5,6]). We have, therefore, investigated the *ff* excitations of CeRh<sub>3</sub>B<sub>2</sub> with high resolution resonant inelastic x-ray scattering (RIXS) at the Ce M<sub>5</sub> edge ( $3d \rightarrow 4f$ ). We show data taken at the I21 beamline at DIAMOND and ID32 at ESRF. The data have been analysed with a full multiplet code (Quanty [7]) and the complete crystal-field level scheme has been determined. We find the intermixing of the  $J=7/2$  multiplet into the ground state increases to few percent upon cooling to 20K but that otherwise the *L-S-J* coupling remains intact. We then compare our results of CeRh<sub>3</sub>B<sub>2</sub> with RIXS results of pseudo-hexagonal CeRh<sub>3</sub>Si<sub>2</sub> ( $T_N < 3.7$ K) [8] that has a substantially larger unit cell. This comparison, and also the comparison of room versus low T data show that the  $J_z=1/2$  state is stabilized as ground state the more the Ce-Ce distances shrink. At the same time, we find that states with electron densities pointing towards the Rh ions are becoming drastically more expensive in energy so that we rule out hybridization of Ce4*f* and Rh4*d* states to be responsible for the unusual properties of CeRh<sub>3</sub>B<sub>2</sub>.

[1] S. K. Dhar *et al.*, J. Phys. C **14**, L321 (1981)

[2] E.V. Sampathkumaran *et al.*, Phys.Rev.B **31** 3185 (1985)

[3] A. Fujimori *et al.*, Phys. Rev. B **41**, 6783 (1990), M Sundermann *et al.*, J. El. Spectrosc. Relat. Phenom. **209**, 1-8 (2016)

[4] K. Yamauchi *et al.*, J. Phys. Soc. Jpn. **79**, 044717 (2010)

[5] S. Raymond *et al.*, Phys. Rev. B **82**, 094416 (2010), F. Givord *et al.*, J. Phys. Cond. Mat. **19** 356208 (2007), F. Givord *et al.*, J. Phys. : Cond. Mat. **19**, 506210 (2007)

[6] K. Takegahara *et al.* J. Phys. Soc. Jpn. **54**, 4743 (1985), T. Kasuya *et al.*, J. Less Comm. Metals **127**, 337 (1987), K. Yamaguchi *et al.*, Phys. Rev. B **51**, 13952 (1995), O. Eriksson *et al.*, Phys. Rev. B **40**, 5270 (1989), T. Jo and S. Imada, J. Phys. Soc. Jpn. **59**, 2312 (1990)

[7] M.W. Haverkort *et al.*, Phys. Rev. B **85**, 165113 (2012)

[8] A. Amorese *et al.*, Phys. Rev. B **105**, 125119 (2022)

# Evidence for a delocalization transition without symmetry breaking in CeCoIn<sub>5</sub>

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The study of quantum phase transitions that are not clearly associated with broken symmetry is a major effort in condensed matter physics, particularly in regard to the problem of high-temperature superconductivity, for which such transitions are thought to underlie the mechanism of superconductivity itself. Here we argue that the putative quantum critical point in the prototypical unconventional superconductor CeCoIn<sub>5</sub> is characterized by the delocalization of electrons in a transition that connects two Fermi surfaces of different volumes, with no apparent broken symmetry. Drawing on established theory of f-electron metals, we discuss an interpretation for such a transition that involves the fractionalization of spin and charge, a model that effectively describes the anomalous transport behavior we measured for the Hall effect.

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[1] N. Maksimovic *et al.*, Science (2022): eaaz4566.

## Study of multi-f electron Kondo effect and magnetic ordering in SmCoIn<sub>5</sub>

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The microscopic mechanism of superconductivity in CeCoIn<sub>5</sub> depends strongly on the delocalization of 4f electrons and the formation of a Kondo lattice. Replacing Ce (4f<sup>1</sup>,  $S=1/2$ ,  $L=3$ ,  $J=5/2$ ) with Sm (4f<sup>5</sup>,  $S=5/2$ ,  $L=5$ ,  $J=5/2$ ), which share the same  $J$ , crosses a quantum critical point and leads to an antiferromagnetic ground state. Nevertheless, we present evidence that SmCoIn<sub>5</sub> retains aspects from the delocalized side of the QCP.

We find evidence for a delocalized 4f component in SmCoIn<sub>5</sub> from measurements of the carrier density, from direct observation of 4f spectral weight in photoemission, and from a temperature-induced crossover in the lattice parameter. In addition, SmCoIn<sub>5</sub> exhibits two magnetically ordered phases. Below  $T_N=12$  K, the antiferromagnetic order is incommensurate with an ordering wave-vector (1/2,0,0.4), and at 2 K it is commensurate with (1/2,0,1/2). The magnetic orders may be multi-q and also include multipolar degrees of freedom.

One feature exhibited by Sm, but not by Ce, is the splitting of the 4f states into many multiplet levels, due to the Coulomb repulsion between 4f electrons. We observe that higher multiplets of Sm may be the ones lying at the Fermi level, suggesting the possibility of a novel delocalization mechanism. Our results show that systems with more than one 4f electron may serve as useful probes of the delocalization conditions near the QCP.

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# Visualization of the Kondo lattice crossover with temperature in $\text{YbRh}_2\text{Si}_2$ with high-resolution Compton scattering

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By studying the prototypical heavy-fermion metal  $\text{YbRh}_2\text{Si}_2$ , we address the long-standing problem of the temperature dependence of the Fermi volume in Kondo lattices. Theory predicts a crossover of the Fermi volume from a so-called *large* Fermi surface to a *small* one upon increasing temperature, as the  $4f$  electron (or hole in Yb-based Kondo lattices) leaves the strong-coupling regime, where its degree of freedom is dissolved into the Fermi sea [1], and becomes effectively localized and decoupled from the conduction band. A direct observation of this transition with temperature has, however, remained elusive, because conventional probes of the Fermi surface, e.g. via de Haas-van Alphen oscillations or ARPES, require high magnetic fields, which might reconstruct the Fermi surface or cannot work reliably at elevated temperatures.

We have employed high-resolution Compton scattering to derive the electron occupation number density (EOND) of  $\text{YbRh}_2\text{Si}_2$  [2], which can be viewed as the projection of the Fermi volume onto a two-dimensional plane in momentum space. Our measurements have revealed pronounced changes in the EOND of  $\text{YbRh}_2\text{Si}_2$  between 14 K and 300 K, which can be attributed to a reconstruction of the Fermi surface with increasing temperature. Comparison to equivalent measurements on  $\text{YbCo}_2\text{Si}_2$ , a reference system for the small Fermi surface, allow to conclude, that the  $\text{YbRh}_2\text{Si}_2$  EOND at 300 K reflects a small Fermi surface, which results from a transition of the Fermi volume from large to small due to the temperature-driven breakdown of the Kondo lattice effect.

[1] M. Güttler *et al.*, Nat. Commun. **10**, 796 (2019).

[2] M. Güttler *et al.*, Phys. Rev. B **103**, 115126 (2021), editor's suggestion.

# CaCu<sub>3</sub>Ru<sub>4</sub>O<sub>12</sub>: A High Kondo-Temperature Transition Metal Oxide

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Kondo physics, a hallmark of the interacting electron physics, is rarely observed in transition-metal oxides. In this talk, we present a comprehensive study for a transition-metal oxide CaCu<sub>3</sub>Ru<sub>4</sub>O<sub>12</sub> using local-density approximation (LDA) + dynamical mean field theory (DMFT). The model parameters in the LDA+DMFT scheme are eliminated by fitting the experimental valence and core-level x-ray photoemission spectra [1] with the aid of a new analysis technique introduced recently [2,3]. The calculated local spin and charge susceptibility show that the transition-metal oxide CaCu<sub>3</sub>Ru<sub>4</sub>O<sub>12</sub> must be classified as a Kondo system, where the localized Cu spin ( $S=1/2$ ) is screened by itinerant Ru  $4d$  electrons. The Kondo temperature is found to be high in the range of 500-1000K that reconciles contradictory conclusions of existing studies (conducted at moderate temperatures) on this compound. The temperature evolution of the Cu  $d$ -electron self-energy and the DMFT hybridization densities reveals the Kondo impurity and Kondo lattice dynamics: both are present in CaCu<sub>3</sub>Ru<sub>4</sub>O<sub>12</sub>. In this talk, we also show the LDA+DMFT result for CaCu<sub>3</sub>Ir<sub>4</sub>O<sub>12</sub>, and discuss how the Kondo temperature can be tuned in this material class CaCu<sub>3</sub>M<sub>4</sub>O<sub>12</sub> by suitably varying the  $M$  constituent.

[1] D. Takegami, C. Y. Kuo, K. Kasebayashi, J. G. Kim, C. F. Chang, C. E. Liu, C. N. Wu, D. Kasinathan, S. G. Altendorf, K. Hofer, F. Meneghin, A. Marino, Y. F. Liao, K. D. Tsuei, C. T. Chen, K.-T. Ko, A. Gunther, S. G. Ebbinghaus, J. W. Seo, D. H. Lee, G. Ryu, A. C. Komarek, S. Sugano, Y. Shimakawa, A. Tanaka, T. Mizokawa, J. Kuneš, L. H. Tjeng, and A. Hariki, *Phys. Rev. X* **12**, 011017 (2022).

[2] A. Hariki, T. Uozumi, and J. Kuneš, *Phys. Rev. B* **96**, 045111 (2017).

[3] K. Higashi, M. Winder, J. Kuneš, and A. Hariki, *Phys. Rev. X* **11**, 041009 (2021).

# Triplet pairing mechanisms from Hund's-Kondo models: applications to heavy fermion superconductors

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A number of heavy-fermion candidate-triplet superconductors share the common structural motif of two or more U/Ce sublattices in the unit-cell separated by an inversion center. We present a pairing mechanism for triplet superconductivity that is enabled by such a locally non-centrosymmetric structure. Extremely high upper critical fields in these materials suggest the importance of local pairing scenarios with coherence lengths comparable to the lattice spacing. For instance, UTe<sub>2</sub> remains superconducting at fields above 60T, suggesting a coherence length shorter than 2nm. A legitimate driver of these local triplet pairing correlations is atomic Hund's coupling, which leads to pre-formed triplet pairs between the electrons trapped inside local moments. The sublattice degree of freedom allows these onsite spin-triplet pairs to acquire odd-parity form factors as they Kondo-hybridize with the dispersive electrons, leading to a pairing instability in a triplet channel. We show how the Hund's coupling modifies the Kondo hybridization leading to an anisotropic "triplet" Kondo coupling. Using a simple two-channel Kondo model, derived from a minimal mixed-valent construction with Hund's coupling, we demonstrate the emergence of odd-parity spin-triplet superconductivity in a mean-field calculation. This unifies the emergence of triplet superconductivity with the Kondo hybridization in a coherent framework, and we present support for this hypothesis from existing experiments.

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# A Testable Theory for High-Tc Superconductivity in Cuprates

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We propose a theory for High-Tc superconductivity in cuprates, which makes quantitative predictions for several observable quantities. We obtain, for instance, analytical expressions for the superconducting (SC) and pseudogap (PG) transition temperatures as a function of doping, respectively,  $T_c(x)$  and  $T^*(x)$ ; for the optimal SC transition temperature as a function of the applied pressure,  $T_{max}(P)$ ; for the resistivity as a function of temperature,  $\rho(T)$  in the pseudogap, strange metal and Fermi liquid phases; and for the magneto-resistivity,  $\rho(H)$ , among other observable quantities. These theoretical predictions are in good agreement with the experimental data for several cuprate materials including LSCO, YBCO, Hg1201, Hg1212, Hg1223, Bi2201, Bi2212, Bi2213. Our theory is, therefore, testable, thus fulfilling one of the first pre-requisites of any acceptable theory.

The pairing mechanism in our theory derives from the ferromagnetic fluctuations part of the Kondo-like magnetic interaction that occurs between the itinerant doped holes (belonging to a sophisticated oxygen p-orbital lattice) and the localized Cu ions. The antiferromagnetic part of the fluctuations leads to the Néel sector, while the PG phenomena stem from the Coulomb repulsion among holes. The main resistivity mechanism results from hole-exciton scattering.

- [1]. E. C. Marino *et al*, Supercond. Sci. Tech. **33**, 035009 (2020).
- [2]. E. C. Marino, R. Arouca, Supercond. Sci. Tech. **34**, 085008 (2021)
- [3]. R. Arouca, E. C. Marino, Supercond. Sci. Tech. **34**, 035004 (2021)



# Unravelling the Nature of Spin Excitations Disentangled from Charge Contributions in a Doped Cuprate Superconductor

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The nature of the spin excitations in superconducting cuprates is a key question toward a unified understanding of the cuprate physics from long-range antiferromagnetism to superconductivity. The intense spin excitations up to the over-doped regime revealed by resonant inelastic X-ray scattering bring new insights as well as problems—like understanding their persistence or their relation to the collective excitations in ordered magnets (magnons). Here, we study the evolution of the spin excitations upon hole-doping the superconducting cuprate  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$  by disentangling the spin from the charge excitations in the experimental cross section [1]. We compare our experimental results against density matrix renormalization group calculations for a  $t$ - $J$ -like model on a square lattice. Our results unambiguously confirm the persistence of the spin excitations, which are closely connected to the persistence of short-range magnetic correlations up to high doping. This suggests that the spin excitations in hole-doped cuprates are related to magnons—albeit short-ranged.

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[1] W. Zhang *et al.*, arXiv:2204.08749 (2022).

# Order-parameter evolution in the Fulde-Ferrell-Larkin-Ovchinnikov phase probed by $^{13}\text{C}$ NMR spectroscopy

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The Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state represents a general concept of pairing in multi-component Fermi liquids with strong population imbalance. Clear experimental realizations of FFLO superconductivity require stringent conditions, such as an orbital critical field much larger than the Pauli paramagnetic limit, and a mean free path larger than the coherence length. In the FFLO state, the spin polarization varies as the modulus of the spatially modulated superconducting gap amplitude, and, thus, its modulation amplitude represents the order parameter. Indeed, NMR experiments of the organic superconductors  $\beta''$ -(ET)<sub>2</sub>SF<sub>5</sub>CH<sub>2</sub>CF<sub>2</sub>SO<sub>3</sub> and  $\kappa$ -(ET)<sub>2</sub>Cu(NCS)<sub>2</sub> showed the emergence of inhomogeneous line broadening, which stems from the spatial modulation of the spin polarization [1-3].

We report on our experimental studies of the temperature-dependent order parameter of the superconducting FFLO state. For that, we utilize  $^{13}\text{C}$  NMR spectroscopy studied in  $\beta''$ -(ET)<sub>2</sub>SF<sub>5</sub>CH<sub>2</sub>CF<sub>2</sub>SO<sub>3</sub>. From a comparison of our experimental results to a comprehensive modeling of the  $^{13}\text{C}$  NMR spectra, we determine the evolution of the local spin-polarization modulation amplitude  $\Delta K_{spin}$  upon condensation of the FFLO state. In the experimentally probed temperature regime,  $\Delta K_{spin}$  yields a mean-field-type evolution of the order parameter. Further, the modeling of the spectra in the superconducting phase allows to quantify the decrease of the average spin polarization, stemming from the spin-singlet coupling of the superconducting electron pairs in the FFLO state of  $\beta''$ -(ET)<sub>2</sub>SF<sub>5</sub>CH<sub>2</sub>CF<sub>2</sub>SO<sub>3</sub>.

[1] J. A. Wright *et al.*, Phys. Rev. Lett. **107**, 087002 (2011).

[2] H. Mayaffre *et al.*, Nat. Phys. **10**, 928 (2014).

[3] G. Koutroulakis *et al.*, Phys. Rev. Lett. **116**, 067003 (2016).

# Orbital FFLO State in a Layer-Coupled Ising Superconductor

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In a conventional superconductor, when both spatial inversion and time-reversal symmetries are respected, electrons form Cooper pairs with both opposite momenta and spins as described by the Bardeen–Cooper–Schrieffer (BCS) theory. Breaking either one of the two aforementioned symmetries can lead to unconventional Cooper pairing with nontrivial spin or momentum configurations. In transition metal dichalcogenides (TMDs), the Ising SOC enhances the paramagnetic limiting field to go beyond the Pauli limit [1–3]. Applying parallel magnetic fields to the  $2H$ -type TMDs may induce an orbital Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase, where Cooper pairs are formed with nonzero momentum, by coupling Ising SOC and orbital effect [4,5].

We report the experimental observation of the orbital effect induced finite momentum superconducting state in a multilayer  $2H$ -type Ising superconductor NbSe<sub>2</sub>. The orbital FFLO phase emerges below a tricritical point  $T^* = 0.84T_{c0}$  and  $B^* = 0.36B_p$ , at which the orbital effect of the parallel  $B$  field couples superconducting layers through Josephson interaction. Compared with the uniform phase below  $B^*$ , the orbital FFLO alters the pinning of vortex when the finite momentum Cooper pairing breaks the translational symmetry of the uniform order parameter in real space. Meanwhile, it also breaks the rotational symmetry, showing a six-fold azimuthal anisotropy of the superconducting critical temperature. Following the distinctive symmetry behavior, we can map out the first-order boundary and establish the phase diagram of orbital FFLO states.

[1] Kormányos, A. et al. Monolayer MoS<sub>2</sub>: Trigonal warping, the  $\Gamma$  valley, and spin-orbit coupling effects. *Phys. Rev. B - Condens. Matter Mater. Phys.* 88, 1–8 (2013).

[2] Lu, J. M. et al. Evidence for two-dimensional Ising superconductivity in gated MoS<sub>2</sub>. *Science* 350, 1353–1357 (2015).

[3] Xi, X. et al. Ising pairing in superconducting NbSe<sub>2</sub> atomic layers. *Nat. Phys.* 12, 1–6 (2015).

[4] Liu, C. X. Unconventional Superconductivity in Bilayer Transition Metal Dichalcogenides. *Phys. Rev. Lett.* 118, 1–5 (2017).

[5] Nakamura, Y. & Yanase, Y. Odd-parity superconductivity in bilayer transition metal dichalcogenides. *Phys. Rev. B* 96, 1–11 (2017).

## Field-angle dependence reveals odd-parity superconductivity in CeRh<sub>2</sub>As<sub>2</sub>

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CeRh<sub>2</sub>As<sub>2</sub> is an unconventional superconductor with multiple superconducting phases and  $T_c = 0.26$  K. When  $H \parallel c$ , it shows a field-induced transition at  $\mu_0 H^* = 4$  T from a low-field superconducting state SC1 to a high-field state SC2 with a large critical field of  $\mu_0 H_{c2} = 14$  T. In contrast, for  $H \parallel ab$ , only the SC1 with  $\mu_0 H_{c2} = 2$  T is observed [1]. A simple model based on the crystal symmetry was able to reproduce the phase-diagrams and their anisotropy, identifying SC1 and SC2 with even and odd parity superconducting states, respectively. However, additional orders were observed in the normal state which might have an influence on the change of the superconducting state at  $H^*$  [2]. Here, we present a comprehensive study of the angle dependence of the upper critical fields using magnetic ac-susceptibility, specific heat and torque on single crystals of CeRh<sub>2</sub>As<sub>2</sub>. The experiments show that the state SC2 is strongly suppressed when rotating the magnetic field away from the  $c$ -axis and it disappears for an angle of 35°. This behavior agrees perfectly with our extended model of a pseudospin triplet state with  $\mathbf{d}$  vector in the plane and hence allows to nail down that SC2 is indeed the suggested odd-parity state.

[1] S. Khim and J. F. Landaeta *et al.* Science **373** (6558), 1012-1016 (2021)

[2] D. Hafner *et al.* Phys. Rev. X **12** (1), 011023 (2022)

# Orbital effects in spin-singlet superconductors: $\pi$ -pairing, Edelstein effect, and orbital vortex phase

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We consider a multi-orbital spin-singlet superconductor without inversion symmetry, e.g. due to crystalline asymmetry as well as to electric fields or mechanical strain. The lack of inversion symmetry yields non-trivial orbital-Rashba couplings in the system that affects the electronic orbital texture at the surface leading to a dramatic impact on the superconductivity. We demonstrate that, by varying the strength of the orbital-Rashba couplings, the superconducting phase can be either suppressed, or undergo a  $0-\pi$  transition, with the  $\pi$ -phase being marked by non-trivial sign change of the superconducting order parameter between different bands[1-2]. The occurrence of orbital dependent phase frustration can naturally account for the observation of the suppression of the critical supercurrent without change in the critical temperature, observed in recent experiments[3-4].

Furthermore, in superconductors that lack inversion symmetry, the flow of supercurrent can induce a non-vanishing magnetization, a phenomenon also known as Edelstein effect. We find that the supercurrent-induced orbital magnetization is more than one order of magnitude greater than that due to the spin, and it is shown to be also sign tunable[5].

Exploring further the role of spatial symmetry breaking, we show that in two-dimensional spin-singlet superconductors with low degree of spatial-symmetry content, a vortex state at zero magnetic field can be energetically stable[6]. This vortex is marked by neutral supercurrents flowing around the core with counterpropagating Cooper pairs with opposite orbital moments.

The overall findings unveil a rich scenario to design heterostructures with superconducting orbitronics effects for the achievement, for instance, of all-electric superconducting devices.

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[1] M. T. Mercaldo, P. Solinas, F. Giazotto, and M. Cuoco, *Phys. Rev. Applied* **14**, 034041 (2020).

[2] M. T. Mercaldo, F. Giazotto, and M. Cuoco, *Phys. Rev. Research* **3**, 043042 (2021).

[3] G. De Simoni, et al., *Nat. Nanotechnol.* **13**, 802 (2018).

[4] L. Bours, M. T. Mercaldo, M. Cuoco, E. Strambini, and F. Giazotto, *Phys. Rev. Research* **2**, 033353 (2020).

[5] L. Chirolli, M.T. Mercaldo, C. Guarcello, F. Giazotto, and M. Cuoco, arXiv:2107.07476.

[6] M. T. Mercaldo, C. Ortix, F. Giazotto, and M. Cuoco, arXiv:2105.09025, *Phys. Rev. B (Letter)* to be published.

# Theory of intrinsic superconducting diode effect

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Nonreciprocal phenomena are attracting attention as new functionalities of matter [1,2]. Examples include the magnetochiral anisotropy (MCA), which has been observed in various materials from (semi)conductors to superconductors. MCA is the inequivalence of the resistance for the rightward and leftward currents. On the other hand, such a drastic situation is possible in superconductors that either one of the leftward and rightward resistance vanishes while the other remains finite: electrons flow individually in one direction while flow with forming the Cooper pairs in the other. Such a superconducting diode effect (SDE) has recently been observed in the Nb/V/Ta superlattice without an inversion center [3]. SDE is a promising building block of dissipationless electric circuits and is a fascinating phenomenon manifesting the interplay of the inversion breaking and superconductivity. However, the mechanisms to cause SDE have not been clarified.

In this work, we propose an intrinsic mechanism to cause SDE by studying the nonreciprocity in the depairing critical current [4]. We clarify the temperature scaling of the nonreciprocal depairing current near the critical temperature [4,5,6] and point out its significant enhancement at low temperatures. It is also found that the nonreciprocal critical current shows sign reversals upon increasing the magnetic field. These behaviors are understood by the nonreciprocity of the Landau critical momentum and the crossover of the helical superconductivity. Thereby, we propose the intrinsic SDE as a promising bulk probe of the helical superconducting states.

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[1] Y. Tokura and N. Nagaosa, *Nat. Commun.* **9**, 3740 (2018).

[2] T. Ideue and Y. Iwasa, *Annu. Rev. Condens. Matter Phys.* **12**, 201 (2021).

[3] F. Ando *et al.*, *Nature* **584**, 373 (2020).

[4] A. Daido, Y. Ikeda, and Y. Yanase, *Phys. Rev. Lett.* **128**, 037001 (2022).

[5] N. Yuan and L. Fu, *PNAS* **119**, e2119548119 (2022).

[6] J. J. He, Y. Tanaka, and N. Nagaosa, arXiv:2106.03575.

# Designer quantum states in van der Waals heterostructures

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Van der Waals (vdW) heterostructures have emerged as a playground for realizing and engineering exotic quantum states not found in naturally occurring materials. Materials with very different physical properties can be combined essentially at will and the desired physics emerges through the engineered interactions between the different components. VdW heterostructures can also be directly incorporated into device structures and potentially allow further control through e.g. electrostatic gating.

I will highlight these concepts through our results on realizing topological superconductivity and heavy-fermion physics in vdW heterostructures [1-3]. We use molecular-beam epitaxy (MBE) in ultra-high vacuum for the sample growth and characterize the resulting samples using low-temperature scanning tunneling microscopy (STM). Topological superconductivity requires combining out of plane ferromagnetism, Rashba-type spin-orbit interactions and s-wave superconductivity and we use monolayer ferromagnet CrBr<sub>3</sub> on a superconducting substrate NbSe<sub>2</sub> to achieve this. I will discuss how the presence of a moiré pattern is an essential ingredient in this system as it profoundly modifies the topological phase diagram and enables the realization of a topological superconducting state that would not be accessible in the absence of the moiré. As another example of a designer vdW system, I focus on our experiments on 1T-TaS<sub>2</sub> / 1H-TaS<sub>2</sub> heterostructures that bring together the building blocks of heavy fermion systems - Kondo coupling between a lattice of localized magnetic moments and mobile conduction electrons [3]. These results highlight the versatility of vdW heterostructures in realizing quantum states that are difficult to find and control in naturally occurring materials.

[1] S. Kezilebieke *et al.*, Topological superconductivity in a van der Waals heterostructure, *Nature* **588**, 424-428 (2020).

[2] S. Kezilebieke *et al.*, Moiré-enabled topological superconductivity, *Nano Lett.* **22**, 328 (2022).

[3] V. Vaño *et al.*, Artificial heavy fermions in a van der Waals heterostructure, *Nature* **599**, 582-586 (2021).

## Anisotropic c-f hybridization in CeRh<sub>6</sub>Ge<sub>4</sub> and CeCu<sub>2</sub>Si<sub>2</sub>

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The Kondo effect, manifested by the hybridization between conduction and f electrons (c-f hybridization), plays a key role in the low-temperature properties in Ce-based heavy fermion systems, although the importance of band/momentum-dependent c-f hybridization remains an important issue. Here we demonstrate the significance of anisotropic c-f hybridization in two prototypical Ce-based heavy fermion systems, CeRh<sub>6</sub>Ge<sub>4</sub> and CeCu<sub>2</sub>Si<sub>2</sub>, using angle-resolved photoemission spectroscopy (ARPES). In CeRh<sub>6</sub>Ge<sub>4</sub>, where a pressure-induced ferromagnetic quantum critical point was recently discovered, we found that strong c-f hybridization takes place already well above the Curie temperature ( $T_c = 2.5$  K), and the hybridization strength was found to be anisotropic in k-space due to the chainlike configuration of Ce [1]. In the canonical heavy fermion superconductor CeCu<sub>2</sub>Si<sub>2</sub>, we directly observed the quasi-two-dimensional heavy electron band near the Brillouin corner [2], predicted by theoretical calculations, which is essential for the emergence of spin density wave and heavy fermion superconductivity. We also found light conduction bands near the Z point, which contain much smaller 4f weight. The momentum/band-dependent c-f hybridization can be important for understanding the emergent phenomena in Ce-based heavy fermion systems.

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[1] Y. Wu *et al.*, Phys. Rev. Lett. **126**, 216406 (2021).

[2] Z. Wu *et al.*, Phys. Rev. Lett. **127**, 067002 (2021).



## Quantum critical point in the high-pressure structure of CeSb<sub>2</sub>

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Ce-based heavy fermion compounds exhibit a variety of exotic states brought about by strong electronic correlations. Their properties are often susceptible to pressure-tuning, which can stabilise new phases and push materials through quantum phase transitions.

CeSb<sub>2</sub> at ambient pressure displays a series of complex magnetic phases and is thought to adopt a ferromagnetic ground state, a rare case in Ce systems which invites further study [1]. Magnetic transitions have been known to depend only weakly on applied pressure up to about 20 kbar, where material properties change abruptly [2]. Using high-pressure powder X-ray diffraction, we have recently demonstrated that this abrupt change can be attributed to a structural transition, and we have resolved the high pressure crystal structure [3]. Here, we focus on the low-temperature properties in the new high-pressure structure.

We have accessed the high-pressure structure of CeSb<sub>2</sub> using both piston-cylinder and anvil pressure cells at mK temperatures. Our resistivity and AC heat capacity data reveal two new phase transition anomalies which move to lower temperatures with increasing pressure. The temperature dependence of the resistivity above the ordering temperature is unusually steep, suggesting a low coherence temperature and very high effective masses. In the pressure region where the transitions extrapolate to zero temperature, we observe non-Fermi liquid behaviour, suggesting the presence of a quantum critical point. We will show data on the temperature-, field- and pressure-dependence of the resistivity in the vicinity of the quantum critical point, and we will discuss our findings in the context of recent experimental and theoretical results in other heavy fermion compounds.

[1] S. L. Bud'ko, P. C. Canfield, C. H. Mielke, and A. H. Lacerda, *Anisotropic Magnetic Properties of Light Rare-Earth Diantimonides*, Phys. Rev. B 57, 13624 (1998).

[2] T. Kagayama, Y. Uwatoko, S. L. Bud'ko, and P. C. Canfield, *Pressure-Induced Collapse of Ferromagnetism in CeSb<sub>2</sub>*, Physica B: Condensed Matter 359–361, 320 (2005).

[3] C. K. de Podesta *et al.*, this conference (2022).

# Electro-nuclear transition in $\text{YbRh}_2\text{Si}_2$ ; evidence for a spin density wave

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The nature of the antiferromagnetic order in the heavy fermion metal  $\text{YbRh}_2\text{Si}_2$ , its quantum criticality, and superconductivity, which appears at low mK temperatures [1], as well as the interplay between magnetism and superconductivity remain open questions. We report measurements of the heat capacity over the temperature range 180  $\mu\text{K}$  - 80 mK, performed in a novel cell which uses current sensing noise thermometry over the full temperature range. Measurements were made at magnetic fields in the range 0 to 70 mT, applied perpendicular to the *c*-axis. In zero magnetic field we observe a sharp heat capacity anomaly at 1.5 mK, which coincides with a transition in superconducting transport. The entropy agrees with the expected Yb nuclear spin entropy. The nuclear moments detect, through the hyperfine interaction, the local magnitude of the electronic moment. This is small above the transition, consistent with  $0.002\mu_B$  along hard *c*-axis, and we precisely determine the quadrupole energy. Below the anomaly the data are well described by an incommensurate electronic spin density wave (SDW) of amplitude  $0.1\mu_B$  at the lowest temperatures. This can be accounted for by a re-orientation of the electronic spins into the *ab*-plane, previously observed under the influence of in plane field [2]. With increasing magnetic field, up to 22 mT, the anomaly in the nuclear spin heat capacity broadens and shifts to lower temperatures. Together these results demonstrate that superconductivity and antiferromagnetism coexist and demonstrate SDW order of as yet unknown *q*-vector.

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[1] E. Schuberth, M. Tippmann, L. Steinke, S. Lausberg, A. Steppke, M. Brando, C. Krellner, C. Geibel, R. Yu, Q. Si, and F. Steglich. Emergence of superconductivity in the canonical heavy electron metal  $\text{YbRh}_2\text{Si}_2$ . *Science* 351, 485, (2016).

[2] M. Brando, L. Pedrero, T. Westerkamp, C. Krellner, P. Gegenwart, C. Geibel, and F. Steglich. Magnetization study of the energy scales in  $\text{YbRh}_2\text{Si}_2$  under chemical pressure. *Physica Status Solidi B* 250, 485, (2013).

## The multi-phase heavy-fermion superconductor CeRh<sub>2</sub>As<sub>2</sub>

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We discovered superconductivity in CeRh<sub>2</sub>As<sub>2</sub> ( $T_c = 0.26$  K) in 2017. It is a rare case of a system with multiple superconducting (SC) phases in which the even-parity SC order parameter can be changed into an odd-parity one by a magnetic field [1]. Meanwhile, a large number of experiments have been performed to understand its SC state and other peculiar properties, namely: i) the presence of a non-magnetic ordered phase believed to be a unique example of quadrupole-density-wave (QDW) order [2], ii) the suspected presence of antiferromagnetic (AFM) order as odd-parity multipoles inside the SC phase [3], and finally the nature of the quantum critical fluctuations observed right above all these ordered phases.

I will present a comprehensive overview of recent experiments and provide new insights into the understanding of this material. In particular, I will focus on the interplay between superconductivity and the QDW and AFM phases with the aim of explaining why CeRh<sub>2</sub>As<sub>2</sub> has still no equals.

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[1] S. Khim, J. F. Landaeta *et al.*, *Science* **373**, 1012 (2021)

[2] D. Hafner *et al.*, *Phys. Rev. X* **12**, 011023 (2022)

[3] M. Kibune *et al.*, *Phys. Rev. Lett.* **128**, 057002 (2022)

# Novel parity transition in strongly correlated superconductor: relation to CeRh<sub>2</sub>As<sub>2</sub>

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The recent discovery of superconductivity in CeRh<sub>2</sub>As<sub>2</sub> clarified an unusual  $H$ - $T$  phase diagram with two superconducting phases [1]. CeRh<sub>2</sub>As<sub>2</sub> crystallizes in the centrosymmetric tetragonal CaBe<sub>2</sub>Ge<sub>2</sub>-type structure with stacking Ce layers and Rh<sub>2</sub>As<sub>2</sub> layers. Importantly, Rh<sub>2</sub>As<sub>2</sub> layers at the top and bottom of the Ce layer have different compositions. Therefore, the inversion symmetry is locally broken at the Ce sites, although the global inversion center exists in the middle of the two Ce sites. Surprisingly, a similar phase diagram was predicted in theoretical work about locally noncentrosymmetric superconductors [2]. The qualitative similarity of the phase diagrams between the experiment [1] and theory [2] suggests that the local inversion symmetry breaking plays an essential role in CeRh<sub>2</sub>As<sub>2</sub> and the superconducting phase in the high magnetic field region is the pair-density-wave (PDW) state. PDW state is an odd parity superconducting state with dominant spin-singlet pairing. We showed that the PDW phase in CeRh<sub>2</sub>As<sub>2</sub> is topological superconductivity [3]. However, there are contradicting points between the weak-coupling theory and experiment. In particular, the parity transition field obtained by the weak-coupling theory is small by a factor of five, and the up-turn structure of the upper critical field in the high-magnetic field region is not observed by the experiment [1].

In this talk, we focus on strong correlation effects in CeRh<sub>2</sub>As<sub>2</sub>. We find  $XY$ -type magnetic fluctuation consistent with a recent NMR study [4]. We also clarify that in the resulting superconducting phase diagram, the parity transition field is significantly enhanced, and the up-turn structure is weakened.

[1] S. Khim *et al.*, *Science* **373**, 1012 (2021).

[2] T. Yoshida, M. Sigrist, and Y. Yanase, *Phys. Rev. B* **86**, 134514 (2012).

[3] K. Nogaki, A. Daido, J. Ishizuka, and Y. Yanase, *Phys. Rev. Research* **3**, L032071 (2021).

[4] S. Kitagawa *et al.*, *J. Phys. Soc. Jpn.* **91**, 043702 (2022).

# Cascade of Fermi surface reconstructions linked to superconductivity inside the CDW phase of TiSe<sub>2</sub>

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The Fermi surface reconstruction induced by a charge density wave (CDW) has drawn interest for a long time. Recently, observations of CDW correlations in cuprates [1] and nickelates [2] have sparked new interest in CDW phases. Moreover, several scenarios for the relation to superconductivity have been proposed in high-temperature superconductors [3].

The transition metal dichalcogenides have been instrumental in the development of CDW models as well as studies of Fermi surface reconstruction [4] and the interplay of CDWs with superconductivity. Here, we study the Fermi surface evolution of TiSe<sub>2</sub> with pressure over the entire CDW phase. Our quantum oscillation experiments reveal not only a reconstruction upon entering the CDW phase, but also a remarkable cascade of further Fermi surface reconstructions within the CDW phase indicated by sharp changes in the observed frequencies.

To interpret these results, we conducted DFT calculations to model the pressure evolution of the Fermi surface, finding good agreement outside the CDW phase where the Fermi surface is unreconstructed. Introducing the CDW gap inspired by recent ARPES results [5], we evolve the Fermi surface inside the CDW phase and find good agreement with our measurements. The obtained model suggests a link between the presence of a large Fermi surface pocket and superconductivity in TiSe<sub>2</sub> [6]. These results help quantitatively understand the interplay between CDW phases and electronic degrees of freedom which give rise to superconductivity.

[228 words, max 250]

[1] C. C. Tam, *et al.* Nature Commun. 13, 570 (2021).

[2] M. Rossi *et al.* arXiv: 2112.02484 (2021).

[3] B. J. Ramshaw, *et al.* Science **348**, 317 (2015).

[4] T. M. Rice and G. K. Scott, Phys. Rev. Lett. 35, 2 (1975).

[5] M. D. Watson, *et al.*, Phys. Rev. Lett. 122, 076404 (2019).

[6] A. F. Kusmartseva, *et al.*, Phys. Rev. Lett. 103, 236401 (2009).

## Laser ARPES measurements of Sr<sub>2</sub>RuO<sub>4</sub> under uniaxial strain

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Sr<sub>2</sub>RuO<sub>4</sub> has evolved into a key-model system for correlated electron physics following the discovery of its superconductivity - long believed to harbour p-wave triplet pairing - 28 years ago. The normal state of Sr<sub>2</sub>RuO<sub>4</sub> is exceptionally well characterized and is generally regarded as the cleanest Fermi-liquid system amongst all transition metal oxides. Recent transport experiments discovered that a compressive strain of  $\sim 0.6\%$  causes the superconducting transition temperature of Sr<sub>2</sub>RuO<sub>4</sub> to increase from 1.5 K to 3.4 K concomitant with the development of a pronounced non-Fermi-liquid behaviour in the normal state. This behaviour is commonly attributed to a Lifshitz transition in one of the three Fermi surface sheets [1–3]. Here, we report a new generation of ARPES experiments under strain based on a thermally actuated strain cell and a micro-structured tapered sample prepared with focused ion beam milling. Coupled with a micro-focused laser source, this allows the measurement of the quasi-continuous variation of strain on a single sample. We use this new capability to image the Lifshitz transition and to monitor the evolution of the quasiparticle dispersion and self-energy upon approaching the non-Fermi-liquid regime.

[1] A. Steppke *et al.*, *Science* **355**, 6321 (2017).

[2] M. Barber *et al.*, *Phys. Rev. Lett.* **120**, 076602 (2018).

[3] V. Sunko *et al.*, *npj Quantum Mater.* **4**, 46 (2019).

## Orbital loop current phase at the surface of Sr<sub>2</sub>RuO<sub>4</sub>

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The layered oxide perovskite Sr<sub>2</sub>RuO<sub>4</sub> is a strongly correlated electron material that has been intensively investigated since its discovery due to its unusual physical properties. Whilst recent experiments have reopened the debate on the exact symmetry of the superconducting state in Sr<sub>2</sub>RuO<sub>4</sub>, a deeper understanding of the normal state appears crucial as this is the background in which electron pairing occurs. We investigate the occurrence of quantum phases at the surface of Sr<sub>2</sub>RuO<sub>4</sub> with breaking of time reversal symmetry due to electronic ordering in the form of orbital loop currents. We use a tight-binding description of the electronic structure of Sr<sub>2</sub>RuO<sub>4</sub> including d-orbitals at the Ru sites and p-orbitals at the planar O sites and consider d-p and p-p Coulomb interactions as responsible for the electronic instabilities yielding the orbital loop current phase. We find that loop currents with vanishing net magnetic flux due to orbital frustration are energetically stable and can account for the hallmark signatures of the observed time-reversal symmetry breaking phase at the Sr<sub>2</sub>RuO<sub>4</sub> surface [1]. The orbital dependent nature of the loop current phase suggests that mechanisms lowering the crystalline symmetry, e.g. strain, can increase the orbital imbalance and result in stronger magnetism. From this point of view, our results can be also linked to the strain-induced magnetism and other magnetic phenomena already observed in the bulk of Sr<sub>2</sub>RuO<sub>4</sub>.

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[1] R. Fittipaldi, M.T. Mercaldo, ..., M. Cuoco, Z. Salman, A. Vecchione, A. Di Bernardo, Nature Communications 12, 5792 (2021)

# Twofold van Hove singularity and origin of charge order in topological kagome superconductor $\text{CsV}_3\text{Sb}_5$

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Recently, kagome lattice compounds have emerged as a novel platform to realize exotic quantum many-body phenomena, combining strong electronic correlation and nontrivial topology. This potential of the kagome lattice originates from its unique symmetry-protected electronic dispersion, composed of Dirac fermions, van Hove singularities (vHS), and flat band.

In late 2020, a series of V-based kagome metal  $AV_3\text{Sb}_5$  ( $A=\text{K,Rb,Cs}$ ) is discovered to exhibit surprisingly rich arrays of entangled symmetry-breaking phases, in close analogy to other strongly correlated systems such as Cu- and Fe-based high-temperature superconductors. The collective phenomena in  $AV_3\text{Sb}_5$  observed so far include translational symmetry breaking  $2\times 2$  charge order, rotational symmetry breaking  $1\times 4$  stripe order, time-reversal symmetry breaking loop current phase, and superconductivity [1].

Here, combining angle-resolved photoemission spectroscopy and density functional theory, we establish the connection between novel collective phenomena realized in  $\text{CsV}_3\text{Sb}_5$  and its underlying kagome electronic structure [2]. We detected multiple kagome-derived vHS coexisting near the Fermi level of  $\text{CsV}_3\text{Sb}_5$ , which are characterized by two distinct *pure* ( $p$ ) and *mixed* ( $m$ ) sublattice flavors. The two types of vHS are unique to the kagome lattice geometry and critically determine the pairing symmetry and ground states emerging in the  $AV_3\text{Sb}_5$  series. We established that among the multiple vHS in  $\text{CsV}_3\text{Sb}_5$ , the  $m$ -type vHS of  $d_{xz}/d_{yz}$  kagome band and the  $p$ -type vHS of  $d_{xy}/d_{x^2-y^2}$  kagome band play an essential role in the electronic symmetry breaking across the charge order transition. Our work lays the groundwork to understand the unconventional many-body phases emerging from the itinerant kagome lattice electrons.

\*This work is supported by the STC Center for Integrated Quantum Materials, NSF.

[1] T. Neupert *et al.*, *Nature Physics* **18**, 137-143 (2022).

[2] M. Kang *et al.*, *Nature Physics* **18**, 301-308 (2022).



## ***Electronic structure of CeTAl<sub>3</sub> (T=Ag, Au, Cu, Pd, Pt) studied with density functional theory***

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The CeTAl<sub>3</sub> family (T=Ag, Au, Cu, Pd, Pt) is prototypical of strongly correlated electron systems with a large variety of different magnetic ordering phenomena [1,2,3,4], such as ferromagnetism in CeAgAl<sub>3</sub> and incommensurate antiferromagnetism in CeAuAl<sub>3</sub>. Further, in CeAuAl<sub>3</sub> [5] and CeCuAl<sub>3</sub> [6] magnetoelastic hybrid excitations between crystal electric fields and phonons have been observed. The electronic structure, and in particular the role of the Ce-4f electron, is key for understanding the mechanism driving these phenomena. We report electronic structure calculations for selected members of the CeTAl<sub>3</sub> family, where the Ce-4f electrons are described either as being itinerant or localized using DFT or DFT+U, respectively. The results of our calculations treating the 4f electrons as localized are in good agreement with the experimental data available.

[1] C. Franz *et al.*, J. Alloy. Comp. **668**, 978 (2016).

[2] D.T. Adroja *et al.*, Phys. Rev. B **91**, 134425 (2015)

[3] M. Klipcera *et al.*, Phys. Rev. B **91**, 224419 (2015)

[4] M. Stekiel *et al.*, arXiv:2106.08194 (2021)

[5] P. Čermák *et al.*, Proc. Natl. Acad. Sci. **116**, 6695 (2019).

[6] D.T Adroja *et al.*, Phys. Rev. Lett. **108**, 216402 (2012).

# ***Disorder-robust phase crystal in high-temperature superconductors from topology and strong correlations***

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Today there exists a strong research focus on topological effects in condensed matter. Initial studies were only focused on non-interacting electronic systems, but attention is now shifting towards the influence of electron-electron interactions and also the broken symmetry states they can generate. Real-world materials bring disorder as a third important component, as many symmetry broken states are sensitive to disorder. Hence, to understand many materials we need to keep a combined focus on topology, electronic correlations, and disorder. Copper oxide high-temperature superconductors (cuprates) with pair breaking edges host a flat band of topological zero-energy states, making them an ideal playground where strong correlations, topology, and disorder are strongly intertwined. Here, we show that the three way interplay in cuprates generates a new phase of matter: a fully gapped "phase crystal" state that breaks both translational and time reversal invariance, characterized by a modulation of the d-wave superconducting phase co-existing with a modulating extended s-wave superconducting order. In contrast to conventional wisdom, this phase crystal state is remarkably robust to omnipresent disorder, but only in the presence of strong correlations, thus giving a clear route to its experimental realization.

\*This work is supported by the the Swedish Research Council (Vetenskapsrådet, Grant No. 2018-03488) and the Knut and Alice Wallenberg Foundation through the Wallenberg Academy Fellows program.

[1] D. Chakraborty *et al.*, npj Quantum Materials 7, 44 (2022).

# Topology, colossal magnetoresistance, and complex magnetic domains in $\text{Eu}_5\text{In}_2\text{Sb}_6$

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The axion insulating state is a paradigm of topological correlated matter which has been particularly difficult to demonstrate in real materials. We found that the non-symmorphic Zintl compound  $\text{Eu}_5\text{In}_2\text{Sb}_6$ , which has previously attracted interest due to its extraordinary thermoelectric and colossal magnetoresistive properties [1], may provide an unprecedented platform to explore and engineer the effects of band topology in narrow-gap magnetic insulators [2,3]. While previous demonstrations of axion insulating states required the growth of artificial heterostructures or were limited by ionic disorder,  $\text{Eu}_5\text{In}_2\text{Sb}_6$  yields high-quality crystals with robust and reproducible physical properties.

Using neutron scattering, resonant elastic x-ray scattering, muon spin-rotation and bulk measurements, we clarify how the combination of co-planar glide symmetries and large  $\text{Eu}^{2+}$  magnetic moments produces an unusual two-step ordering process. At  $T_N = 15$  K, the material first forms a complex non-collinear weak Ising-ferrimagnet, which we identify as a trivial insulator. Below  $T_Z = 7.5$  K, this phase is continuously displaced by a growing volume fraction of a compensated antiferromagnetic arrangement that may have axion insulating character. This discovery also implies the presence of a solitonic antiferromagnetic domain structure on the mesoscale, which demonstrably couples to charge transport and, due to the net magnetization of some domains, should be highly susceptible to manipulation. This will potentially open up a platform to engineer interfaces of trivial and non-trivial insulators on the mesoscale.

[1] P. Rosa *et al.*, npj Quantum Materials 5, 52 (2020).

[2] Y. Xu *et al.*, Nature 586, 702 (2020).

[3] B. J. Wieder *et al.*, Science 361, 246 (2018)

# The Weyl-Kondo semimetal: high-harmonic generation and extreme topological tunability

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Strong correlations between electrons in condensed matter promote the formation of local moments, which lowers the energy scales of external tuning needed to induce quantum and topological phase transitions by a large renormalization of their coupling with the conduction electrons. The heavy fermion systems have been a fruitful platform to study strongly correlated topological semimetals, for which Weyl-Kondo semimetals (WKSM) [1-3] are prototype examples. In [1-5], novel topological probes that can be performed in the strongly correlated regime were developed.

High-harmonic generation (HHG) is a twofold probe of both topology (through inter- and intra-band transitions enabled by nontrivial Berry curvature, and a probe of strong correlations by detecting the coherent excitations or charge dynamics of many-body states. The HHG spectra of the WKSM model is studied in terms of the harmonic orders, intensity and frequency dependence, and across different correlation energy scales. The HHG spectra of several models with no correlations and trivial topology are compared to the spectra of the WKSM in order to elucidate the physical origins of the nonlinear optical processes shaping the signal.

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[1] H.-H. Lai, S. E. Grefe, S. Paschen, Q. Si, Proc. Natl. Acad. Sci. U.S.A. **115**, 1 (2018); S. E. Grefe *et al.*, Phys. Rev. B **101**, 075138 (2020).

[2] L. Chen *et al.* (S. E. Grefe), arXiv:2107.10837 (2021).

[3] S. Dzsaber *et al.*, Phys. Rev. Lett. **118**, 246601 (2017); S. Dzsaber *et al.* (S. E. Grefe), Proc. Natl. Acad. Sci. U.S.A. **118**, 8 (2021).

[4] S. Dzsaber *et al.*, arXiv:1906.01182 (2019).

[5] S. E. Grefe, H.-H. Lai, S. Paschen, Q. Si, arXiv:2012.15841 (2020).

# Physical properties of $\text{Ce}_3\text{Bi}_4\text{X}_3$ beyond the $X = \text{Pt}, \text{Pd}$ case: First study of $\text{Ce}_3\text{Bi}_4\text{Ni}_3$

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The proposal that Kondo insulators could host topologically nontrivial surface states sparked a variety of experimental studies on different candidate materials. It was shown that the archetypal Kondo insulator  $\text{Ce}_3\text{Bi}_4\text{Pt}_3$  can be driven into an exotic strongly correlated topological semimetal state when Pt is substituted by Pd [1]. The fully substituted compound  $\text{Ce}_3\text{Bi}_4\text{Pd}_3$  is the first realization of a Weyl-Kondo semimetal [1-3]. There, a cubic-in-temperature contribution to the electronic specific heat [1] and a giant spontaneous (nonlinear) Hall response [3] are attributed to the presence of Weyl nodes in the bulk band structure, positioned in the immediate vicinity of the Fermi energy. Here we extend the isoelectronic substitution study (5d to 4d) one step further, to the 3d transition element compound  $\text{Ce}_3\text{Bi}_4\text{Ni}_3$ . We report the first successful single crystal growth and present results of chemical and structural analyses and physical property measurements. Interestingly,  $\text{Ce}_3\text{Bi}_4\text{Ni}_3$  shows insulating behavior with a residual resistivity ratio comparable to that of  $\text{Ce}_3\text{Bi}_4\text{Pt}_3$ . Unlike the Pt-to-Pd case, the substitution of Pd by Ni is not isosize and corresponds to positive chemical pressure. Thus, our results not only add to the general knowledge of the large 3-4-3 family, but could also have an impact on the interpretation of pressure effects on  $\text{Ce}_3\text{Bi}_4\text{Pd}_3$  [4].

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[1] S. Dzsaber *et al.*, Phys. Rev. Lett., **118**, 246601 (2017)

[2] H.-H. Lai *et al.*, Proc. Natl. Acad. Sci. U.S.A. **115**, 93 (2018)

[3] S. Dzsaber *et al.*, Proc. Natl. Acad. Sci. U.S.A. **118**, e2013386118 (2021)

[4] M. O. Ajeesh *et al.*, arXiv:2110.08230 (2021)

# Effects of hydrostatic pressure on the Weyl-Kondo semimetal candidate CeRu<sub>4</sub>Sn<sub>6</sub>

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Nontrivial electronic topology in strongly correlated materials is an emerging area of great interest, as it may open a way to realize entirely new quantum phases. A promising platform to explore this regime is the tetragonal, noncentrosymmetric Kondo semimetal CeRu<sub>4</sub>Sn<sub>6</sub>. It was theoretically predicted that CeRu<sub>4</sub>Sn<sub>6</sub> could host Weyl nodes in its electronic band structure near the Fermi level [1], making it a candidate material for the newly discovered Weyl-Kondo semimetal phase [2-4]. With the discovery that CeRu<sub>4</sub>Sn<sub>6</sub> is quantum critical without tuning [5], a natural question arises: Can the Weyl-Kondo semimetal phase nucleate out of quantum critical fluctuations and get further stabilized via tuning? Here we address this question by a study of the specific heat and magnetotransport properties of CeRu<sub>4</sub>Sn<sub>6</sub> single crystals under hydrostatic pressure.

\* The work in Vienna was supported by the Austrian Science Fund (FWF projects I4047, P29279, and I5868-FOR 5249 - QUAST) and the European Microkelvin Platform (H2020 project 824109).

[1] Y. Xu *et al.*, Phys. Rev. X **7**, 011027 (2017)

[2] S. Dzsaber *et al.*, Phys. Rev. Lett. **118**, 246601 (2017)

[3] H.-H. Lai *et al.*, Proc. Natl. Acad. Sci. U.S.A. **115**, 93 (2018)

[4] S. Dzsaber *et al.*, Proc. Natl. Acad. Sci. U.S.A. **118**, e2013386118 (2021)

[5] W. T. Fuhrman *et al.*, Sci. Adv. **7**, eabf9134 (2021)

## Pressure-induced ferromagnetism in the topological semimetal $\text{EuCd}_2\text{As}_2$

Elena Gati<sup>1,2,3</sup>, Sergey L. Bud'ko<sup>2,3</sup>, Lin-lin Wang<sup>2</sup>, Adrian Valadkhani<sup>4</sup>, Ritu Gupta<sup>5</sup>, Brinda Kuthanazhi<sup>2,3</sup>, Li Xiang<sup>2,3</sup>, John M. Wilde<sup>2,3</sup>, Aashish Sapkota<sup>2,3</sup>, Zurab Guguchia<sup>5</sup>, Rustem Khasanov<sup>5</sup>, Roser Valenti<sup>4</sup> and Paul C. Canfield<sup>2,3</sup>

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<sup>2</sup> *Ames Laboratory, US Department of Energy, Iowa State University, Ames, Iowa 50011, USA*

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<sup>5</sup> *Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, 5232 Villigen PSI, Switzerland*

In the search for ideal Weyl semimetals with a minimal number of Weyl nodes close to the Fermi energy,  $\text{EuCd}_2\text{As}_2$  has attracted significant attention, following the theoretical prediction that this material could manifest this physics if it were to order ferromagnetically with moments along the  $c$  axis. However, at ambient pressure,  $\text{EuCd}_2\text{As}_2$  orders antiferromagnetically with moments aligned within the  $ab$ -plane. With the goal to manipulate the magnetic state of  $\text{EuCd}_2\text{As}_2$ , we studied the change of magnetism with hydrostatic pressure. Experimentally, we find that moderate hydrostatic pressures of  $\sim 2$  GPa change the magnetic structure from in-plane antiferromagnetism to in-plane ferromagnetism, which is supported by DFT calculations. The latter also predict that increasing pressure further to  $\sim 23$  GPa might allow to stabilize the sought-for ferromagnetic state with moments along the  $c$  axis if the Eu valence remains unchanged. Overall, this work establishes pressure in  $\text{EuCd}_2\text{As}_2$  as a key tuning parameter to study the interplay of correlated magnetism and topology.

\* This work was carried out at Iowa State University and supported by Ames Laboratory, US DOE, under Contract No. DE-AC02-07CH11358. Parts of this work were supported by the Gordon and Betty Moore Foundation, DOE, Swiss NSF and the DFG.

[1] E. Gati et al., Phys. Rev. B 104, 155124 (2021).

## ALSA – Automatic Laue Sample Aligner

Petr Čermák<sup>1</sup>, Damián Wałoszek<sup>1</sup>, Kryštof Višňák<sup>1</sup>, Ivo Gold<sup>1,2</sup>

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While the evolution of the synchrotron brightness still follows exponential Moore's law [1], the time-integrated flux of the neutron sources reached its maximum 50 years ago at ILL, and it will be only slightly surpassed by the upcoming ESS [2]. Therefore, scientists have been trying for decades to optimize optics, measurement strategies or build multi-detector systems to take advantage of every possible neutron to measure weaker fluctuations on smaller samples.

Another approach is to increase the sample size for inelastic neutron experiments by co-aligning more single crystals. This process is very time-consuming and often not very precise (e.g. [3]). The goal of ALSA is to change it. It will automatize the co-alignment process by using a state-of-the-art X-Ray Laue diffractometer, robotized manipulators, real-time camera recognition, and bespoke neural network software for crystal placing and Laue pattern solving. The device ALSA will be a true game-changer in the field of inelastic neutron scattering because it will drastically speed up sample preparation.

Existing Laue orienting software requires manual input and cannot solve Laue patterns automatically. We will present a multi-layered neural network for the determination of crystal orientation from taken Laue pattern, automatizing this task. To glue small crystals as close to each other as possible, we have developed an online algorithm for irregular polygon stacking; a series of benchmarking tests proved, that it is the most efficient online algorithm available.

In this presentation, we will focus on the hardware and software design of the device and show first automatically co-aligned samples.

[1] Assoufid, L. and Graafsma, H. MRS Bulletin **42**, 418-423 (2017). [doi:10.1557/mrs.2017.118](https://doi.org/10.1557/mrs.2017.118)

[2] Rønnow H.M. et al. Swiss Academies Reports **16**, 7 (2021). [doi:10.5281/zenodo.4637660](https://doi.org/10.5281/zenodo.4637660)

[3] Duan, C. Et al. Nature 600, 636–640 (2021). [doi:10.1038/s41586-021-04151-5](https://doi.org/10.1038/s41586-021-04151-5)



# Integrating Machine Learning with Neutron Scattering

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Quantum materials research requires co-design of theory with experiments and involves demanding simulations and the analysis of vast quantities of data, usually including pattern recognition and clustering. Artificial intelligence is a natural route to optimise these processes and bring theory and experiments together. This talk will discuss a scheme that integrates machine learning (ML) with high-performance simulations and scattering measurements, covering the pipeline of typical neutron experiment [1]. This approach uses nonlinear autoencoders trained on realistic simulations along with a fast surrogate for the calculation of scattering in the form of a generative model. As an example of implementation of these techniques and of the approach, I will discuss how ML can be used to extract an effective Hamiltonian for the highly frustrated magnet  $\text{Dy}_2\text{Ti}_2\text{O}_7$  and how the scheme was used to guide neutron scattering experiment under hydrostatic pressure, extract material parameters and construct a phase diagram.

[1] A. M. Samarakoon, D. A. Tennant, F. Ye, Q. Zhang, and S. A. Grigera, "Integration of Machine Learning with Neutron Scattering: Hamiltonian Tuning in Spin Ice with Pressure". arXiv preprint arXiv:2110.15817 (2021)

[2] A. M. Samarakoon et al. "Machine-learning-assisted insight into spin ice  $\text{Dy}_2\text{Ti}_2\text{O}_7$ ." Nature communications, **11** 1-9 (2020).

# STM at magnetic fields of 20 T: quasiparticle interference and vortex lattices of pnictide superconductors

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Electronic systems showing emergent phenomena generally present varied phase diagrams with intertwined phases. Of great interest are the electronic phases favouring the emergence of high critical temperature (HTc) superconductivity, in particular close to a quantum critical point. Among these, charge density waves, antiferromagnetism and nematic order are identified ubiquitously in relation to superconductivity. Fe-based superconductivity offers ultra-pure materials easily tunable through relevant phases emerging from electron correlations. These phases have different associated length scales and produce intrinsic spatially varying electronic behaviour when the material is tuned to the quantum critical point. Therefore, addressing the problem of electron correlations requires powerful microscopes probing electronic properties down to atomic scale. On the other hand, high magnetic fields are needed to disentangle the electronic correlations, because they enable comparison between normal and superconducting phases and unveil quantum critical behavior and vortex physics.

In this seminar, I will show the efforts made in STM for very high magnetic fields up to 22 T. Then I will present results in different topical systems within the family of Fe-based superconductors (FeSe, KFe<sub>2</sub>As<sub>2</sub>, CaKFe<sub>4</sub>As<sub>4</sub> and P-substitute BaFe<sub>2</sub>As<sub>2</sub>). In particular, I will discuss the vortex lattice in P-substitute BaFe<sub>2</sub>As<sub>2</sub> close to the quantum critical point and quasiparticle interference experiments in the heavy fermion iron-based superconductor KFe<sub>2</sub>As<sub>2</sub>, from which we obtain the band structure as a function of the magnetic field.

\*This work is supported by the ERC Starting Grant PNICTEYES.

# Quantum oscillations and magnetostriction in $\text{Sr}_3\text{Ru}_2\text{O}_7$ studied by a novel capacitive dilatometer

Maximilian T. Pelly<sup>1</sup>, Martin George<sup>1</sup>, Craig V. Topping<sup>1</sup>, Robin S. Perry<sup>2,3</sup> and Andreas W. Rost<sup>1</sup>

<sup>1</sup>*School of Physics and Astronomy, University of St Andrews, UK*

<sup>2</sup>*London Centre for Nanotechnology and Department of Physics and Astronomy, University College London, UK*

<sup>3</sup>*ISIS Neutron and Muon Source, Rutherford Appleton Laboratory, UK*

Magnetostriction and thermal expansion measurements are powerful tools for studying thermodynamic properties and phase transitions of quantum materials at low temperatures and high magnetic fields. Linked to stress and strain via thermodynamic relationships these techniques are especially relevant now with the resurgence of experiments using strain/stress cells. Magnetostriction can predict the evolution of phase transitions under stress while thermal expansion is directly linked to the elastocaloric effect [1].

Capacitive dilatometers are the most common approach to dilatometry. State-of-the-art instruments are complex, requiring delicate sample mounting and often exerting stress [2]. Capacitance plates must also be well aligned and positioned at room temperature, limiting resolution. Here we present a novel approach in which the sample is mounted stress-free above a self-aligning counter electrode placed on a piezo-driven nanopositioner, taking advantage of developments in scanning probe technology. This design makes plate alignment trivial and allows the capacitance to be adjusted in-situ at low temperatures with plate separation controllable on the sub-micron scale. We demonstrate a resolution of  $0.6 \text{ pm}/\sqrt{\text{Hz}}$  resulting in  $\Delta l/l = 6 \times 10^{-10}$  for samples of 1mm length at 30 mK.

Performance of the device is demonstrated using the metamagnet  $\text{Sr}_3\text{Ru}_2\text{O}_7$  which has a well-established low temperature, high field phase diagram [3]. Our newly developed setup has not only reproduced existing results [4], but also allowed the detection of quantum oscillations in magnetostriction in  $\text{Sr}_3\text{Ru}_2\text{O}_7$ . Only Fermi pockets with a strong dependence on  $c$ -axis strain will produce these quantum oscillations, naturally highlighting those pockets most interesting for stress/strain cell experiments.

[1] M.S. Ikeda *et al.*, Rev. Sci. Instrum. **90**, 083902 (2019)

[2] R. Kuchler *et al.*, Rev. Sci. Instrum. **83**, 095102 (2012)

[3] D. Sun *et al.*, Phys. Rev. B **97**, 115101 (2018)

[4] P. Gegenwart *et al.*, Phys. Rev. Lett. **96**, 136402 (2006)

# Two channel Kondo physics in one dimension: algebraic hastatic order and remnants of quantum criticality

Milan Kornjača<sup>1</sup> and Rebecca Flint<sup>1</sup>

<sup>1</sup>*Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA*

The two-channel Kondo lattice likely hosts a rich array of phases, including magnetic orders, composite pair superconductivity and non-Fermi liquids, as well as *hastatic order*, a channel-symmetry breaking heavy Fermi liquid that has been predicted to have a spinorial order parameter[1,2]. We revisit its one-dimensional phase diagram using density matrix renormalization group. In contrast to previous work[3], we find algebraic hastatic orders generically for sufficiently strong coupling[4]. We show that these are heavy Tomonaga-Luttinger liquids with nonanalyticities at Fermi wave-vectors that are well-described by incommensurate hastatic density waves. Intriguingly, we find a recently predicted additional order parameter[2], not present at large-N that arises from RKKY mediated interference between hastatic spinors, and indications of increasingly strong residual repulsive interactions at strong coupling, suggesting that these hastatic orders might be non-Fermi liquids in higher dimensions.

\*This work is supported by the Program Committee.

[1] P. Chandra, P. Coleman, and R. Flint, *Nature* **493**, 621 (2013).

[2] M. Kornjača and R. Flint, arXiv:2012.08511 [cond- mat.str-el] (2020).

[3] T. Schauerte, D. L. Cox, R. M. Noack, P. G. J. van Dongen, and C. D. Batista, *Phys. Rev. Lett.* **94**, 147201 (2005).

[4] M. Kornjača and R. Flint arXiv:2203.07367 [cond- mat.str-el] (2022).



# ***POSTER Program***

**International Conference on Strongly  
Correlated Electron Systems (SCES)**



## Monday 25 July

### Poster session MONP01 13.30 - 15.15 - Ruby Lounge, Room E102

Poster # 1

**Antonio Sergio Teixeira Pires** // *Universidade Federal de Minas Gerais*  
Transport on the Lieb lattice

Poster # 2

**Davi Antonio Zau de Alvarenga** // *Instituto de física "Gleb Wataghin", Unicamp*  
Microscopically unveiling 4f electrons hybridization in the CeCuSb<sub>2</sub> Heavy Fermion

Poster # 3

**Denise Christovam** // *Max-Planck Institute for Chemical Physics of Solids*  
A Sum rule investigation of the 4f ground state of the Kondo semimetal CeNiSn

Poster # 4

**Vivek Kumar** // *Technische Universität München, Garching*  
Anisotropic magnetic and thermodynamic properties of single crystals of antiferromagnetic CePdAl<sub>3</sub>

Poster # 5

**Jörg Sichelschmidt** // *Max Planck Institute for Chemical Physics of Solids, Dresden*  
Optical study of the electronic structure of locally noncentrosymmetric CeRh<sub>2</sub>As<sub>2</sub>

Poster # 6

**Pavlo Khanenko** // *Max Planck Institute for Chemical Physics of Solids, Dresden*  
The quadrupole density wave and its interplay with superconductivity in CeRh<sub>2</sub>As<sub>2</sub>: a thermodynamic study

Poster # 7

**Hiroyuki Hidaka** // *Hokkaido University, Japan*  
Investigation of Anisotropy of Lattice Distortion in CeCoSi

Poster # 8

**André Strydom** // *University of Johannesburg, South Africa*  
The new compound Ce<sub>2</sub>Rh<sub>2</sub>Al: a representative of the monoclinic Pr<sub>2</sub>Co<sub>2</sub>Al structure type

Poster # 9

**Marvin Lenk** // *Physikalisches Institut, Universität Bonn*  
DFT + DMFT study of the two-channel quadrupolar Kondo effect in PrV<sub>2</sub>Al<sub>20</sub>

Poster # 10

**Wolfgang Simeth** // *Paul Scherrer Institut*  
Composition of magnetic interactions in the heavy-fermion system CeIn<sub>3</sub>

Poster # 11

**William Knafo** // *LNCMI Toulouse, France*  
Pulsed-magnetic-field studies of magnetism and superconductivity in UTe<sub>2</sub>

Poster # 12

**Shingo Kuniyoshi** // *University of the Ryukyus*  
Emergence of heavy local Fermi liquid in the underscreened Kondo model with easy-plane anisotropy



Poster # 13

**Magdalena Majewicz** // *Institute of Low Temperature and Structure Research, Polish Academy of Sciences*

Possible Lifshitz point in the magnetic phase diagram of  $\text{UNi}_2\text{Si}_2$  single crystals

Poster # 14

**Tristan Thebault** // *Laboratoire National des Champs Magnétiques Intenses, Toulouse, France*

Anisotropic signatures of the electronic correlations in the electrical resistivity of  $\text{UTe}_2$ .

Poster # 15

**Christian de Podesta** // *University of Cambridge, UK*

High pressure structural instability in  $\text{CeSb}_2$

Poster # 16

**Masashi Ohashi** // *Kanazawa University*

Single crystal growth of  $\text{RNiGe}_2$  (R: rare earth) compounds

Poster # 17

**Samuel Gomes de Mercena** // *Instituto de Física "Gleb Wataghin", Campinas, SP, Brazil*

Effects of chemical substitution of Bi by Sb on the physical properties of  $\text{NdCu}(\text{Bi}_{1-x}\text{Sbx})_2$  compounds

Poster # 18

**Arvind Maurya** // *Max Planck Institute for Solid State Research, Germany*

Large magnetocrystalline energy and electron correlations in  $\text{EuIrSi}_3$

Poster # 19

**Theo Weinberger** // *University of Cambridge*

High pressure structural and electronic instabilities in  $\text{LaSb}_2$

Poster # 20

**Tathamay Basu** // *Rajiv Gandhi Institute of Petroleum Technology (RGIT), India*

Strong 4d-4f correlation in multiferroic compound,  $\text{Ba}_3\text{HoRu}_2\text{O}_9$

Poster # 21

**Corentin Morice** // *University Paris-Saclay, France*

Multi-component charge order

Poster # 22

**Sanjay Kumar Upadhyay** // *Indian Institute of Science Bangalore*

Magnetic study of mixed-metal garnet  $\text{ErFeCuGe}_4\text{O}_{12}$

Poster # 23

**Marius-Adrian Husanu** // *National Institute of Materials Physics, Magurele*

Stabilization mechanisms of opposed ferroelectric states

Poster # 24

**Youjin Lee** // *Seoul National University*

Magnetic exciton in a multiferroic 2D van der Waals antiferromagnet

Poster # 25

**Fengqi Zhang** // *Delft University of Technology, The Netherlands*

Reduced hysteresis and enhanced GMCE in B-doped all-d-metal Ni-Co-Mn-Ti based Heusler materials



Poster # 26

**Mahieddine Lahoubi** // *University of Badji Mokhtar Annaba, Algeria*  
Low temperature anomalies in the mixed dysprosium-yttrium iron garnets with a connection to the magnetodielectric property of DyIG

Poster # 27

**Vadim Sikolenko** // *Karlsruhe Institute of Technology*  
Neutron scattering studies of multiferroics based on bismuth ferrites

Poster # 28

**Sonu Chhillar** // *School of Basic Sciences, Indian Institute of Technology*  
Magnetodielectric coupling as a manifestation of metamagnetic transition and structural distortion in  $Ba_3RRu_2O_9$  ( $R = Gd, Dy$ )

Poster # 29

**Gurpreet Kaur** // *Indian Institute of Technology*  
Magnetic properties and magnetodielectric coupling in mixed metal oxide  $NdCr_{0.5}Co_{0.5}O_3$

Poster # 30

**Boglarka Toth** // *Budapest University of Technology and Economics*  
Spin excitations of the high temperature transverse conical phase in multiferroic  $BiFeO_3$

Poster # 31

**Masahiro Shinozaki** // *Shimane University, Japan*  
Study for Physical Properties and Magnetoelectric Response of  $Ce_3TiSb_5$

Poster # 32

**Dana-Georgeta Popescu** // *National Institute of Materials Physics*  
Impact on Ferroelectricity and Band Alignment of Gradually Grown metal on  $BaTiO_3$

Poster # 33

**Xiaotian Zhang** // *University of Cambridge, UK*  
Magnetoelectric coupling of rare-earth orthotantalates

Poster # 34

**Ina Park** // *POSTECH (Pohang University of Science and Technology)*  
Manifestation of Hund's rule effect in the optical conductivity near the metal-insulator transition of  $NiS_2$ .

Poster # 35

**Arwin Kool** // *High Field Magnet Laboratory, Radboud University*  
Disorder study of the anomalous magnetoresistance in  $2H-NbSe_2$

Poster # 36

**Prachi Telang** // *University of Augsburg, Augsburg, Germany*  
Novel metallic phases in pyrochlore iridates

Poster # 37

**Jaroslav Valenta** // *National Institute for Materials Science, Japan*  
Low temperature criticality at  $YbCo_2$  compound

Poster # 38

**Ruo Hibino** // *Hokkaido University, Japan*  
Elemental Dilution Effect on the Ultrasonic Dispersion of the Non-Kramers Systems  $Y_{1-x}Pr_xIr_2Zn_{20}$

Poster # 39

**Rikako Yamamoto** // *Hiroshima University, Japan*  
Feasibility of Two-channel Kondo Effect in Diluted Nd Compounds  $Y_{1-x}Nd_xCo_2Zn_{20}$  for  $x < 0.1$





Poster # 40

**Benny Lau** // *University of Toronto*

Revealing an anisotropic electronic scattering rate in the “non-metallic” metal FeCrAs through the Hall effect

Poster # 41

**Francesco Gabriele** // *"Sapienza" University of Rome, Rome (Italy)*

Density fluctuations and generalized plasma waves in layered cuprates

Poster # 42

**Pratyay Ghosh** // *Julius-Maximilians-Universität Würzburg*

Another exact ground state of a 2D quantum antiferromagnet

Poster # 43

**Dylan Behr** // *University College London*

Weak Ferromagnetism and Spin Reorientation in Antiferroelectric BiCrO<sub>3</sub>

Poster # 44

**Darren Peets** // *IFMP, Technische University Dresden*

Hidden Charge Order in an Iron Oxide Square-Lattice Compound

Poster # 45

**Sheetal Devi** // *Indian Institute of Technology Mandi, India*

Field-induced spin freezing and low-temperature heat capacity of Ho<sub>2</sub>Zr<sub>2</sub>O<sub>7</sub>

Poster # 46

**Belen Elizabeth Zuniga Cespedes** // *Max Planck Institute for Chemical Physics of Solids, Germany*

Anomalous Hall Effect in Single-Crystals of the Noncollinear Antiferromagnet Mn<sub>3</sub>Pt

Poster # 47

**Akihisa Koga** // *Tokyo Institute of Technology, Japan*

Majorana-mediated spin transport in Kitaev model at finite temperatures

Poster # 48

**Arjun Unnikrishnan** // *Indian Institute of Science, Bangalore (present); Indian Institute of Science Education and Research, Thiruvananthapuram (former)*

Singlet ground state in the alternating spin-1/2 chain compound NaVOAsO<sub>4</sub>

Poster # 49

**Leonardo Facheris** // *Laboratory for Solid State Physics, ETH Zurich, Switzerland*

Magnetization plateaux in the distorted triangular quantum antiferromagnet Cs<sub>2</sub>CoBr<sub>4</sub> /

Poster # 50

**Kazuyuki Matsuhira** // *Kyushu Institute of Technology*

Anisotropic magnetic phase diagram of geometrically frustrated iridate Ca<sub>5</sub>Ir<sub>3</sub>O<sub>12</sub>

Poster # 51

**Bin Shen** // *University of Augsburg, Germany*

Pressure-tuning of Li<sub>2</sub>IrO<sub>3</sub> Kitaev materials

Poster # 52

**Denis Arčon** // *Institute Jožef Stefan*

pi-orbital order coupled to the spin-1/2 pyrochlore lattice in alkali-sesquioxides



Poster # 53

**Takuto Fujii** // *Max Planck Institute for Chemical Physics of Solids*

Field induced magnetic order and quantum spin liquid on planar triangular lattice,  $\text{TlYbSe}_2$

Poster # 54

**Dr. Rajib Sarkar** // *Technical University of Dresden*

Low temperature spin dynamics in the  $S = 2$  kagome magnet  $\text{Fe}_4\text{Si}_2\text{Sn}_7\text{O}_{16}$ : An AC susceptibility, NMR and  $\mu\text{SR}$  study

Poster # 55

**Matthias Peschke** // *University of Amsterdam, The Netherlands*

Competing states in the two-dimensional Kondo-Necklace model on the triangular lattice

Poster # 56

**Ryota Yambe** // *The University of Tokyo, Japan*

Classification of anisotropic exchange interactions in momentum space toward understanding multiple- $Q$  instability

Poster # 57

**Heejun Yang** // *Seoul National University, Republic of Korea*

Unusual thermal Hall effect in the 3d cobalt Kitaev system  $\text{Na}_2\text{Co}_2\text{TeO}_6$

Poster # 58

**Kazuki Okigami** // *The University of Tokyo, Japan*

Engineering skyrmion crystal in centrosymmetric ferromagnetic/antiferromagnetic bilayers

Poster # 59

**Ranjith Kumar Kizhake Malayil** // *LNCMI-CNRS, Grenoble, France*

NMR evidence against spin-nematic nature of the presaturation phase in frustrated magnet  $\text{SrZnVO}(\text{PO}_4)_2$

Poster # 60

**Dirk Wulferding** // *Seoul National University, Korea*

Colossal spin-phonon coupling and Higgs-amplitude fluctuations in  $\text{Nd}_2\text{Ru}_2\text{O}_7$

Poster # 61

**Sven Luther** // *Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, Germany*

Exchange anisotropy and field-induced magnetic order of the triangular-lattice delafossites  $\text{NaYbCh}_2$  ( $\text{Ch} = \text{O}, \text{S}, \text{Se}$ )

Poster # 62

**E.V. Sampathkumaran** // *HBCSE (TIFR)*

Magnetic field induced magnetic disorder in honeycomb lattice,  $\text{Tb}_5\text{Si}_3$

Poster # 63

**Toshihiro Sato** // *Universität Würzburg, Germany*

Quantum Monte Carlo simulations of generalized Kitaev models: applications to  $\alpha\text{-RuCl}_3$

Poster # 64

**Július Bačkai** // *Slovak Academy of Sciences, Slovakia*

Angle-resolved magnetoresistance in strongly anisotropic quantum magnet  $\text{TmB}_4$

Poster # 65

**Yasuyuki Kato** // *University of Tokyo*

Magnetic field-temperature phase diagrams and spin excitation spectra for topological multiple- $Q$  magnetic orders



Poster # 66

**Deepak Singh Kathyat** // *Harish-Chandra Research Institute*  
Engineering antiferromagnetic skyrmions and antiskyrmions at metallic interfaces

Poster # 67

**Dipranjan Chatterjee** // *Université Paris-Saclay, France*  
From quantum spin liquid to long range order in the distorted kagome compound,  $Y_3Cu_9(OH)_{18}OCl_8$

Poster # 68

**Somesh K** // *Indian Institute of Science Education and Research, India*  
Quantum magnetism of ferromagnetic spin dimers in  $\alpha$ -KVOPO<sub>4</sub>

Poster # 69

**Lingjia Shen** // *Lund University*  
Revealing the Impact of Interchain Exchange Interactions on the Magnetic Quasiparticles in a Tomonaga-Luttinger Liquid

Poster # 70

**Mitchell Bordelon** // *Los Alamos National Laboratory*  
Crystal structure, electronic properties, and unusual antiferromagnetism in tetragonal CeLiBi<sub>2</sub>

Poster # 71

**Fumiya Hori** // *Kyoto University, Japan*  
Magnetic ground state in semiconducting Yb-based compounds with a zigzag-chain structure

Poster # 72

**Sebin Joseph Sebastian** // *Indian Institute of Science Education and Research (IISER), India*  
Collinear order in the spin-5/2 triangular-lattice antiferromagnet Na<sub>3</sub>Fe(PO<sub>4</sub>)<sub>2</sub>.

Poster # 73

**Beom Hyun Kim** // *Korea Institute for Advanced Study*  
Field-angle anisotropy of magnon specific heat in proximate Kitaev systems under an in-plane magnetic field

Poster # 74

**Alexander Engelhardt** // *Technical University of Munich, Germany*  
Thermodynamic Signatures of the Soliton Lattice in Single-Crystal TbFeO<sub>3</sub>

Poster # 75

**Deok-Yong Cho** // *Jeonbuk National University, Republic of Korea*  
Effects of electron-phonon coupling on the interfacial carriers in Al<sub>2</sub>O<sub>3</sub>/TiO<sub>2</sub> heterostructure

Poster # 76

**Mucio Amado Continentino** // *Centro Brasileiro de Pesquisas Fisicas, Brazil*  
Thermoelectric properties of topological chains coupled to a quantum dot

Poster # 77

**Grace Causer** // *Technical University of Munich*  
Magnetic-Field Controlled Cascade of Soliton Layers in Epitaxial MnSi

Poster # 78

**Mahammad Tahir** // *Indian Institute of Technology Kanpur, India*  
Observation of giant spin pumping in Ferromagnet - organic semiconductor heterostructures



Poster # 79

**Carlos Rosário** // *University of Twente, The Netherlands*  
Scanning SQUID microscopy studies of ferromagnetism in LaMnO<sub>3</sub> thin films grown on SrTiO<sub>3</sub>

Poster # 80

**Ravi Kaushik** // *Italian Institute of Technology, Genova, Italy*  
First-principles study of momentum-forbidden excitons in bulk 2H-MoX<sub>2</sub> (X= S, Se).

Poster # 81

**Xing Gao** // *Faculty of Science and Technology and MESA+ Institute for Nanotechnology, University of Twente, The Netherlands*  
Multi-level operation in vanadium dioxide-based resistive switching devices

Poster # 82

**Akira Kofuji** // *Department of Physics, Graduate School of Science, Kyoto University, Japan*  
Relation between anomalous gap dependence of high harmonic generation and extremely strong light-matter coupling

Poster # 83

**Kimoon Lee** // *Department of Physics, Kunsan National University, Republic of Korea*  
Hole transporting conductor designed by polarizability encouraged strongly correlated oxide

Poster # 84

**SoRa Yun** // *Kunsan National University, The Republic of Korea*  
Thin-film deposition of Cu-substituted NiWO<sub>4</sub> by electron beam evaporation and its device application

Poster # 85

**Inseo Kim** // *Kunsan national university of Gunsan, Republic of Korea*  
Large polaronic conduction in strongly correlated Cu-substituted NiWO<sub>4</sub>

Poster # 86

**Xingchen Chen** // *Leiden University, The Netherlands*  
NbSe<sub>2</sub>-Based van der Waals Heterostructure Josephson Junction

Poster # 87

**Craig Topping** // *University of St Andrews, UK*  
Nanocalorimetry of Quantum Materials

Poster # 88

**Fei Sun** // *Max Planck Institute for Chemical Physics of Solids*  
A spatially resolved optical method to measure thermal diffusivity

Poster # 89

**Petr Čermák** // *Charles University Prague*  
MGML.eu - Material Growth & Measurement Laboratory

Poster # 90

**Han-Jin Noh** // *Chonnam National University*  
Fine details of sixfold Dirac fermions in a pyrite structured PdSb<sub>2</sub>

Poster # 91

**Jelle Lorenz** // *University of Amsterdam, The Netherlands*  
Uniaxial strain effects on the magnetoresistance and Fermi surface of the Dirac nodal-line semimetal ZrSiS



Poster # 92

**Venus Rai** // *Jülich Centre for Neutron Science (JCNS-2), Forschungszentrum Jülich, Germany*

Transport and magnetic properties of the topological (Weyl) semimetal: Hexagonal -  $(\text{Mn}_{1-\alpha}\text{Fe}_\alpha)_3\text{Ge}$

Poster # 93

**Ankur Das** // *Weizmann Institute of Science*

The Phase puzzle of  $\nu = 0$  (charge neutrality) Graphene

Poster # 94

**Ivica Zivkovic** // *EPFL, Switzerland*

The origin of the second transition in the Weyl semimetal  $\text{Co}_3\text{Sn}_2\text{S}_2$

Poster # 95

**Myung-Hwa Jung** // *Sogang University, South Korea*

Berry paramagnetism in the Dirac semimetal  $\text{ZrTe}_5$

Poster # 96

**Nico Huber** // *Technical University Munich, Germany*

Network of topological charges in the electronic structure of  $\text{CoSi}$

Poster # 97

**Mario Novak** // *University of Zagreb*

Nodal-line driven anomalous susceptibility in  $\text{ZrSi}_5$

Poster # 98

**Bruno Gudac** // *Faculty of Science, University of Zagreb, Croatia*

Quantum oscillations in  $\text{Zr}_{1-x}\text{Hf}_x\text{Si}_5$

Poster # 99

**Jaime ferreira de oliveira** // *Centro Brasileiro de Pesquisas Físicas*

Analyse of Anti-symmetric component in the magnetoresistance in Sb-doped tellurium using Fourier analysis

Poster # 100

**Stanislaw Galeski** // *University of Bonn, Germany*

Signatures of a magnetic field induced Lifshitz transition in the ultra-quantum limit of the topological semi-metal  $\text{ZrTe}_5$

Poster # 101

**Monika Lužnik** // *Institute of Solid State Physics, TU Wien*

Thermal and electrical transport in  $\text{Ce}_3\text{Bi}_4\text{Pd}_3$

Poster # 102

**Dariusz Kaczorowski** // *Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Poland; Institute of Molecular Physics, Polish Academy of Sciences, Poland*

Thermodynamic and transport properties of  $\text{EuZn}_2\text{As}_2$  single crystals

Poster # 103

**Rafal Wawrzynczak** // *Max Planck Institute for Chemical Physics of Solids, Germany*

Ultrasound propagation in candidate material for electron hydrodynamics, Weyl semimetal  $\text{WTe}_2$

Poster # 104

**Ayako Ohmura** // *Niigata University, Japan*

Structural and superconducting properties of  $\text{PdTe}_2$  under high pressure



## Tuesday 26 July

### Poster session TUEP02

13.30 - 15.15 - Ruby Lounge, Room E102

Poster # 105

**Cristian Mauricio Borja Peña** // *Universidad de Los Andes, Colombia*

Superconductivity and Charge Density Wave in the Extended Fermi-Hubbard Model with Disorder

Poster # 106

**Yoshihiro Takahashi** // *Osaka Metropolitan University, Japan*

Resonant inelastic x-ray scattering of hematite Fe<sub>2</sub>O<sub>3</sub>: LDA+DMFT analysis

Poster # 107

**Adam Kłosiński** // *University of Warsaw*

Can we kill a hole quasiparticle in an Ising antiferromagnet on a Bethe lattice? /

Poster # 108

**Ryszard Radwanski** // *Center of Solid State Physics, Poland*

Physics of strong-electron correlations: CoTiO<sub>3</sub>, Ba<sub>2</sub>YMoO<sub>6</sub> and CeRh<sub>2</sub>Si<sub>2</sub>

Poster # 109

**Koji Inui** // *University of Tokyo*

Inverse Hamiltonian design by automatic differentiation

Poster # 110

**Roberto Franco Peñaloza** // *Departamento de Física - Universidad Nacional de Colombia - Colombia*

Seeking for conditions that could improve the thermoelectric efficiency in quantum dots systems

Poster # 111

**Floris Balm** // *Leiden University, The Netherlands*

Universality of Transport in Holographic Lattices

Poster # 112

**Nicolas Chagnet** // *Leiden University*

Holographic quasinormal modes and cuprates physics

Poster # 113

**Masataka Kawano** // *Technical University of Munich, Germany*

Sine-square deformed mean-field theory and its application to spin-orbit coupled systems

Poster # 114

**Patrick Vlaar** // *University of Amsterdam, The Netherlands*

Tensor network algorithms for 3D quantum systems with applications to the Shastry-Sutherland model

Poster # 115

**Beatriz Pérez-González** // *Science Material Institute of Madrid (ICMM-CSIC), Spain*

Tight-binding models coupled to quantum light



Poster # 116

**Songyang Pu** // *University of Leeds, England*

Anderson localization in fractional quantum Hall effect at  $\nu = n/(2n+1)$

Poster # 117

**Jose Soto** // *Delft University of Technology, The Netherlands*

Quantum Kibble-Zurek mechanism and incommensurate-commensurate phase transitions in chains of Rydberg atoms

Poster # 118

**Min-Chul Cha** // *Hanyang University ERICA, South Korea*

Critical Properties of 1-dim Bose-Hubbard model with a Limited Amount of Entanglement

Poster # 119

**Daniel Flavian Blasco** // *ETH Zurich, Switzerland*

Critical dielectric susceptibility at a magnetic BEC quantum critical point

Poster # 120

**Krzysztof Wójcik** // *Maria Curie-Skłodowska University in Lublin, Poland*

Spin-liquid of 2 Kondo impurities driven by RKKY coupling with or without frustration

Poster # 121

**Manuel Brando** // *Max Planck Institute for Chemical Physics of Solids, Germany*

Electronuclear quantum criticality

Poster # 122

**Rajesh Tripathi** // *ISIS Facility, STFC, Rutherford Appleton Laboratory, United Kingdom, and Jawaharlal Nehru Centre for Advanced Scientific Research, India*

Quantum critical fluctuations in the non-Fermi liquid system CeRh<sub>4</sub>Al<sub>15</sub> investigated using muon spin relaxation

Poster # 123

**Jereson Silva** // *Universidad Nacional de Colombia, Colombia*

The effect of next-neighbor interactions on the ground-state of Bose-Fermi mixtures

Poster # 124

**Cornelius Krellner** // *Physikalisches Institut, Goethe University Frankfurt/Main, Germany*

Isotopically pure YbRh<sub>2</sub>Si<sub>2</sub> single crystals with <sup>171</sup>Yb, <sup>173</sup>Yb, and <sup>174</sup>Yb

Poster # 125

**Kai Grube** // *Karlsruhe Institute of Technology, Germany*

Lock-in Behavior of the Partially Frustrated Order in CePdAl

Poster # 126

**Huanzhi Hu** // *Huanzhi Hu, University College London, UK*

Effects of Kondo Fluctuations on the Néel Quantum Phase Transition

Poster # 127

**Mikolaj Uryszek** // *University College London, United Kingdom*

Effects of disorder on quantum phase transitions of two-dimensional Dirac semimetals

Poster # 128

**Andreas W. Rost** // *University of St Andrews, UK*

Tuning the Van Hove singularity in Sr<sub>3</sub>Ru<sub>2</sub>O<sub>7</sub>

Poster # 129

**Emine Bakali** // *Technical University of Vienna*



Electrical transport in MBE-grown YbRh<sub>2</sub>Si<sub>2</sub> thin films at mK temperatures

Poster # 130

**Hermann Suderow** // *Universidad Autonoma de Madrid*

Tunneling spectroscopy through the magnetic phases of Ce(Ru<sub>0.92</sub>Rh<sub>0.08</sub>)<sub>2</sub>Si<sub>2</sub>

Poster # 131

**Fusako Kon** // *Hokkaido University, Japan*

Correlation between Antiferromagnetic and Charge-Density-Wave Order in UPt<sub>2</sub>Si<sub>2</sub>  
Studied by Resonant X-Ray Scattering

Poster # 132

**Hiroshi Amitsuka** // *Hokkaido University, Japan*

Observation of current-induced magnetization in the antiferromagnetic state of UPt<sub>2</sub>Si<sub>2</sub>

Poster # 133

**Maria Szlawska** // *Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Wrocław, Poland*

Properties of UPd<sub>2</sub>Si<sub>2</sub> close to putative Lifshitz point

Poster # 134

**Tatsuya Yamaguchi** // *Osaka Metropolitan University, Japan*

Metal-insulator transition in A-site ordered perovskite oxides ACu<sub>3</sub>Fe<sub>4</sub>O<sub>12</sub> /

Poster # 135

**Farzin Abadizaman** // *Masaryk University*

Optical signature of strain-induced ferromagnetism in LaCoO<sub>3</sub> thin film

Poster # 136

**Andrea Leon** // *Technical University of Dresden, Dresden, Germany*

Ca<sub>3</sub>Ru<sub>2</sub>O<sub>7</sub>: Interplay among degrees of freedom and role of the exchange and correlation

Poster # 137

**Keita Kojima** // *Aoyama Gakuin University, Japan*

Development of vanadium zigzag chains in layered LiVSe<sub>2</sub> under high pressure

Poster # 138

**Adam Dubroka** // *Masaryk University, Czech Republic*

Photo-induced insulator-to-metal transition and coherent acoustic phonon propagation in LaCoO<sub>3</sub> explored by femtosecond ellipsometry

Poster # 139

**Diana Csontosova** // *Masaryk University, Czech Republic*

Dynamical mean-field study of collective modes in antiferromagnetically ordered systems

Poster # 140

**Cauê Kaufmann Ribeiro** // *Laboratory for Quantum Matter Under Extreme Conditions, Institute of Physics, University of São Paulo, Brazil*

Investigation of role of disorder in pristine cage compound FeGa<sub>3</sub>

Poster # 141

**Claude Ederer** // *Materials Theory, ETH Zurich, Switzerland*

Charge disproportionation and "Hund's insulating" behavior in different transition metal oxides by DFT+DMFT

Poster # 142

**Sungkyun Park** // *Pusan National University*

Modified orbital occupancy induced phase transition of VO<sub>2</sub>





Poster # 143

**José Guimarães** // *Max Planck Institute for Chemical Physics of Solids, Germany*  
Ionic based gate control of quantum phase transitions on ZrS<sub>2</sub>

Poster # 144

**Mohamamdmehti Torkzadeh** // *Sorbonne Université, Paris*  
Large-gap insulating phase induced by magnetic ordering in a two-dimensional material at low temperature

Poster # 145

**Carolina Burger** // *Technical University of Munich, Germany*  
High-mobility surface conduction in FeSi at low temperatures

Poster # 146

**Dorsa Fartab** // *Max Planck Institute for Chemical Physics of Solids, Dresden, Germany*  
Gate-tunable insulator-metal transition and weak antilocalization in two-dimensional tellurium

Poster # 147

**Maria Helena Carvalho da Costa** // *Universidade Estadual de Campinas, IFGW*  
Electron spin resonance on FeSi crystals

Poster # 148

**Remko Fermin** // *Universiteit Leiden*  
Universal size-dependent nonlinear charge transport in single crystals of the Mott insulator Ca<sub>2</sub>RuO<sub>4</sub>

Poster # 149

**Kazuki Yamamoto** // *Kyoto University, Japan*  
Universal properties of dissipative Tomonaga-Luttinger liquids: A case study of a non-Hermitian XXZ spin chain

Poster # 150

**Momoka Hayashida** // *Kyushu Institute of Technology, Japan*  
Current induced hysteresis phenomena in resistivity of spin-orbit coupled iridate Ca<sub>5</sub>Ir<sub>3</sub>O<sub>12</sub>

Poster # 151

**Yuri Pusep** // *University of Sao Paulo*  
Diffusion of photo-excited holes in viscous electron fluid

Poster # 152

**Anand Manaparambil** // *Adam Mickiewicz University in Poznan, Poland*  
Nonequilibrium Seebeck coefficient of a correlated molecular junction

Poster # 153

**Xuanbo Feng** // *University of Amsterdam, The Netherlands*  
Cascade of charge density wave transitions in selenium doped 1T-TaS<sub>2</sub> probed with optics

Poster # 154

**Shun Okumura** // *The University of Tokyo, Japan*  
Recombination of Weyl points in periodically driven Dirac semimetals

Poster # 155

**Jinhong Park** // *Institute for Theoretical Physics, University of Cologne, Germany*  
Thermal Hall response: violation of gravitational analogues



Poster # 156

**Hironobu Yoshida** // *The University of Tokyo, Japan*

Exact analysis of the Liouvillian gap for the SU(N) Fermi-Hubbard model with two-body loss

Poster # 157

**Sota Kitamura** // *University of Tokyo, Japan*

Floquet topological superconductivity induced by chiral many-body interactions

Poster # 158

**Michael Lampl** // *Technical University of Munich, Germany*

Pump-Probe AC Susceptibility of LiHoxY1-xF4 (x = 4.5 %)

Poster # 159

**Vladimir Ohanesjan** // *Leiden University*

Quantum thermodynamics of strongly correlated systems

Poster # 160

**Mahima M Kurian** // *Indian Institute of Technology Madras, India*

Exchange bias effect and inhomogeneous magnetism in 6H Ba<sub>3</sub>CoFeRuO<sub>9</sub>

Poster # 161

**Daniel Keith Brattan** // *Ecole Polytechnique*

A hydrodynamic description for transport in the strange metal phase of cuprates

Poster # 162

**Beomjoon Goh** // *Pohang University of Science and Technology*

Metal-insulator transition in the Hubbard model under external field

Poster # 163

**Koudai Sugimoto** // *Keio University*

Analysis of pump-probe spectroscopy in the extended Hubbard model in the infinite matrix-product-states representation

Poster # 164

**Jianfeng Ge** // *Leiden University*

Local shot noise of the putative vortex Majorana modes in FeTe<sub>0.55</sub>Se<sub>0.45</sub>

Poster # 165

**Debarchan Das** // *Paul Scherrer Institute, Switzerland*

Disentangling charge order and superconductivity in correlated kagome superconductor CsV<sub>3</sub>Sb<sub>5</sub>

Poster # 166

**Dr. Ankita Singh** // *Tata Institute of Fundamental Research, Mumbai, India*

Structural and magnetic anisotropy in YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub>/ La<sub>0.67</sub>Sr<sub>0.33</sub>MnO<sub>3</sub> bilayer film on SrTiO<sub>3</sub> substrate

Poster # 167

**Hiroto Tanaka** // *Kyoto University, Japan*

Nonlinear optical responses in two-dimensional superconductors

Poster # 168

**Anas Abdelwahab** // *Leibniz University Hannover*

Enhancement of pair correlations in the asymmetric Hubbard ladder

Poster # 169

**Taisei Kitamura** // *Kyoto University, Japan*



Enhancement of the superconductivity due to quantum geometry in monolayer FeSe

Poster # 170

**Mac Curtis** // *University of Bristol*

Effect of hopping anisotropy on the critical temperature of unconventional, superconducting pairing states

Poster # 171

**Shiki Ogata** // *Kyoto University, Japan*

Microscopic evidence of the superconducting multiphase in the noncentrosymmetric heavy-fermion superconductor CeRh<sub>2</sub>As<sub>2</sub>

Poster # 172

**Marc Salis** // *University of Amsterdam, The Netherlands*

Heat capacity study of the type-I to type-II superconducting transition in the Dirac semimetal PdTe<sub>2</sub>

Poster # 173

**Tatsuya Miki** // *Saitama University, Japan*

Odd-frequency pairing in the system with Bogoliubov Fermi surface

Poster # 174

**Maciej Fidrysiak** // *Jagiellonian University, Kraków, Poland*

Quantum spin and charge excitations in high-T<sub>c</sub> cuprates: Variational theory and quantitative comparison with experiment

Poster # 175

**Tsuyoshi Imazu** // *Hirosaki University, Japan*

The edge currents and spin polarization of the chiral superconductor in the checkerboard triangular lattice

Poster # 176

**Ram Prakash Pandeya** // *Department of Condensed Matter Physics & Material Science, Tata Institute of Fundamental Research, Mumbai*

Emergence of singlet states with superconductivity in CaFe<sub>2</sub>As<sub>2</sub>

Poster # 177

**Charles Tam** // *University of Bristol, UK*

Charge density waves and Fermi-surface reconstruction in the clean overdoped cuprate superconductor Tl<sub>2</sub>Ba<sub>2</sub>CuO<sub>6+δ</sub>

Poster # 178

**Ahmed Alshemi** // *Lund University, Sweden*

Investigation of the vortex lattice in NbS<sub>2</sub> – a potential FFLO candidate

Poster # 179

**Jiasen Niu** // *Leiden University, The Netherlands*

1e shot noise below T<sub>c</sub> in superconducting tunnel junctions

Poster # 180

**You-Sheng Li** // *Max Planck Institute for Chemical Physics of Solids, Germany*

Elastocaloric determination of the phase diagram of Sr<sub>2</sub>RuO<sub>4</sub>

Poster # 181

**Ashley Weiland** // *Los Alamos National Laboratory*

Correlating Structure with Superconductivity Variations in UTe<sub>2</sub> [t](#)



Poster # 182

**Gyanendra Singh** // *ICMAB-CSIC*

Gate-tunable unconventional superconductivity in 2D oxide interfaces nanodevices

Poster # 183

**Sanu Mishra** // *Los Alamos National Laboratory, Los Alamos, USA*

Grain boundaries investigation in the heavy fermion superconductor CeCoIn<sub>5</sub>

Poster # 184

**Damla Yesilpinar** // *Czech Academy of Sciences*

Growth of FeSe on in-situ cleaved SnSe<sub>2</sub> (001) surfaces

Poster # 185

**Henri Menke** // *Friedrich-Alexander-Universität Erlangen-Nürnberg*

Spin susceptibility and multiband effects in the Emery model of the cuprate superconductors

Poster # 186

**Javier Landaeta** // *Max Planck Institute for Chemical Physics of Solids*

Field-angle dependence reveals odd-parity superconductivity in CeRh<sub>2</sub>As<sub>2</sub>

Poster # 187

**Yuhei Ikeda** // *Kyoto University, Kyoto*

Impurity effect on superconducting diode effect

Poster # 188

**Mohamed Oudah** // *University of British Columbia*

Type-I Superconductivity in Non-centrosymmetric LaRhGe<sub>3</sub>

Poster # 189

**Klaus Hasselbach** // *University Grenoble Alpes, CNRS, Institut Néel, 38000 Grenoble, France*

Observation of Chiral Superconductivity in UPt<sub>3</sub> by scanning SQUID Microscopy

Poster # 190

**Kim Lefmann** // *University of Copenhagen, Denmark*

Investigation of the evolution of magnetic fluctuations in LSCO, measured in the quasi-elastic region

Poster # 191

**Adrien Rosuel** // *CEA Grenoble, Phelips, France*

Thermodynamic evidence for two superconducting phases at ambient pressure in UTe<sub>2</sub>

Poster # 192

**Willem Tromp** // *Leiden University, The Netherlands*

Puddle formation, persistent gaps, and non-mean-field breakdown of superconductivity in overdoped (Pb,Bi)<sub>2</sub>Sr<sub>2</sub>CuO<sub>6+δ</sub>

Poster # 193

**Vivek Kumar Anand** // *University of Petroleum and Energy Studies, Dehradun, India*

Superconductivity in CaPd<sub>2</sub>Ge<sub>2</sub> and CaPd<sub>2</sub>As<sub>2</sub>: A  $\mu$ SR study

Poster # 194

**Marta Fernández-Lomana Gómez-Guillamón** // *Universidad Autónoma de Madrid, Spain*

Tunneling spectroscopy at very high magnetic fields in the iron based superconductor KFe<sub>2</sub>As<sub>2</sub>



Poster # 195

**Amber Mozes** // *Leiden University, The Netherlands*

Exploring the limits of unconventional superconductivity with a novel complex impedance scanning tunneling microscope

Poster # 196

**Pascal Reiss** // *Max Planck Institute for Solid State Research, Stuttgart, Germany*

High Pressure-Tuning of Electron-Doped Cuprate Superconductors

Poster # 197

**Andreas Kreisel** // *University of Leipzig*

Superconducting Instabilities in Strongly-Correlated Infinite-Layer Nickelates

Poster # 198

**Raquel Sánchez-Barquilla** // *Universidad Autónoma de Madrid*

mK STM studies of FeSe

Poster # 199

**Xie Chengrog** // *Tohoku University, Japan*

Majorana zero modes on parallel one-dimensional p-wave superconducting wires

Poster # 200

**Chang-Youn Moon** // *Korea Research Institute of Standards and Science*

Pairing symmetries in Sr<sub>2</sub>RuO<sub>4</sub> from first-principles

Poster # 201

**Malte Grosche** // *University of Cambridge*

Effect of pressure on normal and superconducting states of YFe<sub>2</sub>Ge<sub>2</sub>

Poster # 202

**Grzegorz Litak** // *Lublin University of Technology*

Cooper pairs sizes in two orbital superconductor with d-wave pairing



## Thursday 28 July

### Poster session THUP03

13.30 - 15.15 - Ruby Lounge, Room E102

Poster # 203

**Seungho Seong** // *The Catholic University of Korea, Korea*

Temperature-dependent angle resolved photoemission spectroscopy study of the possible topological Kondo insulator CeNiSn

Poster # 204

**Maxime Debertolis** // *Institut Néel*

Numerical study of screening clouds around quantum impurities subject to disorder and anisotropy

Poster # 205

**Bernd Wolf** // *Goethe University Frankfurt, Germany*

From magnetic order to valence-change crossover in  $\text{EuPd}_2(\text{Si}_{1-x}\text{Ge}_x)_2$  using He-gas pressure

Poster # 206

**Marius Peters** // *Goethe University, Frankfurt, Germany*

Valence fluctuations and structural collapse in Eu-based phosphides  $\text{EuT}_2\text{P}_2$

Poster # 207

**Michal Kwasigroch** // *University College London & Trinity College*

Magnetic hard-direction ordering in anisotropic Kondo systems

Poster # 208

**Michael Turaev** // *University of Bonn*

Kondo systems with periodically driven dipole transitions

Poster # 209

**Petr Král** // *Charles University, Faculty of Mathematics and Physics, Department of Condensed Matter Physics, Czech Republic*

Microscopic essence of magnetism in  $\text{Ce}_2\text{Pd}_2\text{In}$  at ambient and elevated pressures

Poster # 210

**Piotr Majek** // *Adam Mickiewicz University, Poland*

Thermoelectric signatures of Majorana-Kondo interplay in double quantum dots

Poster # 211

**Jannis Willwater** // *IPKM, TU Braunschweig, Germany*

Magnetic phase diagram and novel electronic phase in  $\text{U}_2\text{Rh}_3\text{Si}_5$

Poster # 212

**Ricardo Urbano** // *State University of Campinas, Gleb Wataghin Institute of Physics, Brazil*

Orbital anisotropy probed by hyperfine couplings in Kondo lattice materials

Poster # 213

**Yuka Kusanose** // *Hiroshima University*

Quadrupole phase transition in a cubic  $4f^2$  compound  $\text{PrCdNi}_4$  with a non-Kramers doublet ground state



Poster # 214

**Henrique Pizzi** // Instituto de física "Gleb Wataghin", Universidade Estadual de Campinas

Magnetic properties of TbCuBi<sub>2</sub> Intermetallic compound

Poster # 215

**Shun Yanagiya** // Hokkaido University

Detailed magnetic phase diagram in CeCoSi for single crystal

Poster # 216

**Owen Moulding** // Institut Neel, France

Crystal-Electric-Field excitations of CeCoSi unveiled by Raman spectroscopy

Poster # 217

**Gabriel Silva Freitas** // University of Campinas

Crystalline electric field effect and anisotropic magnetic interactions in RTBi<sub>2</sub> (R=Ce, Pr, Nd; T=Cu, Au)

Poster # 218

**Nicolas Gauthier** // Université de Sherbrooke, Canada

Probing field-induced CEF mixing in CeRhIn<sub>5</sub> with field-angle dependence measurements

Poster # 219

**David Sviták** // Charles University, Faculty of Mathematics and Physics, Department of Condensed Matter Physics

Magnetoelastic coupling in PrNi<sub>5</sub>

Poster # 220

**Abhijit Bhat Kademane** // UNiversity of Stavanger

Crystal fields and Magnetic frustration in SrTm<sub>2</sub>O<sub>4</sub>

Poster # 221

**Pallavi Kushwaha** // CSIR- National Physical Laboratory, India

Cobalt substitution induced ferromagnetism in PdCrO<sub>2</sub>

Poster # 222

**Katsuki Nihongi** // Osaka University, Japan

High field magnetism of the triangular lattice antiferromagnet CsFeCl<sub>3</sub> under high pressure

Poster # 223

**Kwang-Yong Choi** // Sungkyunkwan University, South Korea

Gauge-flux-driven Kondo screening in  $\alpha$ -Ru<sub>1-x</sub>Cr<sub>x</sub>Cl<sub>3</sub>

Poster # 224

**Russell Ewings** // ISIS Pulsed Neutron and Muon Source

Metastable antiphase boundary ordering in CaFe<sub>2</sub>O<sub>4</sub>

Poster # 225

**Aritro Mukherjee** // University of Amsterdam, The Netherlands

Probing Flat Band Physics in Spin Ice Systems via Polarized Neutron Scattering.

Poster # 226

**Geoffroy Haeseler** // ENSL, CNRS, Laboratoire de physique, F-69342 Lyon, France.

Kasteleyn Transition in Coulomb phase



Poster # 227

**Sreejith Thamban** // *Helmholtz-Zentrum Berlin, Germany and Technical University Berlin, Germany*

Single Crystal Growth and Physical Properties of Distorted Triangular Lattice quantum magnet La<sub>2</sub>CuGe<sub>2</sub>O<sub>8</sub>

Poster # 228

**Andrej Pustogow** // *Institute of Solid State Physics, TU Wien, Vienna, Austria*

Thirty-Year Anniversary of  $\kappa$ -(BEDT-TTF)<sub>2</sub>Cu<sub>2</sub>(CN)<sub>3</sub>: Reconciling the Spin Gap in a Spin-Liquid Candidate

Poster # 229

**Nina Stilkerich** // *Max Planck Institute for Chemical Physics of Solids, Germany*

Nonlinear stress-strain relation of PdCrO<sub>2</sub>

Poster # 230

**Margherita Parodi** // *University of Genova, Italy*

Magnon contributions to thermal conductivity in non-collinear magnets

Poster # 231

**Michael Graf** // *Dept. of Physics, Boston College*

A muSR study of novel magnetic ordering in LiYbO<sub>2</sub>

Poster # 232

**Arnob Mukherjee** // *University of Tennessee, Knoxville, USA*

Engineering antiferromagnetic skyrmions and antiskyrmions at metallic interfaces

Poster # 233

**Markus Drescher** // *Technische Universität München, Germany*

Dynamical Spin Structure Factor of the spin-1/2 J<sub>1</sub>-J<sub>2</sub> Heisenberg Model on the Triangular Lattice

Poster # 234

**Hui-Ke Jin** // *Technical University of Munich*

Possible chiral spin liquid state in the S = 1/2 kagome Heisenberg model

Poster # 235

**Takanori Kida** // *Osaka University*

Pressure effects on the magnetism of the S = 1/2 spin ladder Cu(DEP)Br<sub>2</sub>

Poster # 236

**Simon Rousseau** // *Laboratoire National des Champs Magnétiques Intenses, Grenoble, France*

The Skyrmion Phase of the Chiral Antiferromagnet EuPtSi Studied by Transport Measurements

Poster # 237

**Julian Sereni** // *Low Temperature Division, Centro Atómico Bariloche, Argentina*

Evidences for a Skyrmion phase formation in Eu<sub>2</sub>Pd<sub>2</sub>Sn

Poster # 238

**Kavipriya Thangavel** // *University of Leipzig, Germany*

EPR and SQUID Interrogations of Chromium Trimer Complexes in the MIL-101(Cr) and MIL-100(Al/Cr) MOFs

Poster # 239

**Akmal Hossain** // *Indian Institute of Science, India*

Y<sub>2</sub>CuTiO<sub>6</sub>: A novel low temperature dynamic correlated 3D-paramagnet on a randomly diluted planar triangular lattice





Poster # 240

**Christoph Resch** // *Technical University Munich, Germany*  
Single-crystal growth and low temperature properties of ErB<sub>2</sub>

Poster # 241

**Aleksandr Sukhanov** // *Technische Universität Dresden*  
Frustration model and spin excitations in the helimagnet FeP

Poster # 242

**Noah Winterhalter-Stocker** // *University of Augsburg, Germany*  
Low temperature thermodynamic characterization of the spin-1/2 triangular antiferromagnet Na<sub>2</sub>BaCo(PO<sub>4</sub>)<sub>2</sub>

Poster # 243

**Kazuya Miyagawa** // *University of Tokyo, Japan*  
NMR studies of the spin liquid candidate material, k-(ET)<sub>2</sub>Cu<sub>2</sub>(CN)<sub>3</sub>, with varying magnetic field and pressure

Poster # 244

**Toru Sakai** // *University of Hyogo*  
Quantum spin nematic liquid in the low-dimensional anisotropic magnets

Poster # 245

**Kiyu Fukui** // *The University of Tokyo, Japan*  
Feasibility study of Kitaev quantum spin liquid for ultracold polar molecules and higher spin materials

Poster # 246

**Shin Miyahara** // *Fukuoka University, Japan*  
Theory of absorption in Shastry-Sutherland material SrCu<sub>2</sub>(BO<sub>3</sub>)<sub>2</sub>

Poster # 247

**Lukas Worch** // *Technical University of Munich, Germany*  
Vibrating-coil and membrane-based-Faraday magnetometry of the magnetic phase diagram of Gd<sub>3</sub>Ga<sub>5</sub>O<sub>12</sub> at low temperatures

Poster # 248

**Edward Riordan** // *Institut Néel CNRS, Grenoble, France*  
Advanced magnetocaloric materials for adiabatic demagnetization Spin dynamics of the quantum dipolar magnet Yb<sub>3</sub>Ga<sub>5</sub>O<sub>12</sub>

Poster # 249

**Kento Kojima** // *Aoyama Gakuin University, Japan*  
A cluster extension of the spin wave theory for spin excitation spectra

Poster # 250

**Yoshito Watanabe** // *The University of Tokyo, Japan*  
Bose-Einstein Condensations in quasi-2D Diluted S = 3/2 Quantum Magnets

Poster # 251

**Wilhelm Kadow** // *Technical University of Munich, Germany*  
Hole Spectral Function of a Chiral Spin Liquid in the Triangular Lattice Hubbard Model

Poster # 252

**Gervasi Herranz** // *Institute for Materials Science of Barcelona, ICMAB-CSIC, Spain*  
Spin-orbit mixed states in an electromagnetic field



Poster # 253

**Josse Muller** // *University of Groningen, Netherlands*

Three-Dimensional Skyrmions in chiral non-collinear antiferromagnets

Poster # 254

**Sopheak Sorn** // *Karlsruhe Institute of Technology, Germany*

Fractonic behaviors of skyrmions in chiral magnets

Poster # 255

**Aman Kumar** // *Tata Institute of Fundamental Research, India*

Thermal Hall transport calculations in Kitaev-Heisenberg model

Poster # 256

**Emma Ynill Lenander** // *University of Copenhagen, Denmark*

ClassiC, a package for simulating classical spin dynamics at finite temperatures

Poster # 257

**Guratinder Kaur** // *The University of Edinburgh, UK*

Tuning exchanges in frustrated diamond-lattice antiferromagnet:  $\text{MnSc}_2\text{Se}_4$

Poster # 258

**Piyush Jeena** // *CNRS - Laboratoire Ondes et Matière d'Aquitaine, Bordeaux*

Engineering magnetic frustration with impurities

Poster # 259

**Matúš Orendáč** // *Institute of Experimental Physics, Slovak Academy of Sciences, Slovakia*

Quantum oscillations in heat capacity and charge transport of the unconventional insulator  $\text{SbM}_6$

Poster # 260

**Maria Victoria Ale Crivillero** // *Max Planck Institute for Chemical Physics of Solids, Dresden, Germany*

Exploring  $\text{Eu}_5\text{In}_2\text{Sb}_6$ , a non-symmorphic antiferromagnet: from macroscopic to atomic length scales

Poster # 261

**Po-Ya Yang** // *Max Planck Institute for Chemical Physics of Solids, Germany*

Orbital Differentiation in  $\text{Sr}_2\text{RuO}_4$  under Uniaxial Stress

Poster # 262

**Yuki Utsumi Boucher** // *Institute of Physics, Croatia*

Angle-resolved photoelectron spectroscopy of  $\text{Yb}(\text{Ni}_{1-x}\text{Co}_x)_3\text{Ga}_9$

Poster # 263

**Izidor Benedičič** // *University of St Andrews, United Kingdom*

Compass-like manipulation of nematicity in  $\text{Sr}_3\text{Ru}_2\text{O}_7$

Poster # 264

**Jasper Linnartz** // *HFML, Radboud University, Netherlands*

Fermi surface and nested magnetic breakdown in  $\text{WTe}_2$

Poster # 265

**Simli Mishra** // *Max Planck Institute for Chemical Physics of Solids, Dresden, Germany*

Investigation of temperature dependent thermal transport in  $\text{Sr}_2\text{RuO}_4$  and  $\text{Sr}_3\text{Ru}_2\text{O}_7$  over a wide temperature range



Poster # 266

**Minjae Kim** // *Korea institute for advanced study, South Korea*  
Emergent Phase Diagram of Ruthenates : SrRuO<sub>3</sub>-SrTiO<sub>3</sub> Heterostructure

Poster # 267

**Shingo Araki** // *Okayama University, Japan*  
Localized-to-itinerant crossover in CeIn<sub>3</sub>

Poster # 268

**Rahul Mahavir Varma** // *Indian Institute of Science, India*  
Electronic structure across the antiferromagnetic transition of NiO

Poster # 269

**Michelle Hollricher** // *Technical University of Munich, Germany*  
Investigation of de Haas-van Alphen oscillations under temperature modulation in Bi

Poster # 270

**Sven Friedemann** // *University of Bristol, United Kingdom*  
Mutually stabilised electronic and structural transition in high-pressure sulphur

Poster # 271

**Saumya Mukherjee** // *University of Amsterdam, The Netherlands*  
Nodes of different speeds: anisotropy of the nodal electronic structure in single-layered Pb-Bi<sub>2</sub>201 high-T<sub>c</sub> superconductors

Poster # 272

**Susanne Schulz** // *TU Dresden, Germany*  
Cubic Rashba effect and 2D-ferromagnetism at the iridium-silicide surfaces of antiferromagnetic GdIr<sub>2</sub>Si<sub>2</sub> and mixed-valent EuIr<sub>2</sub>Si<sub>2</sub>

Poster # 273

**Marcin Mucha-Kruczynski** // *University of Bath, UK*  
Lifshitz transition-induced tuning of charge density waves in 2H-TaSe<sub>2</sub>

Poster # 274

**Paweł Starowicz** // *Jagiellonian University, Poland*  
Electronic structure of the Ce<sub>3</sub>PdIn<sub>11</sub> heavy fermion system with two inequivalent Ce sites

Poster # 275

**Shailja Sharma** // *Indian Institute of Technology Mandi, India*  
Quantum Oscillations and ARPES Studies of PdxBi<sub>2</sub>Te<sub>3</sub> Topological Insulator

Poster # 276

**Sonika Bagga** // *School of Basic Sciences, Indian Institute of Mandi, India*  
Planar Hall effect in Cu intercalated PdTe<sub>2</sub>

Poster # 277

**Charles Mielke III** // *Paul Scherrer Institute, Switzerland*  
Intriguing magnetism of the topological kagome magnet TbMn<sub>6</sub>Sn<sub>6</sub>

Poster # 278

**Ayanesh Maiti** // *Indian Institute of Science*  
Temperature dependence of Dirac Fermions in SnTe

Poster # 279

**Indranil Roy** // *Weizmann Institute of Science, Israel*  
Imaging Chern mosaic and Berry-curvature magnetism in magic-angle graphene



Poster # 280

**Davide Pizzirani** // *Radboud University - IMM - HFML*  
Magneto-resistance and quantum oscillations in thin ZrSiSe flakes

Poster # 281

**Orest Pavlosiuk** // *Institute of Low Temperature and Structure Research, Polish Academy of Sciences*  
Magnetotransport properties of half-Heusler antiferromagnets SmPtBi and DyPtBi

Poster # 282

**Takanori Sugimoto** // *Osaka University, Japan*  
High-dimensional Hofstadter butterfly induced by aperiodic magnetic field in quasicrystalline topological insulator

Poster # 283

**Pantelis Bampoulis** // *University of Twente, The Netherlands*  
Is epitaxial germanene a two-dimensional topological insulator?

Poster # 284

**Thies Jansen** // *University of Twente*  
Topological insulating bilayers and related interface effects

Poster # 285

**Tomasz Toliński** // *Institute of Molecular Physics, Polish Academy of Sciences*  
Magnetic properties of the higher-order topological insulator Euln<sub>2</sub>As<sub>2</sub>

Poster # 286

**L K Saini** // *Department of Physics, SV NIT, Surat India*  
Coulomb drag study of inhomogeneous dielectric medium: Hole-hole dynamic screening in 2D-GaAs DQW

Poster # 287

**Rui Aquino** // *Rio de Janeiro State University*  
Exceptional Points in Fermi Liquids with multipolar interactions

Poster # 288

**Dongwook Kim** // *Pohang University of Science and Technology, South Korea*  
Drastic Magnetic Anisotropy Change Under Electric Field in Fe<sub>n</sub>GeTe<sub>2</sub> (n=3, 4) Monolayers: Density Functional Theory Perspective

Poster # 289

**Michal Kiaba** // *Masaryk University*  
Structural and magnetic properties of LaFeO<sub>3</sub>/SrTiO<sub>3</sub> superlattices

Poster # 290

**Orion Ciftja** // *Prairie View A&M University, USA*  
The energy of a two-dimensional electron gas with finite thickness

Poster # 291

**Jae-Ho Chung** // *Korea University, Republic of Korea*  
Topological Dirac magnons in honeycomb ferromagnets

Poster # 292

**Shroya Vaidya** // *University of Warwick, England*  
Electronic and Magnetic Properties of Fe<sub>3</sub>GeTe<sub>2</sub> at High Magnetic Fields

Poster # 293

**Herwig Michor** // *Institute of Solid State Physics, TU Wien, Austria*  
Single Crystal Studies of Charge Density Wave Physics in Quasi-1D Metals RNiC<sub>2</sub>



Poster # 294

**Marta Roman** // *Gdansk University of Technology, Poland*

Single-crystal studies of the charge density wave and magnetism in TmNiC<sub>2</sub>

Poster # 295

**Debasmita Pariari** // *Indian Institute of Science, India*

Understanding the electronic structure of MoS<sub>2</sub>: Effect of chemical exfoliation and mechanical strain

Poster # 296

**Tatsuto Hatanaka** // *University of Tokyo, Japan*

First-principles study of intercalated transition metal dichalcogenides

Poster # 297

**Sreya Suresh** // *Indian Institute of Technology, Madras, India*

Signatures of Correlated Quantum Transport in Spintronic Heterostructures

Poster # 298

**Sreejith P K** // *Indian Institute of Technology Madras, India*

Interplay of weak localization and magnetism in strongly correlated PrCo<sub>0.5</sub>Ni<sub>0.5</sub>O<sub>3</sub> thin films grown on SrTiO<sub>3</sub> substrates

Poster # 299

**Evgeny Stepanov** // *CPHT, CNRS, Ecole Polytechnique, France*

Coexisting charge density wave and magnetic instabilities in monolayer InSe and Pb/Si(111) systems

Poster # 300

**Aditya Putatunda** // *Istituto Italiano di Tecnologia*

Magnetism in strongly correlated twisted bilayers from first principles

Poster # 301

**Noah Meyer** // *University of Cambridge*

Pressure-induced structural phase transitions in 2D van der Waals material NiPS<sub>3</sub>

Poster # 302

**Jinwon Lee** // *Leiden University, The Netherlands*

Atomic adsorbate identifying a correlated Mott insulator

Poster # 303

**Fernando Passos** // *University of São Paulo, São Paulo*

Magnetic, electronic, and structural investigation of the strongly correlated Sm<sub>1-x</sub>Y<sub>x</sub>Co<sub>5</sub> system

Poster # 304

**Jesla P K** // *Indian Institute of Technology Madras, India*

Magnetic properties of a multicomponent intermetallic compound  
Tb<sub>0.25</sub>Dy<sub>0.25</sub>Ho<sub>0.25</sub>Er<sub>0.25</sub>Al<sub>2</sub>

Poster # 305

**Manuel Nunez-Regueiro** // *Institute NEEL CNRS*

Possible high temperature superconducting transitions in bulk twisted graphite

Poster # 306

**O Hamutu** // *Delft University of Technology, The Netherlands*

Exploration in new room temperature magnetocaloric materials: structure and magnetocaloric properties in Mn<sub>5</sub>(Si,P)B<sub>2</sub> compounds



Poster # 307

**Ho Keun Lee** // *Kangwon National University, Republic of Korea*

Effects of Lead sulfate doping on the formation and superconducting properties of  $(\text{Bi}_{2-x}\text{Pbx})\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_z$  superconductors

Poster # 308

**Thomas Gruner** // *University of Cambridge, UK*

Solid-state refrigeration with enormous heat absorption to less than 120mK: Application of metallic magnetocaloric

Poster # 309

**Thom Ottenbros** // *High Field Magnet Laboratory, Radboud University Nijmegen, Netherlands*

Thermal Expansion and Magnetostriction of  $\text{GdTe}_3$

# Transport on the Lieb lattice

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The Lieb lattice, also known as face-centered square lattice, has attracted a lot of attention in the last decade due to its topological properties and the fact that its band structure features two dispersive bands and a perfectly dispersionless flat band, and flat bands have been of interest for a long time. The two-dimensional Lieb lattice has been an essential building block in many three-dimensional perovskite materials with complex phase diagrams and strong electron-electron correlations. Several materials have their atoms arranged on the Lieb lattice. A typical example is the  $\text{CuO}_2$  planes of cuprate superconductors. Other examples are  $\text{La}_4\text{Ba}_2\text{Cu}_2\text{O}_{10}$ ,  $\text{LaCO}_5$ ,  $\text{CePt}_5$ , and the Pphthalocyanine-based metal compounds. It can also be realized in optical lattices, and the bulk and edge transport of light in photonic Lieb lattices have been observed experimentally. We employ the Hubbard model at the mean-field level at finite temperature. The intrinsic spin-orbit coupling term does not affect the flat band. Still, it opens the gap between the flat and upper and lower dispersive bands generating a nontrivial intrinsic Berry phase that leads to topological features. We present calculations for the longitudinal and transverse dynamical Hall conductivities at finite temperatures. The Drude weight as a function of temperature is also calculated.

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# Microscopically unveiling 4f electrons hybridization in the CeCuSb<sub>2</sub> Heavy Fermion

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Previous results in the CeCuBi<sub>2</sub> [1] heavy-fermion samples showed a low hybridization between the Ce<sup>3+</sup> 4f<sup>1</sup> electrons and the Cu atoms in the material. Therefore, a new compound was grown with the substitution of Sb in the Bi site, aiming to increase the interaction between the Ce<sup>3+</sup> magnetic moments and the Cu atoms. It led to the synthesis of monocrystalline samples of CeCuSb<sub>2</sub>.

In this work, we performed systematic nuclear magnetic resonance NMR measurements in this latter sample, focusing on the <sup>63</sup>Cu hyperfine coupling constant B<sub>hf</sub>. We then compared these results with the previously obtained for the undoped samples of CeCuBi<sub>2</sub>. Afterward, we contrasted the B<sub>hf</sub> observed on each compound with their  $\alpha$  constant values, which comprises the contribution of the spin  $\pm 5/2$  to the Ce<sup>3+</sup> 4f<sup>1</sup> electronic orbitals, as it has been done previously in [2] for another heavy fermion family.

Surprisingly, despite the suppression in  $\alpha$  with the Sb substitution, which indicates a less planar 4f<sup>1</sup> orbital and thus should favor an increase in B<sub>hf</sub>. Our results exhibit a slight decrease in the hyperfine coupling in the <sup>63</sup>Cu. This odd behavior suggests that the Ce<sup>3+</sup> magnetic moments are very localized, hence leading to an inexpressive contribution to the hyperfine coupling constant arising from the shape of the 4f<sup>1</sup> orbitals.

Furthermore, our Knight shift results revealed the onset of the antiferromagnetic transition at T<sub>N</sub>  $\approx$  8K, which is above T<sub>N</sub> = 5.8K found via magnetic susceptibility measurements. It implies some degree of magnetic frustration or incommensurability in the magnetic structure of this compounds. This conclusion is then further reinforced by the fast depletion of the main resonance line below T = 8K with the remanence of its spin-echo signal even below the temperature of the AFM onset.

Finally, our spin-lattice relaxation T<sub>1</sub> data exhibited slow relaxation rates, indicating a weak interaction between the magnetic moments. These results, point to localized weakly interacting magnetic moments in this family of compounds. It enables us to conclude that, even though weak, the RKKY interaction is the dominant mechanism behind the AFM ordered ground-state. Lastly, this study comes to enlighten our understanding of the relevant magnetic properties of this heavy fermion family and aid the search for new materials with related physics.

[1] Adriano, C., Rosa, P.F.S., Jesus, C.B.R., Mardegan, J.R.L., Garitezi, T.M., Grant, T., Fisk, Z., Garcia, D.J., Reyes, A.P., Kuhns, P.L. and Urbano, R.R., 2014. Physical properties and magnetic structure of the intermetallic CeCuBi<sub>2</sub> compound. *Physical Review B*, 90(23), p.235120.

[1] Menegasso, P., Souza, J.C., Vinograd, I., Wang, Z., Edwards, S.P., Pagliuso, P.G., Curro, N.J. and Urbano, R.R., 2021. Hyperfine couplings as a probe of orbital anisotropy in heavy-fermion materials. *Physical Review B*, 104(3), p.035154.



# A Sum rule investigation of the 4f ground state of the Kondo semimetal CeNiSn

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CeNiSn has been intensively studied in the context of Ce-based Kondo insulators. CeNiSn shows a notably narrow hybridization gap near the Fermi level, and a slight overlap between valence and conduction bands, placing it as a Kondo semimetal, or as *failed* Kondo insulator. It crystallizes in an orthorhombic space group with monoclinic point symmetry, thus displaying strongly anisotropic magnetic, transport and thermal properties [1]. Theoretical attempts to describe the formation of such a pseudogap highlight the importance of the ground state (GS) wave function [2-4], but unfortunately the strong hybridization of 4f and conduction electrons prevented inelastic neutron scattering (INS) experiments from resolving the crystal-field (CF) excitations in CeNiSn [5,6], leaving the CF scheme and GS of this compound undetermined.

We have now performed polarization-dependent X-ray absorption spectroscopy (XAS) at the Ce M<sub>4,5</sub> edge (3d→4f) of CeNiSn [7]. Analyzing the linear polarized XAS data with respect to the expectation values of  $J_x^2$ ,  $J_y^2$  and  $J_z^2$  and we find more than one solution. We then measured also isostructural and isoelectronic CePtSn with XAS [8], because its 4f electrons are more localized so that the crystal-field scheme of CePtSn is well described by the single crystalline INS work of Janoušová *et al.* [9]. Comparing the XAS solutions we are now able to provide a ground state wave function for CeNiSn.

[1] Takabatake *et al.*, Phys. Rev. B **41**(13) 9607 (1990).

[2] K. A. Kikoin, *et al.*, Phys. Rev. B **59** 15070 (1999).

[3] H. Ikeda and K. Miyake, J. Phys. Soc. Jpn. **65** 1769 (1996).

[4] J. Moreno and P. Coleman, Phys. Rev. Lett. **84** 342 (2000).

[5] M. Kohgi *et al.*, Physica B **186-188** 409-411 (1993)

[6] J.-Y. So *et al.*, Phys. Rev. B **71**, 214441 (2005)

[7] Beamline ID08 at ESRF, Grenoble, France

[8] Beamline TPS 45A, NSRRC, Taiwan

[9] B. Janoušová *et al.*, Phys. Rev. B **69**, 220412(R) (2004).

# Anisotropic magnetic and thermodynamic properties of single crystals of antiferromagnetic CePdAl<sub>3</sub>

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Recently, Ce-based intermetallic compounds with the structure formula CeTAl<sub>3</sub> (with *T* being a transition metal) [1] attracted considerable scientific attention due to the observation of vibronic bound states and magneto-elastic hybrid excitations in CeCuAl<sub>3</sub> [2] and CeAuAl<sub>3</sub> [3]. Here, we report a study of the magnetic and thermodynamic properties of single-crystal CePdAl<sub>3</sub> grown by means of the optical floating zone technique. Depending on the growth conditions, either a tetragonal (space group *I4mm*) or an orthorhombic (space group *Cmc2<sub>1</sub>*) modification crystallizes. Twinning occurs in the orthorhombic crystals with twins differing in their orientation in the basal plane formed by the <100> and <010> crystallographic axes, while sharing a common <001> hard axis. While the tetragonal compound remains nonmagnetic down to the lowest temperatures studied, the orthorhombic compound develops antiferromagnetic order below a Néel temperature of 5.6 K. In this state, the localized cerium moments align antiparallel along the magnetically easy <100> axes. The magnetic properties exhibit a pronounced anisotropy, with magnetic fields along the easy axes inducing a spin-flop transition at 5 T at 2 K. The electronic contribution to the specific heat is described by a Sommerfeld coefficient of 121 mJ K<sup>-2</sup> mol<sup>-1</sup>, characteristic of moderate heavy-fermion behavior. Magnetic phase diagrams are inferred, providing a solid point of reference for further studies of this compound.

[1] C. Franz *et al.*, J. Alloys Compd. **688**, 978 (2016).

[2] D. Adroja *et al.*, Phys. Rev. Lett. **108**, 216402 (2012).

[3] P. Čermák *et al.*, Proc. Natl. Acad. Sci. U.S.A. **116**, 6695 (2019).

# Optical study of the electronic structure of locally noncentrosymmetric $\text{CeRh}_2\text{As}_2$

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$\text{CeRh}_2\text{As}_2$  has recently been discovered as a novel heavy-fermion superconductor ( $T_C = 0.26$  K) [1]. Its  $\text{CaBe}_2\text{Ge}_2$ -type structure lacks a local inversion symmetry of the Ce and one of the Rh and As sites while maintaining a global inversion center [2]. The electronic structures of  $\text{CeRh}_2\text{As}_2$  and the reference material  $\text{LaRh}_2\text{As}_2$  have been investigated by using optical conductivity spectra and first-principal DFT calculations [3]. The low-temperature spectra of  $\text{LaRh}_2\text{As}_2$  revealed, after subtraction of the free-carrier Drude contribution, background- and peak features which could nicely be reproduced in the DFT-spectra, implying a conventional metallic nature. In  $\text{CeRh}_2\text{As}_2$  two mid-IR peaks which correspond to the unoccupied Ce- $4f_{5/2}$  and  $4f_{7/2}$  states, respectively, strongly develop with decreasing temperature, suggesting the emergence of the hybridization states between conduction- and  $4f$ - electrons. We compared the temperature dependence of these mid-IR peaks with corresponding data from  $\text{CeCu}_2\text{Si}_2$  and  $\text{CeNi}_2\text{Ge}_2$  in the  $\text{ThCr}_2\text{Si}_2$ -type structure to examine a possible impact of local inversion symmetry breaking on electronic structures.

[1] S. Khim et al., *Science* 373, 1012 (2021).

[2] A. Pourret and G. Knebel, *Science* 373, 962 (2021).

[3] S. Kimura, J. Sichelschmidt, and S. Khim, *Phys. Rev. B.* 104, 245116 (2021).

# The quadrupole density wave and its interplay with superconductivity in CeRh<sub>2</sub>As<sub>2</sub>: a thermodynamic study

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The newly discovered [1] heavy-fermion CeRh<sub>2</sub>As<sub>2</sub> is a rare case of multi-phase superconductor ( $T_c = 0.26$  K) located in the vicinity of a quantum-critical-point (QCP). Two different superconducting (SC) phases are observed for a magnetic field applied along the  $c$ -axis ( $B \parallel c$ ) of the tetragonal locally-non-centrosymmetric crystalline structure. The two SC phases are separated by a 1<sup>st</sup>-order line located at  $B^* \approx 4$  T which has been interpreted as the transition between an even-parity to an odd-parity SC order parameter [1]. Accordingly, the upper critical field for this field direction is huge,  $H_{c2} = 14$  T, compared to  $T_c$  but with field along the basal  $ab$ -plane ( $B \perp c$ ) only a single SC phase is observed with  $H_{c2} = 2$  T. In addition, thermodynamic measurements have detected another non-magnetic phase transition at  $T_0 = 0.4$  K. The phase below  $T_0$  was interpreted as a unique quadrupole-density-wave (QDW) state [2].

A study of the evolution of both phases with a field  $B \perp c$  has shown that the SC phase is included in the QDW phase because  $T_0$  increases with  $B \perp c$ . However, unpublished experiments indicate that  $T_0$  decreases with  $B \parallel c$  and disappears for fields close to  $B^*$ , suggesting that the QDW might intersect the SC phase at a field near  $B^*$ .

In this poster, we present new zero-field-cooled and field-cooled specific heat and thermal expansion measurements on a single crystal of CeRh<sub>2</sub>As<sub>2</sub> with  $B \parallel c$  and  $B \perp c$ . These allow to draw a more precise phase diagram for  $B \parallel c$  and to discuss in more detail the interplay between the SC and the QDW phases.

[1] S. Khim, J. F. Landaeta *et al.*, *Science* **373**, 1012 (2021)

[2] D. Hafner *et al.*, *Phys. Rev. X* **12**, 011023 (2022)

# Investigation of Anisotropy of Lattice Distortion in CeCoSi

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The Ce-based intermetallic compound CeCoSi crystallizes into the tetragonal CeFeSi-type structure ( $P4/nmm$ ,  $D_{4h}^7$ , No. 129), where the spatial inversion symmetry is locally broken at the Ce site [1]. It shows an antiferromagnetic (AFM) ordering at  $T_N = 9.4$  K [2,3] and another phase transition at  $T_0 \sim 12$  K [4], whose order parameter is unidentified. The Co-NQR/NMR measurements have suggested that the ordering at  $T_0$  is an antiferroquadrupole one [5], whereas very recent x-ray diffraction measurements revealed that a triclinic lattice distortion takes place below  $T_0$  [6]. Thus, the order parameter of the  $T_0$  ordering is still controversial. In addition, it has been revealed that each ordering state has a high magnetic-field region when the magnetic field is applied the [100] and [001] directions, suggesting a change in the symmetry of the order parameter or domain alignment under high magnetic field [7].

In the present research, we performed the linear thermal expansion measurements along the [100] and [110] directions in the tetragonal structure under magnetic field up to 14 T for a single crystalline CeCoSi in order to investigate anisotropy of the lattice distortion in the (001) plane below  $T_0$ . We will report the details of the experimental results and discuss the symmetry of the order parameter of the  $T_0$  ordering including the high-field ordering regions.

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[1] O. I. Bodak *et al.*, J. Struct. Chem. **11**, 283 (1970).

[2] E. Lengyel *et al.*, Phys. Rev. B **88**, 155137 (2013).;

[3] S. E. Nikitin *et al.*, Phys. Rev. B **101**, 214426 (2020).

[4] H. Tanida *et al.*, J. Phys. Soc. Jpn. **88**, 054716 (2019).

[5] M. Manago *et al.*, J. Phys. Soc. Jpn. **90**, 023702 (2021).

[6] T. Matsumura *et al.*, arXiv:2203.03879.

[7] H. Hidaka *et al.*, arXiv:2203.09754.

# The new compound $\text{Ce}_2\text{Rh}_2\text{Al}$ : a representative of the monoclinic $\text{Pr}_2\text{Co}_2\text{Al}$ structure type

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We have recently demonstrated the dimorphic nature of the gallium compound  $\text{Ce}_2\text{Rh}_2\text{Ga}$ , which forms either in an ordered version of the orthorhombic  $\text{La}_3\text{Ni}_2$  structure type or in the monoclinic  $\text{Pr}_2\text{Co}_2\text{Al}$  structure type, depending on the heating conditions administered during annealing [1].  $\text{Ce}_2\text{Rh}_2\text{Ga}$  in the  $\text{La}_3\text{Ni}_2$  structure type suffers a temperature hysteretic but reproducible crystal structure transformation at  $T^*=130$  K, which we have shown to be driven by strong  $4f$ -electron hybridization and a valence transition among the Ce ions [2]. At  $T^*$  the crystal structure changes from the space group  $Cmce$  to the monoclinic, centrosymmetric  $C2/m$ , accompanied by non-merohedral twinning [3].

As part of our ongoing research into the 2:2:1 stoichiometry of cerium-based compounds, we present here the results of exploratory studies of a polycrystalline sample of the new compound  $\text{Ce}_2\text{Rh}_2\text{Al}$ . This compound shows an electrical resistivity  $\rho(T)$  that is characteristic of metallic behaviour with electron-phonon scattering dominating towards room temperature. Below 30 K there is Kondo-like spin charge-carrier scattering evident with an increase in the  $4f$ -electron derived resistivity  $\rho_{4f}(T)$  as temperature is further lowered. At  $T_C = 4$  K a distinct knee in  $\rho(T)$  separates the paramagnetic higher temperature phase from a ferromagnetic ground state, as confirmed by magnetization results. Between  $T_C$  and 1.9 K the resistivity decreases by a factor of more than 2. The phase transition in  $\text{Ce}_2\text{Rh}_2\text{Al}$  is further manifested as a lambda-type peak in its temperature dependence of specific heat. We demonstrate the results of resistivity and specific heat measured in various applied magnetic fields.

[1] S. Nesterenko, A. Tursina, M. Pasturel, S. Xhakaza, and A. Strydom, *J. Alloys. Comp.* **844**, 155570 (2020).

[2] H. Sato, T. Matsumoto, N. Kawamura, K. Maeda, T. Takabatake, and A. Strydom, *Phys. Rev. B* **105**, 035113 (2022).

[3] A. Dudka, S. Nesterenko, and A. Tursina, *J. Alloys Comp.* **890**, 161759 (2022).

# DFT + DMFT study of the two-channel quadrupolar Kondo effect in $\text{PrV}_2\text{Al}_{20}$

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Praseodymium-based cubic 1-2-20 materials like  $\text{PrV}_2\text{Al}_{20}$  exhibit a strong coupling between Pr 4f states and conduction electrons. They experimentally show traces of a two-channel quadrupolar Kondo effect in competition with quadrupolar ordering and superconductivity [1]. Valence fluctuations on the Pr atom occur between the magnetic quadrupole  $4f^2 \Gamma_3$  doublet and the excited  $4f^3$  configuration with a dipole Kramers-doublet  $\Gamma_7$ . This leads to an exotic two-channel quadrupolar Kondo effect, where the channel carries a dipole moment and the Kondo degree of freedom a quadrupolar moment. Additionally, the first excited triplet of the  $4f^2$  configuration turns out to be crucial in describing the magnetic response over a wide temperature range. This is due to it carrying a dipole moment and being only 40K above the  $4f^2$  ground state doublet.

We develop a dynamical mean-field theory (DMFT) with a non-crossing approximation (NCA) local impurity solver, that is able to faithfully capture the exotic two-channel Kondo physics in this class of materials, including a momentum-dependent hybridization. This method is then combined with a density functional theory (DFT) calculation, allowing us to quantitatively compare the results to experimental data down to the Kondo regime. Within this approximation, we calculate several temperature dependent quantities: density of states, band structure and magnetic susceptibility.

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[1] For review, see: T. Onimaru and H. Kusunose, J. Phys. Soc. Jpn. 85, 082002 (2016)

## Composition of magnetic interactions in the heavy-fermion system CeIn<sub>3</sub>

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We report high-resolution neutron spectroscopy on the archetypal heavy fermion material CeIn<sub>3</sub> that exhibits an antiferromagnetic (AFM) order below  $T_N = 10.1$  K. Increasing pressure suppresses the AFM state to zero temperature resulting in a quantum critical point, the critical fluctuations of which are believed to mediate unconventional superconductivity. Previous neutron results with moderate resolution reported a substantial spin gap of about 1 meV, which suggest a substantial magnetic anisotropy, in contrast to the observed bulk properties. Our results unambiguously demonstrate that CeIn<sub>3</sub> does not exhibit a spin gap. Instead, we find that the spin waves disperse quasi-vertically up to almost 1 meV. We show that via ab-initio band structure calculations fed into the multi-orbital periodic Anderson model can predict the magnetic excitation spectrum quantitatively. Our results show that this model can be renormalized to a simple Kondo lattice model decorated with short-range super exchange interactions to account for the formation of magnetic order. This microscopically-derived modified Kondo lattice model quantitatively reproduces the low-energy magnetic soft modes in CeIn<sub>3</sub>, which are key to understanding unconventional superconductivity.

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## Pulsed-magnetic-field studies of magnetism and superconductivity in $\text{UTe}_2$

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During the last three years, we have dedicated a large experimental effort in studying the interplay between magnetism and superconductivity in  $\text{UTe}_2$  under extreme conditions. In particular, pulsed magnetic fields were needed to access to magnetic and superconducting phases stabilized in this compound beyond 45 T. Here, a synthesis of experiments performed at the LNCMI-Toulouse under different sets of combined conditions: pulsed magnetic fields up to 70 T at temperatures down to 1.4 K, up to 60 T at temperatures down to 100 mK or at pressures up to 4 GPa and temperatures down to 1.4 K, will be presented.

The observation of multiple superconducting phases induced by a magnetic field in the vicinity of metamagnetic transitions at field  $H_m$  will be considered [1-4]. Different domains of stability of the field-induced superconducting phases are observed, but not understood so far. At ambient pressure superconductivity exists in fields either only below  $H_m$  for  $\mathbf{H} \parallel \mathbf{b}$ , or can be stabilized beyond  $H_m$  for  $\mathbf{H}$  tilted by  $30^\circ$  from  $\mathbf{b}$  towards  $\mathbf{c}$ . In the vicinity of the critical pressure  $p_c = 1.5\text{-}1.7$  GPa, field-induced superconductivity was also observed for  $\mathbf{H} \parallel \mathbf{c}$ . In these different configurations, an enhancement of the Fermi-liquid  $T^2$ -resistivity coefficient  $A$  is found and proposed to result from critical magnetic fluctuations, which are suspected to drive to field-induced superconductivity. A recent high-field investigation of the electrical resistivity measured with different current directions, and of a related anisotropic coefficient  $A$ , will be also presented [5].

### References:

- [1] Knafo et al., J. Phys. Soc. Jpn. **88**, 063705(2019).
- [2] Knebel et al., J. Phys. Soc. Jpn. **88**, 063707 (2019).
- [3] Knafo et al., Commun. Phys. **4**, 40 (2021).
- [4] Vališka et al., Phys. Rev. B **104**, 214507 (2021).
- [5] Thébault et al., to be published.

# Emergence of heavy local Fermi liquid in the underscreened Kondo model with easy-plane anisotropy

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The low-temperature properties of Eu compounds have recently been attracting renewed interest owing to the discoveries of a new type of heavy fermion, complex magnetic orders, and quantum phase transitions associated with the valence crossover phenomena. To clarify the microscopic origin of the heavy fermion state in the Eu system, we have introduced an effective impurity Anderson model considering a valence fluctuating Eu ion (Eu-IAM) [1]. In this presentation, we focus on the divalent Eu ion having the half-filled 4*f* shell and study an effective underscreened Kondo Hamiltonian with easy-plane anisotropy, on the basis of the Eu-IAM,

$$H = \sum_{k\sigma} \varepsilon_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma} + J\boldsymbol{\sigma} \cdot \mathbf{S} + \Delta S_z^2.$$

Here,  $S$  represents the impurity spin operator of  $S = 7/2$ . The Kondo coupling constant  $J$  and the crystal field strength  $\Delta$  are assumed to be positive. We have analyzed the model particularly for  $T_K \gg \Delta$  by using the numerical renormalization group method. It is found that the effective spin  $\tilde{S} = 3$  is formed by the Kondo coupling in the intermediate-temperature region; the crystal field term is relevant to the  $\tilde{S}$  multiplet at low enough temperatures, resulting in a singlet ground state. We show that a local Fermi liquid state with a significant mass enhancement is stabilized in the course of such a singlet formation, indicative of realizing a non-trivial ground state [2]. The mechanism of the heavy fermion formation will be studied in terms of the singular Fermi liquid concept [3]. The relationship of the results with real Eu compounds will also be discussed.

[1] S. Kuniyoshi and R. Shiina, J. Phys. Soc. Jpn. **89**, 124711 (2020).

[2] S. Kuniyoshi and R. Shiina, J. Phys. Soc. Jpn. **90**, 123702 (2021).

[3] P. Coleman and C. Pepin, Phys. Rev. B **68**, 220405 (2003).

# Possible Lifshitz point in the magnetic phase diagram of UNi<sub>2</sub>Si<sub>2</sub> single crystals

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UNi<sub>2</sub>Si<sub>2</sub> is a ternary silicide crystallizing with the tetragonal ThCr<sub>2</sub>Si<sub>2</sub>-type structure, which belongs to the intensively studied UT<sub>2</sub>M<sub>2</sub> family (T = d-electron transition metal, M = Si, Ge). The compound shows complex magnetic properties [1,2]. In zero magnetic field, it undergoes a series of subsequent magnetic phase transitions from paramagnetic (PM) to incommensurate spin-density-wave (ICSDW) to simple body centered antiferromagnetic (AF), and eventually to ferrimagnetic (UAF) states. Application of external magnetic field causes metamagnetic transitions and stabilizes the UAF state. In high magnetic fields, PM, ICSDW and UAF phases tend to meet at a single point that may bear features of bicritical Lifshitz point (LP), which exhibits critical behavior strikingly different from any other [3].

With the main aim to verify the LP hypothesis, we performed comprehensive reinvestigation of UNi<sub>2</sub>Si<sub>2</sub> on high-quality single crystals grown using Czochralski pulling technique. Physical properties of the compound were studied in the temperature range 2 – 300 K and in magnetic fields up to 14 T, aligned along the crystallographic *c*-axis that is the easy magnetic direction in the system. The results of our magnetic, electrical transport and heat capacity measurements confirmed the existence of multiple magnetic phases, and the tendency to mearging the PM-ICLSW and ICLSW-UAF phase boundaries in the magnetic phase diagram constructed. However, up to 14 T, no clear evidence for LP was obtained. Further detailed study of this interesting compound in stronger magnetic fields is indispensable.

\* This work was supported by the National Science Centre (Poland), grant no. 2018/31/D/ST3/03295.

[1] P. Svoboda, P. Javorský, F. Honda, V. Sechovský, A. Menovsky, *Centr. Eur. J. Phys.* **2**, 397 (2004).

[2] P. Svoboda, P. Javorský, V. Sechovský, A. Menovsky, *Physica B* **686**, 276 (2000).

[3] R. M. Hornreich, M. Luban, S. Shtrikman, *Phys. Rev. Lett.* **35**, 1678 (1975).

# Anisotropic signatures of the electronic correlations in the electrical resistivity of $\text{UTe}_2$

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We present a thorough study by electrical resistivity of the superconductor  $\text{UTe}_2$  in its paramagnetic regime. Configurations with electrical currents  $\mathbf{I} \parallel \mathbf{a}, \mathbf{c}$  combined with magnetic fields  $\mu_0\mathbf{H} \parallel \mathbf{a}, \mathbf{b}, \mathbf{c}$  up to 70 T are investigated. Two temperatures characterizing the electronic correlations are identified at 12.5 K and 35 K. Their evolutions with magnetic fields along the three crystallographic directions are determined, allowing the construction of magnetic-field-temperature phase diagrams. At low temperature, an anisotropic Fermi-liquid-like coefficient  $A$  is extracted from the  $T^2$  dependence of the resistivity. The magnetic-field variations of  $A$  are revealed up to 60 T for the three field directions. Near the metamagnetic transition induced at  $\mu_0H_m = 35$  T for  $\mathbf{H} \parallel \mathbf{b}$ , differences in the field-variations of  $A$  for  $\mathbf{I} \parallel \mathbf{a}$  and  $\mathbf{I} \parallel \mathbf{c}$  are observed. Our data will be discussed in relation with the high-field stabilization of superconductivity near  $H_m$  in this material.

## High pressure structural instability in CeSb<sub>2</sub>

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Ambient pressure CeSb<sub>2</sub> is a rare instance of a Ce-based Kondo lattice material with a ferromagnetic ground state [1], as well as at least two further magnetic states in a complex field-temperature phase diagram. This invites closer examination under applied hydrostatic pressure, which can often be used as a tuning parameter to explore quantum phase transitions where magnetism is suppressed. Previous studies showed that the magnetic phase diagram is initially robust under the application of moderate pressure but changes abruptly above ~15 kbar [2].

Extensive high-pressure transport measurements reveal that this abrupt change coincides with a pronounced hysteretic anomaly in the resistivity of the material, which suggests a first-order structural transition. We investigate the structural origin of this anomaly in diamond anvil cell powder X-ray diffraction measurements, up to 80 kbar at 300 K. Our findings indicate that above ~10 kbar, CeSb<sub>2</sub> undergoes a first-order structural transition from the “SmSb<sub>2</sub>-type” *Cmca* low-pressure structure [3], to the “EuSb<sub>2</sub>-type” *P2<sub>1</sub>/m* structure. This new symmetry corresponds to a translation between the now offset neighboring Ce-Sb planes, and a compression in the perpendicular *c*-axis.

In the high-pressure state, the Ce atoms lie closer together in zig-zag chains, producing a profoundly different electronic structure to that of ambient pressure CeSb<sub>2</sub>. A detailed investigation of transport and thermodynamic properties within the “EuSb<sub>2</sub>-type” high pressure state of CeSb<sub>2</sub> reveals a very low-lying maximum in the electrical resistivity at < 4 K, indicating a low coherence temperature, high carrier effective mass, and two new transition anomalies, which are continuously suppressed by further increased pressure [4].

[1] S. L. Bud'ko, P. C. Canfield, C.H. Mielke, A. H. Lacerda, *Phys. Rev. B* **57**, 13624 (1998).

[2] T. Kagayama, G. Oomi, S. L. Bud'ko, P. C. Canfield, *Physica B* **281–282**, 90 (2000).

[3] R. Wang, H. Steinfink, *Inorg. Chem.* **6**, 1685 (1967).

[4] O. P. Squire *et al.*, this conference (2022).

## Single crystal growth of $RNiGe_2$ (R: rare earth) compounds

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$RTX_2$  (R: Rare earth, T: transition metals, X: Si, Ge) has an orthorhombic crystal structure [space group Cmc<sub>2</sub>m]. There are not so many reports on single crystal growth due to the difficulty in obtaining single phase samples. On the other hand, the magnetic properties of polycrystals of  $CeT_xGe_2$  (T: Fe, Co, Ni, Cu,  $0 < x < 1$ ) have been investigated in a previous study [1], and it seems to be easier to grow polycrystals when the amount of T is reduced. In this study, we focused on  $RTX_2$ , which has not been reported for single crystal growth.

At first, polycrystalline samples were prepared by arc melting from starting materials at least 99.9 % purity. The lattice constants were determined by powder X-ray diffraction measurements. The compositions were determined at Venture Business Laboratory by JEOL SEM and Oxford Instrument EDX. As for  $CeT_xGe_2$  (T=Mn, Fe, Cu), it was found that  $CeGe_{1.66}$  was formed, and it was difficult to grow single-phase samples.  $CeT_xSi_2$  (T=V, Cr, Mn, Fe, Cu) also had  $CeSi_2$  secondary phase, and it was difficult to grow single-phase samples.

On the other hand single-phase samples were obtained for  $RNi_xGe_2$  when  $x < 0.8$ . Here, single-crystals of  $RNi_xGe_2$  (R=Pr, Nd,  $x=0.2\sim 0.8$ ) were grown by the Czochralski method. The magnetization of  $PrNi_xGe_2$  show that there is a ferromagnetic transition at low temperatures, and no difference in the transition temperature or saturation magnetization is observed. The fact that the measured magnetization does not exceed the saturation magnetization of  $Pr^{3+}$  ions and the value of the effective Bohr magneton number obtained suggests that localized electrons affect the magnetism.

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[1] C.N.R. Rao. Solid State Communications, **83** 765 (1992).

# Effects of chemical substitution of Bi by Sb on the physical properties of $\text{NdCu}(\text{Bi}_{1-x}\text{Sb}_x)_2$ compounds

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In this work, we investigated the effect of the chemical substitution of Bi by Sb on the physical properties of the  $\text{NdCuBi}_{2-x}\text{Sb}_x$  intermetallic compounds. The samples were grown by the self-flux method. The characterization was performed using powder X-ray diffraction, magnetization as a function of field, susceptibility as a function of temperature, and specific heat measurements. The experimental data shows that the entry of Sb at the Bi site is responsible for the increment of the  $c/a$  ratio and the enhancement of the magnetic anisotropy. We believe these effects are associated with the crystalline electric field (CEF) changes at the rare-earth site caused by the chemical substitution. In this case, the Sb substitution causes a decrease in the magnetic frustration of the compound and provides a ground state wave function with predominantly planar characteristics. These effects lead to an enhancement of the Néel temperature. The CEF effects were investigated from experimental data simulations using a mean-field model that considers the CEF effects and anisotropic magnetic exchanges between the first and second neighbors. The good agreement between the model adjustments and the experimental data, adding to the results obtained and those previously reported in the literature for this family of compounds, reinforces the reliability of our proposal [1-6].

[1] C. B. R. Jesus, M. M. Piva, P. F. S. Rosa, C. Adriano, and P. G. Pagliuso, *J. of App. Phys.* **115**, 17E115 (2014).

[2] C. B. R. Jesus, M. M. Piva, P. F. S. Rosa, C. Adriano, Z. Fisk, and P. G. Pagliuso, *Physics Procedia* **75**, 618 - 624 (2015).

[3] C. Adriano, P. F. S. Rosa, C. B. R. Jesus, J. R. L. Mardegan, T. M. Garitezi, T. Grant, Z. Fisk, D. J. Garcia, A. P. Reyes, P. L. Kuhns, R. R. Urbano, C. Giles, and P. G. Pagliuso, *Phys. Rev. B* **90**, 235120 (2014).

[4] C. Adriano, P. F. S. Rosa, C. B. R. Jesus, T. Grant, Z. Fisk, D. J. Garcia, and P. G. Pagliuso, *J. of App. Phys.* **117**, 17C103 (2015).

[5] G. S. Freitas, M. M. Piva, R. Gross, C. B. R. Jesus, J. C. Souza, D. S. Christtovam, N. F. Oliveira Jr., J. B. Leão, C. Adriano, J. W. Lynn and P. G. Pagliuso, *Physical Review B* **102**, 155129 (2020).

[6] M. M. Piva, R. Tartaglia, G. S. Freitas, J. C. Souza, D. S. Christova, S. M. Thomas, J. B. Leão, W. Ratcli, J. W. Lynn, C. Lane, J. X. Zhu, J. D. Thompson, P. F. S. Rosa, C. Adriano, E. Granado and P. G. Pagliuso, *Physical Review B* **101**, 214431 (2020).

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# Large magnetocrystalline energy and electron correlations in EuIrSi<sub>3</sub>

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In crystalline materials, the magnetic field at which magnetization saturates is primarily determined from magnetocrystalline anisotropy energy, which in turn is determined from spin-orbit coupling. For the case of Eu<sup>2+</sup> ( $J=S=7/2$ ,  $L=0$ ) the magnetocrystalline anisotropy is expected to be small. We uncover a large saturation magnetic field in EuIrSi<sub>3</sub>, in which magnetization saturates at 40 T, a way larger than typical  $S$ -state magnetic systems. We conjecture that anisotropic hybridization between the  $LS$ -coupled ground state  $4f$ -orbitals and conduction electrons via enhanced electron correlations is potentially responsible for this astounding phenomenon. Moreover, the large transition temperatures together with enhanced saturation field fits altogether with the exceptional density of electronic states at the Fermi level, as already gestured by an enhancement in the Sommerfeld coefficient in specific heat ( $30.5 \text{ mJ}\cdot\text{mol}^{-1}\cdot\text{K}^{-2}$ ), large hyperfine field at the europium site (52 T) in Mössbauer spectroscopy, a large spin-disorder scattering in electrical transport ( $240 \mu\Omega \text{ cm}$ ) and the largest magnetic ordering temperature (51.8 K) among ‘113’ systems crystalizing in non-centrosymmetric BaNiSn<sub>3</sub>-type crystal structure [1-4]. Moreover, EuIrSi<sub>3</sub> exhibits a cascade of two successive phase transitions, from a paramagnet to incommensurate magnetic order at  $T_{N1}=51.8 \text{ K}$ , followed by squiring it up at  $T_{N2} = 43.1 \text{ K}$  [1]. Our high field magnetization data measured at 1.4 K reveals spin-reorientation transitions occurring at 15 T and 33 T with saturation of the magnetic moment at 40 T. The metamagnetic-transitions infer a closure of the phase boundaries corresponding to the successive phase transitions at  $T_{N1}$  and  $T_{N2}$ .

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[1] A. Maurya, P. Bonville, A. Thamizhavel, and S. K. Dhar, J. Phys.: Condens. Matter **27**, 366001 (2015).

[2] A. Maurya, P. Bonville, A. Thamizhavel, and S. K. Dhar, J. Magn. Magn. Mater. **823**, 401 (2016).

[3] A. Maurya, P. Bonville, A. Thamizhavel, and S. K. Dhar, J. Phys.: Condens. Matter **26**, 216001 (2014).

[4] X. Fabrèges, A. Gukasov, P. Bonville, A. Maurya, A. Thamizhavel, and S. K. Dhar, Phys. Rev. B **93**, 214414 (2016).



## High pressure structural and electronic instabilities in LaSb<sub>2</sub>

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LaSb<sub>2</sub> is a member of the rare-earth diantimonides which, under ambient conditions, forms in the SmSb<sub>2</sub>-type (*Cmca*) structure. It undergoes a superconductive transition below 1 K [1] and is reported to exhibit a resistive anomaly stemming from a structural distortion at 355 K [2]. This is believed to be a consequence of charge density wave (CDW) order, as evidenced by LaSb<sub>2</sub>'s large, anisotropic, linear magnetoresistance up to high fields, and a Fermi surface which is prone to nesting [1]. Further, CDW signatures were found in La<sub>0.5</sub>Ce<sub>0.5</sub>Sb<sub>2</sub> through X-ray scattering and scanning tunneling microscopy measurements [3].

Recent work on the pressure-induced structural instability in strongly-correlated isostructural compound, CeSb<sub>2</sub>, suggests the potential for a similar pressure-induced transition in LaSb<sub>2</sub> [4]. Density Functional Theory (DFT) calculations indicate that at 0 kbar the SmSb<sub>2</sub>-type structure is energetically more favourable. However, application of a moderate hydrostatic pressure of ~5 kbar favours the EuSb<sub>2</sub>-type (*P2<sub>1</sub>/m*) structure. The associated transition corresponds to a shift in the La-Sb planes and a resultant collapse of the *c*-axis.

Piston cylinder cell measurements allow for the 355 K, 0 kbar resistive anomaly to be studied under pressure, where it is found to become highly hysteretic, indicative of a first-order transition. Further, this transition is suppressed to absolute zero by ~5 kbar.

Low-temperature resistivity measurements find that the superconducting transition temperature,  $T_c$ , is highly pressure-dependent where initial pressurisation increases  $T_c$  and sharpens the transition. A peak in  $T_c$  is seen at ~2 kbar before further increases in pressure suppress it. We discuss the evolution of superconducting and normal states in LaSb<sub>2</sub> with applied pressure and their interplay with the high-temperature transition anomaly, as it is suppressed towards absolute zero.

[1] K. F. F. Fischer, N. Roth, and B. B. Iversen, *J. Appl. Phys.* **125**, 045110 (2019).

[2] J. F. DiTusa *et al.*, *J. Phys. Conf. Ser.* **273**, 012151 (2011).

[3] R. F. Luccas *et al.*, *Phys. Rev. B* **92**, 235153 (2015).

[4] C. K de Podesta *et al.*, this conference (2022).

## Strong 4d-4f correlation in multiferroic compound, Ba<sub>3</sub>HoRu<sub>2</sub>O<sub>9</sub>

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We demonstrate complex magnetism in a 6H-perovskite multiferroic system, Ba<sub>3</sub>HoRu<sub>2</sub>O<sub>9</sub>, via comprehensive magnetic and neutron powder diffraction measurements. This system undergoes long-range antiferromagnetic ordering at  $T_{N1} \sim 50$  K (with a propagation wave vector of  $K_1 = \frac{1}{2} 0 0$ ) followed by another phase transition at  $\sim 10$  K ( $T_{N2}$ ). Both Ru and Ho-moments order simultaneously below  $T_{N1}$ , followed by spin-reorientations at lower temperatures, demonstrating strong Ru(4d)-Ho(4f) magnetic correlation [1,2]. Below  $T_{N2}$  two magnetic phases co-exist, in which one magnetic phase containing an up-up-down-down structure (with a propagation wave vector of  $K_1 = \frac{1}{4} \frac{1}{4} 0$ ) is predicted to be responsible for spatial inversion symmetry breaking to govern ferroelectricity below  $T_{N2}$ . Further, we have investigated the title compound under external pressure ( $\sim 1$  GPa) through neutron diffraction. The preliminary results reveal substantial changes in the lattice and magnetic structure under the application of high pressure, which will be discussed in detail.

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[1] T. Basu, et al., Phys. Rev. Materials, 3, 114401 (2019).

[2] T. Basu, et al., Phys. Rev. B, 102, 020409(R) (2020).

# Multi-component charge order

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Charge order is a key ingredient of modern condensed matter physics. Going well beyond its role as an elementary model for emergence, it also plays a crucial role in the materials physics of many real materials, including the layered Van der Waals materials with their rich phase diagrams, as well as cuprate superconductors, which harbour fluctuating charge density waves (CDW) within their pseudogap phase. Charge order moreover plays an indispensable part in various modern applied settings, such as the proposed creation of next-generation transistors functionalizing heterostructures including CDW materials.

Despite this central role of charge order throughout material science, the study of complex charge-ordered phases is much less developed than that of, for example, the closely related magnetically ordered phases, where elaborate structures such as skyrmion lattices and helical spin waves have led to many advances in both fundamental and applied research. The fact that equally elaborate structures remain to be explored in the realm of charge order was recently highlighted by the discovery of spiral CDW phase [1,2].

Here, we will present a unified picture for constructing and exploring multi-component charge density wave phases, which allows us to simultaneously obtain an integrated understanding of various known CDW phases and predict new phases, in relation with experimental data.

[1] Europhys. Lett. 96, 67011 (2011)

[2] arXiv:2105.13195

## Magnetic study of mixed-metal germanates $\text{ErFeCuGe}_4\text{O}_{12}$

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Arsenates, phosphates, sulfates and germanates are among the important class of compounds, who are mainly studied due to its interesting magnetic properties related to super exchange interaction that involves various magnetic as well nonmagnetic pathways. Among them germanates are interesting for their rich physics as well as for their application in luminescent industries [1-2]. Recently Xu et. al. has synthesized a new magnetic germanates  $\text{ErFeCuGe}_4\text{O}_{12}$ , where all the three cation Er, Fe and Cu are magnetic in nature and orders anti-ferromagnetically at 20 K [3]. However, by detailed magnetic measurements in various protocols, we find the evidence of a new magnetic transition in  $\text{ErFeCuGe}_4\text{O}_{12}$ . In the present work detailed dc magnetization and  $^{57}\text{Fe}$  Mössbauer, measurements on a new magnetic germanates  $\text{ErFeCuGe}_4\text{O}_{12}$ , crystallizing in tetragonal structure with space group  $P4/nbm$  has been reported. Our present results establish the new magnetic transition around 12 K, along with the previously reported antiferromagnetic transition at 20 K. The metamagnetic type behavior is only observed below the new magnetic transition at 12 K. Temperature dependent  $^{57}\text{Fe}$  Mössbauer measurements corroborated with our magnetic study.

- [1] G.J. Long, G. Longworth, P. Battle, A.K. Cheetham, R.V. Thundathil, D. Beveridge, *Inorg. Chem.*, **18**, 624 (1979).
- [2] B. Forsyth, J.P. Wright, M.D. Marcos, J.P. Attfield, C. Wilkinson, *J. Phys. Condens. Matter*, **11**, 1473 (1999).
- [3] D. Xu, M. Avdeev, P. D. Battle, *Journal of Solid State Chemistry*, **269**, 107 (2019).

## Stabilization mechanisms of opposed ferroelectric states

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Perovskite oxides extend in application prospects from electronics to energy conversion and catalysis. Such abundant functionalities are a direct consequence of the rich physics emerging from the interplay of their multiple degrees of freedom. Ferroelectrics (FEs) in particular are promising to catalysis and energy conversion due to their intrinsic property of efficiently separating the electrons and holes as a requirement to stabilize a well-defined ferroelectric state. Deriving the most fundamental electronic properties of ferroelectrics as encoded in their experimental band structure is challenging due to their insulating character and surface band bending potential. Here we record for the first time the ferroelectric-dependent three-dimensional electronic structure of ferroelectric  $\text{PbZr}_x\text{Ti}_{1-x}\text{O}_3$   $x=0.2$  - PZT prepared in opposite out of plane ferroelectric states by using k-resolved soft X-ray photoelectron spectroscopy (SX-ARPES). The band structure extracted across the whole Brillouin zone reveals the distinct mechanisms involved in the stabilization of the well-defined ferroelectric state. For PZT prepared with the FE polarization  $P^+$ , pointing away from the surface, oxygen vacancies and the accompanying free electrons released from the chemical bond accumulate close to the surface to screen the depolarizing field. Opposite FE state,  $P^-$ , requires positive charge accumulation close to the interface with the substrate, and this is achieved by altering the ideal stoichiometry and creation of cation vacancies. These results clarify fundamental aspects concerning the functionality of the ferroelectrics, with implications in efficient device design.

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# Magnetic exciton in a multiferroic 2D van der Waals antiferromagnet

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Two-dimensional magnetic van der Waals materials have recently attracted significant interest due to the enormous potential in low-dimensional devices. The vdW material NiI<sub>2</sub> was reported as a multiferroic material in bulk and even in the 2d limit [1,2,3]. In our work, we demonstrate that the multiferroicity in NiI<sub>2</sub> enables the novel magnetic exciton

We observed magnetic excitons in NiI<sub>2</sub> using optical absorption and resonant inelastic X-ray scattering (RIXS). We identify this magnetic exciton arises from a transition between quantum entangled Zhang-Rice triplet (ZRT) to Zhang-Rice singlet (ZRS) state. The many-body calculation based on a configuration interaction theory supports this result. The NiI<sub>2</sub> is a second example of such an entangled quantum state following vdW antiferromagnet NiPS<sub>3</sub>, which has ZRT ground state and magnetic exciton from ZRT to ZRS transition [4].

\*This work is supported by the Leading Researcher Program of the National Research Foundation of Korea.

[1] Kurumaji, T. et. al, *Phys. Rev. B* ,**87**(1), 014429 (2013).

[2] H. Ju. et al, *Nano Lett.* **21**, 5126-5132 (2021)

[3] Song, Q. et al, *Nature* **602**, 601-605 (2022)

[4] Kang, S. et al., *Nature* **583**, 785-789 (2020)

# Reduced hysteresis and enhanced giant magnetocaloric effect in B-doped all-*d*-metal Ni-Co-Mn-Ti based Heusler materials

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Recently [1], the all-*d*-metal Ni(Co)MnTi based Heusler alloys have been found to show a giant magnetocaloric effect near room temperature and are thereby potential materials for solid-state refrigeration [2,3]. However, the relative large thermal hysteresis and the moderate ferromagnetic magnetization provide limitations for real applications. In the present study, we demonstrate that introducing interstitial B atoms within Ni<sub>36.5</sub>Co<sub>13.5</sub>Mn<sub>35</sub>Ti<sub>15</sub> alloys can effectively decrease the thermal hysteresis  $\Delta T_{hys}$  (down to 4.4 K), and simultaneously improve the saturation magnetization (maximum 40% enhancement) for low concentrations of B doping (up to 0.4 at.%). In comparison to the undoped reference material, the maximum magnetic entropy change ( $\Delta S_m$ ) for the Ni<sub>36.5</sub>Co<sub>13.5</sub>Mn<sub>35</sub>Ti<sub>15</sub>B<sub>0.4</sub> alloy shows a remarkable improvement from 9.7 to 24.3 Jkg<sup>-1</sup>K<sup>-1</sup> for an applied magnetic field change ( $\Delta\mu_0H$ ) of 5 T (30.2 Jkg<sup>-1</sup>K<sup>-1</sup> for  $\Delta\mu_0H = 7$  T). Additionally, due to the obtained low thermal hysteresis  $\Delta T_{hys}$ , the maximum reversible  $\Delta S_m^{rev}$  amounts to 18.9 Jkg<sup>-1</sup>K<sup>-1</sup> at 283 K for  $\Delta\mu_0H = 5$  T (22.0 Jkg<sup>-1</sup>K<sup>-1</sup> at 281 K for  $\Delta\mu_0H = 7$  T), which is competitive to the traditional NiMn-*X* based Heusler alloys (*X* = Ga, In, Sn, Sb). The enhancement of the magnetic moments by B doping is also observed in first-principle calculations. These calculations clarify the atomic occupancy of B (as the O-I octahedral interstitial site) and the changes in the electronic configuration. Our current study indicates that interstitial doping with a light element (boron) is an effective method to improve the magnetocaloric effect in these all-*d*-metal NiCoMnTi based magnetic Heusler compounds.

## References:

- [1] Z. Wei *et al.*, Appl. Phys. Lett **107**, 022406 (2015).
- [2] H.N. Bez *et al.*, Acta. Mater **173**, 225 (2019).
- [3] A. Taubel *et al.*, Acta. Mater **201**, 425 (2020).

# Low temperature anomalies in the mixed dysprosium-yttrium iron garnets with a connection to the magnetodielectric property of DyIG

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The occurrence of the low-temperature anomaly due to the ‘Belov point’  $T_B = 42$  K in DyIG [1] was observed in the temperature variations of some parameters pertinent to the magnetic and magneto-optical properties [2], [3]. However, such  $T_B$ -point should be well exhibited in the mixed dysprosium-yttrium iron garnets  $Dy_xY_{3-x}Fe_5O_{12}$  (or  $Dy_xY_{3-x}$ IGs) where the  $Dy^{3+}$  ions were partially replaced by the nonmagnetic  $Y^{3+}$  ions.

We report in this work, isothermal magnetizations  $M_T(H_{ex})$  measured in the 4.2-300 K range under high external DC magnetic fields  $H_{ex}$  up to 16 T applied on two single crystal samples with  $x = 1.5$  and  $2.5$  which are allowed to rotate freely (Free). The compensation temperature ( $T_{comp}$ ) was found equal to 117 and 190 K, respectively. In the range between 4.2 K and  $T_{SR}(x) = 14.62$  K, the transition temperature of the spontaneous spin reorientation  $\langle 111 \rangle \leftrightarrow \langle uuw \rangle$  [4], the curves  $M_T(H_{ex})$  versus  $H_{ex}$  are always greater in the case ‘Free’ than when  $H_{ex}$  is applied along  $\langle 111 \rangle$  whereas a total equality is found above. Anomalies appear in the temperature variations of the derivative of the spontaneous magnetization and magnetic susceptibility at  $T_{SR}(x)$  and  $T_B(x) = 42$  K  $\pm$  (few K). The Dionne’ models [5] are used to improve the  $T_B$ -formula taking into account the anisotropy of both crystal field and exchange interactions. All results are discussed in connection with the magnetodielectric property revealed before in DyIG [6, 7, 8] together with some concomitant effects due to the Schottky anomaly [2], [3] which occurs around the  $T_B$ -region.

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[1] K. P. Belov, Phys. Usp. **39**, 623 (1996).

[2] A. Boutaba, M. Lahoubi, V. Varazashvili, and S. Pu, J. Magn. Magn. Mater. **476**, 551 (2019).

[3] A. Boutaba, M. Lahoubi, V. Varazashvili, and S. Pu, J. Supercond. Nov. Magn. **32**, 3087 (2019).

[4] T. Zhu, W. Wang, M. Lahoubi, and A. Boutaba, AIP Advances **9**, 035326 (2019).

[5] G. F. Dionne, Ferrimagnetism, Chapter 4 in Magnetic Oxides, <https://doi.org/10.1007/978-1-4419-0054-8> Springer-Verlag US (2009) pp.151–199

[6] K. M. Song *et al.*, Phys. Rev. B **83**, 012404 (2011).

[7] P. D. Rogers *et al.*, Phys. Rev. B **83**, 174407 (2011).

[8] T. D. Kang *et al.*, Phys. Rev. B **86**, 144112 (2012).



## Neutron scattering studies of multiferroics based on bismuth ferrites

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Bismuth-based perovskites are ferroelectrics and also have a magnetic ordering. We have studied a temperature and external pressure dependence of a series of doped bismuth ferrites with a method of neutron diffraction as a direct method to study magnetic ordering as well as with a complementary method of X-ray diffraction at synchrotron radiation source in order to find a phase transition from rhombohedral to nonpolar orthorhombic structure and find an influence of doping and external conditions to magnetic properties of these multiferroics. An origin of magnetic interaction is discussed

# Magnetodielectric coupling as a manifestation of metamagnetic transition and structural distortion in $\text{Ba}_3\text{RRu}_2\text{O}_9$ (R = Gd, Dy)

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The 6H-perovskites  $\text{Ba}_3\text{RRu}_2\text{O}_9$  (R = Rare Earth) exhibit complex magnetism and have been extensively studied recently for their magnetodielectric (MD) properties [1,2]. Here, we present a detailed study of structural, magnetic, thermodynamic and MD properties of 6H-perovskites  $\text{Ba}_3\text{RRu}_2\text{O}_9$  (R = Gd, Dy) [3,4]. Long range Antiferromagnetic (AFM) ordering sets at  $\sim 14.8$  K and  $\sim 5.8$  K for Gd and Dy compounds respectively, which is evident from the magnetization and heat capacity studies.

The AFM ordering for  $\text{Ba}_3\text{GdRu}_2\text{O}_9$  shift towards low temperature besides showing the splitting of peak on the application of magnetic field. Low temperature magnetic isotherms for  $\text{Ba}_3\text{GdRu}_2\text{O}_9$  exhibit three metamagnetic transitions with opening of small hysteresis in different regions which are attributed to spin reorientation of AFM magnetic lattice. Entropy change corresponding to AFM ordering indicates the simultaneous alignment of both Ru and Gd moments. On the other hand  $\text{Ba}_3\text{DyRu}_2\text{O}_9$  shows two additional field dependent anomalies at  $\sim 28$  K ( $T_1$ ) and  $\sim 33$  K ( $T_2$ ) besides AFM ordering at  $\sim 5.8$  K in the heat capacity. These anomalies are feebly reflected in the derivative of magnetization curve and dielectric response as well. Low temperature crystal structures of the compound show distortion of  $\text{Ru}_2\text{O}_9$  octahedra near  $T_2$ . Our investigation suggest that  $\text{Ru}_2\text{O}_9$  is distorted at  $T_2$  which in turn forces Ru moments to exhibit magnetic correlations.

Dielectric response recorded at zero and 80 kOe field exhibits the development of MD coupling well above  $T_N$  due to presence of short-range magnetic correlations. These compounds show a large value of MD coupling in comparison to other counterparts in 6H-perovskite family. Our studies suggest that the metamagnetic transition and structural distortion in  $\text{Ru}_2\text{O}_9$  octahedra play an important role in inducing large magnetodielectric coupling in these compounds.

[1] Y. Doi *et al.*, J. Mat. Chem. C. **12**, 1792-95 (2002).

[2] T. Basu *et al.*, Phys. Rev. Mat. **3**, 114401 (2019).

[3] S. Chhillar *et al.*, J. Phys.: Cond. Matter **33**, 285801 (2021).

[4] S. Chhillar *et al.*, J. Phys.: Cond. Matter **34**, 145801 (2022).

# Magnetic properties and magnetodielectric coupling in mixed metal oxide $\text{NdCr}_{0.5}\text{Co}_{0.5}\text{O}_3$

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Mixed-metal oxides are interesting due to novel magnetic phases exhibited by them [1]. Here we report the magnetization, heat capacity and dielectric properties of  $\text{NdCr}_{0.5}\text{Co}_{0.5}\text{O}_3$  compound. X-ray diffraction studies reveal that  $\text{NdCr}_{0.5}\text{Co}_{0.5}\text{O}_3$  crystallizes in orthorhombic structure with  $Pbnm$  space group. This compound undergoes paramagnetic to antiferromagnetic transition around  $T_N \sim 106$  K due to  $\text{Cr}^{3+}$ - $\text{Cr}^{3+}$  interactions; as confirmed by dc, ac magnetisation and heat capacity measurements. The second magnetic transition due to ordering of Nd moments has been observed around  $T^* \sim 6$  K. In the heat capacity curve, a broad shoulder close to  $T^*$  is noted, which is ascribed to the Schottky effect arising from crystal field effect of  $\text{Nd}^{3+}$  cations. The temperature dependent dielectric permittivity shows anomaly around 40 K where metamagnetic transition has also been observed. The observed anomaly in dielectric permittivity gets suppressed by applying magnetic field of 80 kOe, implying the presence of magnetodielectric coupling in this compound. Additionally, double thermal relaxor behaviour above  $T_N$ , with activation energy of 0.24 eV and 0.32 eV are observed due to polaron hopping and Maxwell Wagner effect respectively.

[1] L. H. Yin *et al.*, Mater. Res. Bull. **48**, 4016 (2013)

[1] F. Bartolome *et al.*, Phys. Rev. B **62**, 2 (2000).

[2] Z. Jirak *et al.*, J. Appl. Phys. **115**, 17E118 (2014).

# Spin excitations of the high temperature transverse conical phase in multiferroic BiFeO<sub>3</sub>

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Magnetoelectric multiferroic materials with coexisting ferroelectric and magnetic orders have received much attention in recent years as they may find applications in low power consumption magnetoelectric memories and data storage devices. Among these materials, BiFeO<sub>3</sub> is a unique compound as its multiferroic phase is stable even at room temperature, which is a prerequisite of all applications. The  $S = 5/2$  spins of Fe<sup>3+</sup> ions form a non-trivial antiferromagnetic (AFM) order below  $T_N \approx 640$  K. Neutron diffraction [1] and small-angle neutron scattering (SANS) experiments showed [2] that the non-centrosymmetric crystal structure gives rise to long-wavelength cycloidal modulation of the G-type antiferromagnetic order in zero-field, characterized by the modulation vector  $\mathbf{q}$ . Kawachi et al. [3] have discovered a new magnetic phase at high temperatures: the transverse conical state, when they applied a magnetic field in the (111) plane above 150 K. This novel phase with homogenous AFM component shows remarkably strong linear magnetoelectric effect. We investigated the spin excitations of the transverse conical phase in the THz range at and above room temperature. We found several spin-wave excitations shifting with the magnetic field. We determined the selection rules of the modes for the conical as well as for the high-field canted antiferromagnetic phase. In the conical phase, we also observed directional dichroism: a non-reciprocal absorption difference, which is a finite frequency manifestation of the magnetoelectric effect. Furthermore, at high temperatures, the hysteresis at the cycloidal-conical transition becomes much broader, and the conical phase may remain (meta)stable in zero-field.

[1] I. Sosnowska, et al., J. Phys. C **15**, 4835 (1982).

[2] M. Ramazanoglu, et al., Phys. Rev. Lett. **107**, 207206 (2011).

[3] S. Kawachi, et al., Phys Rev Materials. **1**, 024408 (2017).

# Study for Physical Properties and Magnetoelectric Response of $\text{Ce}_3\text{TiSb}_5$

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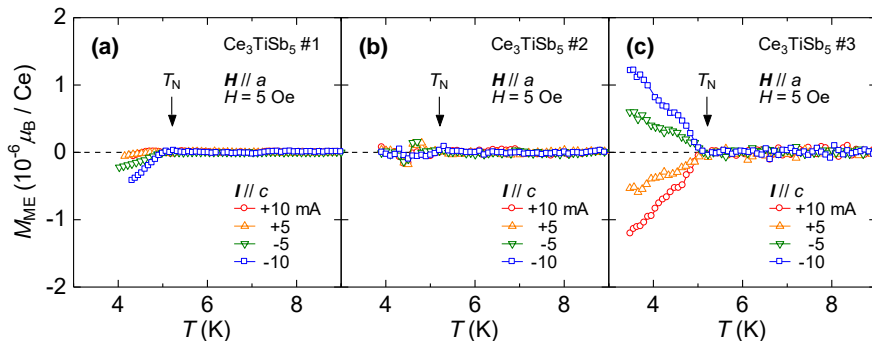
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Odd-parity multipoles have attracted great attention owing to various unique properties such as the cross-correlation phenomena [1]. An antiferromagnetic (AFM) compound with broken local inversion symmetry at magnetic ion site is an ideal system for studying odd-parity multipole ordering. Recently, current-induced magnetization ( $M_{\text{ME}}$ ) is observed on AFM compounds  $\text{UNi}_4\text{B}$  [2] and  $\text{Ce}_3\text{TiBi}_5$  [3].

$\text{Ce}_3\text{TiSb}_5$  has no local inversion symmetry at Ce site and shows an AFM ordering at  $T_N = 5.2$  K [4]. This magnetic ordering is suggested to be an incommensurate AFM ordered state from the results of neutron scattering experiment [5]. Because of this incommensurate AFM ordering, it is not expected that ferroic odd-parity multipole ordering and  $M_{\text{ME}}$  emerge in  $\text{Ce}_3\text{TiSb}_5$ . Meanwhile, there are some problems in which the anisotropy of  $M_{\text{ME}}$  is not consistent with theoretical prediction on  $\text{UNi}_4\text{B}$  and  $\text{Ce}_3\text{TiBi}_5$ . Thus, we are verifying the existence of  $M_{\text{ME}}$  even in  $\text{Ce}_3\text{TiSb}_5$ . Figures show temperature dependences of  $M_{\text{ME}}$  on several samples of  $\text{Ce}_3\text{TiSb}_5$ . In Fig. (c), the magnitude of  $M_{\text{ME}}$  is finite below  $T_N$  and is proportional to applied electric current value. These features suggest that observed  $M_{\text{ME}}$  in Fig. (c) are similar phenomena on  $\text{Ce}_3\text{TiBi}_5$  originating from the odd-parity multipole ordering. However, it is not observed clear  $M_{\text{ME}}$  in Fig. (a) and (b). Due to this large sample dependence, the reproducibility of  $M_{\text{ME}}$  is being checked continuously.

On the other hand, not only electric field but also magnetic field, pressure, and temperature are important controllable physical parameters for activating cross-correlation phenomena. Thus, it is important to proceed physical property measurements under various conditions in parallel. In order to discuss the ordered state, we will report physical properties of  $\text{Ce}_3\text{TiSb}_5$  and a reference compound  $\text{Sm}_3\text{TiSb}_5$  under magnetic field and pressure in this presentation.



**Figure:** Temperature dependences of current-induced magnetization of  $\text{Ce}_3\text{TiSb}_5$ . Figures (a) to (c) show the results of each sample on different batch.

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[1] S. Hayami *et al.*, Phys. Rev. B **98**, 165110 (2018).

[2] H. Saito *et al.*, J. Phys. Soc. Jpn. **87**, 033702 (2018).

[3] M. Shinozaki *et al.*, J. Phys. Soc. Jpn. **89**, 033703 (2020).

[4] M. Shinozaki *et al.*, J. Phys. Conf. Ser. **2164**, 012040 (2021).

[5] C. Ritter *et al.*, J. Phys. Cond. Matter. **33**, 245801 (2021).

# Impact on Ferroelectricity and Band Alignment of Gradually Grown metal on BaTiO<sub>3</sub>

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Developing a predictability electronics field based on ferro-functional materials, one need to control the ferroelectric system switching between different polarization states through bias applied to metallic contacts. This requires understanding of the growth mechanisms and electronic properties at the interface; whether the major contribution at the interface band alignment comes from the work function difference or from the ferroelectric state. Here we investigate the band alignment from the very first stages of metal deposition on BaTiO<sub>3</sub> using X-ray photoelectron spectroscopy. The band bending at metal/ferroelectric interface is given by the shift of core levels (Ba 3d, Ti 2p) as a function of the metal thickness. We show how the interface band alignment mechanism is influenced both by the work function difference and by the polarization orientation. Combining the measurements with *ab-initio* calculations, we envisage the complex microscopic picture of metal/ferroelectric interface formation, elucidating the growth mechanism, valence alteration, ferroelectric-dependent electrostatic potential and thickness – dependent compensation mechanisms of ferroelectricity with application in non-volatile memory storage devices, in ferroelectric capacitors, sensors and actuators.

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## Magnetoelectric coupling of rare-earth orthotantalates

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Quantum multiferroic materials form a new and emerging area of physics where one expects to find emergence of novel quantum phases induced by subtle coupling between spin and charge degrees of freedom at low temperatures [1-2]. Experimental study of such phenomena is limited by the lack of model materials where magnetism and dielectric properties can be tuned using magnetic fields at low temperatures.

In a recent breakthrough, we found that TbTaO<sub>4</sub> exhibits enhancement in dielectric response below 2 K on application of magnetic field, indicating magnetoelectric coupling. Previously, using susceptibility and heat capacity measurements we showed that TbTaO<sub>4</sub> orders at  $T_N = 2.25$  K; powder neutron diffraction (PND) was used to solve the magnetic structure, which is A-type antiferromagnetic [3]

These rare-earth tantalates LnTaO<sub>4</sub> (Ln = Y, La-Lu) are of wide interest as a result of their luminescent, proton-conducting, oxide-ion-conducting and dielectric properties [4]. In addition, in the monoclinic M polymorph of the tantalates with Ln = Nd-Er, the magnetic Ln<sup>3+</sup> ions are arranged on an elongated diamond lattice [3]. Materials with such a magnetic lattice have the potential for unusual magnetic behaviour owing to the interplay of the crystal electric field with the (possibly competing) J<sub>1</sub> and J<sub>2</sub> interactions: for example, LiYbO<sub>2</sub> has incommensurate spiral order [5].

[1] C. Morice et al., Physical Review B 96(24), 245104 (2017).

[2] A. Narayan et al., Nature Materials 18(3), 223-228 (2019).

[3] N. D. Kelly et al., Physical Review Materials 6, 044410 (2022).

[4] P. Sarin et al., J. Am. Ceram. Soc. 97(10), 3307 (2014).

[5] M. M. Bordelon et al., Physical Review B 103(1), 014420 (2021).

# Manifestation of Hund's rule effect in the optical conductivity near the metal-insulator transition of NiS<sub>2</sub>

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In recent decade, the effect of Hund's coupling  $J$  in multi-band system has been studied with much attention. Hund's coupling affects the energy scale of the system by nature, as can be understood from that it determines the energy scale of spin Kondo screening. This phenomena was prominent in non-half-filled and non-singly-filled multi-orbital case, but recently, the similar Hund's physics has also been observed evidently in half-filled NiS<sub>2-x</sub>Se<sub>x</sub> system. [1] It was demonstrated that the kink in the spectral function is produced by Hund  $J$ , and it is closely interconnected to the quasiparticle coherence-incoherence crossover temperature. Here, we will present our study of pressurized NiS<sub>2</sub>, in correlated metallic phase, to investigate the Hund's physics in half-filled multi-band system. We will visit how the energy scales are determined, and in particular we will examine how Hund's effect is manifested in the optical conductivity. The anomalous frequency dependence away from the Drude behavior was observed, and it is produced by the kink in the spectral function. Our results propose that half-filled multi-band system can be also a good ground to study rich fundamentals such as the Hund's physics.

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[1] Bo Gyu Jang *et al.*, Nat. Commun. **12**, 1208 (2021).



## Disorder study of the anomalous magnetoresistance in $2H\text{-NbSe}_2$

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The transition metal dichalcogenide (TMDC)  $2H\text{-NbSe}_2$  has been studied extensively, due to the interesting interplay that exists between the superconducting (SC) and charge density wave (CDW) states and their evolution with pressure [1] and disorder [2]. Another peculiarity of the normal state of  $2H\text{-NbSe}_2$  is its robust  $H$ -linear magnetoresistance (MR) that is found to persist over a wide field range [3]. Such a quadrature form of the MR, with a high-field slope that is relatively independent of temperature, has become a very active topic of research in the field of strongly correlated electron systems [4], though its origin remains elusive [5]. Of particular interest is the notion that the  $H$ -linear MR may be insensitive not only to temperature but also to disorder. This behaviour is in marked contrast to the strong (Kohler-like) scaling of the MR as a function of disorder found in more conventional metals.

A recent disorder study showed that  $T_c$  is robust to disorder as long as the CDW itself is not destroyed [2]. The effects of disorder on the magneto-resistive properties of  $2H\text{-NbSe}_2$  in the normal metallic state, however, have not yet been investigated. In this work, we perform a study of the high-field MR of bulk  $2H\text{-NbSe}_2$  single crystals with varying degrees of disorder and map the evolution of  $T_c$ ,  $H_{c2}$  as well as the form of the MR as a function of the residual resistivity.

[1] Moulding, O. *et al.*, *Phys. Rev. Res.* **2**, 043392 (2020).

[2] Cho, K. *et al.*, *Nat Commun* **9**, 2796 (2018).

[3] Naito, M. and Tanaka, S. *J. Phys. Soc. Japan* **51**, 228-236 (1982).

[4] Alexandradinata, A. *et al.*, *arXiv:2010.00584* (2020).

[5] Hinlopen, R. D. H. *et al.*, *arXiv:2201.03292* (2022).

## Novel metallic phases in pyrochlore iridates

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Emergent electronic phases are expected in pyrochlore iridates  $A_2Ir_2O_7$  ( $A$  = rare earth, post transition metal ions) as a result of electronic correlations, and strong spin orbit coupling. Further, the interpenetrating corner-shared tetrahedral network between  $A$  and  $Ir$  site in the cubic structure leads to geometric frustration. The ground state properties of the members of this family are highly sensitive to the choice of  $A$ -site ion as well as chemical and/or physical pressure, where an effective increase in the  $A$ -site ionic radius leads to a metallic ground state [1].

Interestingly, the metallic members, despite minor structural variations, exhibit distinct novel ground states [2][3]. Here, we compare the electronic and magnetic properties of pristine as well as doped metallic pyrochlore iridates and comment on the driving forces that lead to such a variety of novel metallic phases in this family of compounds.

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[1] N. P. Armitage, *Rev. Mod. Phys.* 90, 015001(2018).

[2] Tokiwa *et al.*, *Nat. Mater.* 13, 356–359 (2014).

[3] P. Telang *et al.*, *Phys. Rev. B* 99, 201112(R) (2019).

## Low temperature criticality at YbCo<sub>2</sub> compound

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The electrical resistivity, magnetization and specific heat data of YbCo<sub>2</sub> are reported for the first time. The effective magnetic moment observed from Curie-Weiss fit shows not only expected Yb<sup>3+</sup> magnetic moment, observed by microscopic measurement in Ref [1], but also Co magnetic moment  $\sim 2.94 \mu_B$  in paramagnetic state. Despite these observations, the magnetic ordering is not observed down to 0.3 K. On the other hand, Kondo screening is manifested in electrical resistivity and specific heat data by low temperature anomalies. Unfortunately, Kondo temperature can't be easily determined because of divergence of  $C_p/T$  and  $\chi$  which point to critical behavior in low temperature state.

Application of magnetic field revealed tiny metamagnetic-like transition in magnetization curves and well pronounced field induced transition-like anomaly in all measurements. By the increasing of magnetic field, the anomaly shifts to higher temperatures and points to ferromagnetic character. It is opposite than for many of Yb-based heavy fermion compounds which are antiferromagnets and possess quantum criticality.

The YbCo<sub>2</sub> seems to be complex case which contains Kondo effect, Yb 4*f*-local moments and Co 3*d*-itinerant moments. The presentation will discuss origin of the observed properties in comparison with other Yb-based compounds.

[1] O. V. Chernysheva, A. P. Menushenkov, A. V. Tsvyashchenko, L. N. Fomicheva, A. A. Ivanov, A. V. Kuznetsov, *Journal of Physics: Conference Series* **747**, 012028 (2016)

# Elemental Dilution Effect on the Ultrasonic Dispersion of the Non-Kramers Systems $Y_{1-x}Pr_xIr_2Zn_{20}$

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$PrT_2X_{20}$  ( $T = Ir, Rh, V,$  and  $Ti$ ;  $X = Al, Zn,$  and  $Cd$ ) systems, crystallizing in the cubic  $CeCr_2Al_{20}$ -type structure ( $Fd\bar{3}m, O^7_h$ , No. 227), show exotic phenomena originating from a non-Kramers doublet ground state in the crystalline electric field (CEF), in which the  $\Gamma_3$ -type electric quadrupoles can be active [1, 2]. The compound  $PrIr_2Zn_{20}$  shows antiferroquadrupolar order and superconducting transitions at  $T_Q = 0.11$  K and  $T_c = 0.05$  K, respectively [1]. Y dilution has systematically been studied to search for the experimental evidence for the quadrupolar Kondo effect [3, 4]. Recently, we found that the elastic constant  $(C_{11}-C_{12})/2$ , corresponding to a  $\Gamma_3$ -symmetry multipolar response, on  $Y_{0.63}Pr_{0.37}Ir_2Zn_{20}$  (Pr-37%) shows a  $+\sqrt{T}$  dependence below 0.15 K, which corresponds to a quadrupolar Kondo "lattice" model [5, 6]. In addition, we discovered an ultrasonic dispersion (UD) for the Pr-37% system between 0.15 and 2 K [6], the origin of which is not clarified yet.

Here, we present results of our ultrasonic measurements on  $Y_{1-x}Pr_xIr_2Zn_{20}$  for several Pr concentrations ( $x = 0, 0.08, 0.37,$  and  $1.0$ ) and report how the UD changes with Pr concentration. We observed UDs only for the higher Pr concentrations ( $x = 0.37$  and  $1.0$ ). In the presentation, we discuss the magnetic-field dependence of the UDs and propose that the origin of the UD in the Pr-37% system is related to  $\Gamma_3$  quadrupolar degrees of freedom in the CEF ground state.

- [1] T. Onimaru *et al.*, Phys. Rev. Lett. **106**, 177001 (2011).
- [2] A. Sakai and S. Nakatsuji, J. Phys. Soc. Jpn. **80**, 063701 (2011).
- [3] Y. Yamane *et al.*, Phys. Rev. Lett. **121**, 077206 (2018).
- [4] T. Yanagisawa *et al.*, Phys. Rev. Lett. **123**, 067201 (2019).
- [5] A. Tsuruta and K. Miyake, J. Phys. Commun. **6**, 015006 (2022).
- [6] R. Hibino *et al.*, SCES Poster: 141089, 2020/21 (Brazil, online).

# Feasibility of Two-channel Kondo Effect in Diluted Nd Compounds $Y_{1-x}Nd_xCo_2Zn_{20}$ for $x < 0.1$

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The two-channel Kondo model for a single impurity is one of the scenarios to understand non-Fermi liquid (NFL) behavior of both the magnetic susceptibility  $\chi(T)$  and the magnetic specific heat  $C_m(T)$ , and the presence of the residual entropy of  $(1/2)R\ln 2$  at  $T=0$  [1,2]. Recently, manifestation of the NFL behavior due to the two-channel Kondo effect was theoretically proposed in cubic Nd compounds with a  $\Gamma_6$  doublet state [3]. In such a compound  $NdCo_2Zn_{20}$ , the electrical resistivity  $\rho(T)$  shows a convex downward curvature on cooling below 4 K [4], which is ascribed to the two-channel Kondo effect.

We have measured the magnetic and transport properties of diluted Nd compounds  $Y_{1-x}Nd_xCo_2Zn_{20}$  for  $x < 0.1$  to extract single-site NFL properties. The paramagnetic Curie temperature estimated from the  $\chi(T)$  data for  $T < 1.8$  K is almost zero, indicating negligible magnetic interaction between the Nd moments. On cooling below 0.2 K, both  $\chi(T)$   $C_m(T)/T$  increase as  $-\ln T$ . These NFL behaviors agree with those theoretically predicted by the single-site two-channel Kondo model [2]. Furthermore, the magnetic entropy remains as  $(3/4)R\ln 2$  at 0.08 K. Therefore, the residual entropy of  $(1/2)R\ln 2$  could conceal itself below 0.08 K as proposed for the two-channel Kondo scenario.

[1] P. Nozières and A. Blandin, *J. Phys. (Paris)* **41**, 293 (1980).

[2] P. D. Sacramento and P. Schlottmann, *Phys. Rev. B* **43**, 13294 (1991).

[3] T. Hotta, *J. Phys. Soc. Jpn.* **86**, 083704 (2017).

[4] R. Yamamoto *et al.*, *J. Phys. Soc. Jpn.* **88**, 044703 (2019).

# Revealing an anisotropic electronic scattering rate in the “non-metallic” metal FeCrAs through the Hall effect

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FeCrAs presents a curious puzzle in the physics of metals: at room temperature the magnitude of its resistivity is that of a typical metal, but yet, due to a strange, non-metallic temperature dependence (from above 800 K to below 100 mK) [1], the low temperature resistivity becomes unusually large. Along with this oddity in its electronic transport, FeCrAs plays host to frustrated Cr moments that reside on a distorted Kagomé lattice. We believe that magnetic frustration leads to stiff magnetic fluctuations that survive far beyond the energy scale of its antiferromagnetic ordering temperature,  $T_N \sim 125$  K [2]. As such, it is tempting to draw a connection between the exotic electronic scattering and robust magnetic fluctuations.

Here, we report the results of ordinary Hall effect measurements between  $\sim 2$  and 300 K in FeCrAs. We observe a strong temperature dependence in the low-field Hall coefficient below  $T_N$ , where two sign-reversals occur as the sample is cooled. By relating these results to prior optical conductivity experiments [3], we suggest that there are two different scattering rates in FeCrAs: one that is responsible for the “non-metallic” temperature dependence across the large temperature range, and the other, an anisotropic (i.e. momentum-dependent) scattering rate that is much more sensitive to the static magnetic order.

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[1] W. Wu *et al.*, Europhys. Lett. **85**, 17009 (2009).

[2] K. W. Plumb *et al.*, Phys. Rev. B **97**, 184431 (2018).

[3] A. Akrap *et al.*, Phys. Rev. B **90**, 125115 (2014).

# Density fluctuations and generalized plasma waves in layered cuprates

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Recent Electron Energy Loss Spectroscopy experiments in layered cuprates have shown that the strange metal, i.e. the peculiar, and still not completely understood, metallic phase occurring in optimally doped cuprates, does not have plasmons. Indeed, the density-density response function measured in such phase displays, as a function of the energy, a featureless momentum-independent peak, which cannot be linked to a well defined collective mode [1,2]. A theoretical explanation of such feature is still lacking. Another fundamental issue regards the description of density fluctuations in such systems, which usually relies on the RPA renormalization of the free-electron density-density function with respect to the Coulomb potential, which mediates the electrostatic interaction between electrons. Whilst this approximation is good for isotropic systems, where longitudinal (plasmons) and transverse (e.m. waves) degrees of freedom are uncoupled, it breaks down in layered systems, where the anisotropy along the out-of-plane direction causes longitudinal and transverse degrees of freedom to get mixed, so that the role of the electron-electron interaction is not exhausted by the electrostatic potential alone and retardation effects come in [3].

In this talk I will discuss how a complete description of density fluctuations in layered systems, including both Coulomb interaction and retardation effects, can be achieved, and how this general framework predicts not only the emergence of two generalized plasmons, with mixed longitudinal and transverse character, in the density spectrum [3], but also the peculiar density-spectrum shape found experimentally in the strange-metal phase.

[1] Mitrano, M., et al. "Anomalous density fluctuations in a strange metal." *Proceedings of the National Academy of Sciences* 115.21 (2018): 5392-5396.

[2] Husain, Ali A., et al. "Crossover of charge fluctuations across the strange metal phase diagram." *Physical Review X* 9.4 (2019): 041062.

[3] Gabriele, F., C. Castellani, and L. Benfatto. "Generalized plasma waves in layered superconductors." *arXiv preprint arXiv:2110.06772* (2021).

# ANOTHER EXACT GROUND STATE OF A 2D QUANTUM ANTIFERROMAGNET

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We present the exact dimer ground state of a quantum antiferromagnet on the maple-leaf lattice [1]. A coupling anisotropy for one of the three inequivalent nearest neighbor bonds is sufficient to stabilize the dimer state. Together with the Shastry-Sutherland Hamiltonian [2], we show that this is the only other model with an exact dimer ground state for all two-dimensional lattices with uniform tilings.

[1] P. Ghosh, T. Müller, R. Thomale, arXiv:2112.05137 (2021).

[2] B. S. Shastry and B. Sutherland, Physica B+C 108, 1069 (1981)



## ***Weak Ferromagnetism and Spin Reorientation in Antiferroelectric BiCrO<sub>3</sub>***

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BiCrO<sub>3</sub> is an antiferroelectric perovskite known to exhibit an unconventional spin reorientation transition between antiferromagnetic structures, accompanied by a large jump in weak ferromagnetism [1,2,3,4,5]. Using a combination of neutron powder diffraction, magnetometry, and symmetry analysis, we confirm the dominant G-type antiferromagnetic order below  $T_N = 111$  K and identify the magnetic phase transition with a spontaneous rotation of Cr<sup>3+</sup> moments from the *b*-axis to a particular direction in the *ac*-plane. We demonstrate the role of antiferroelectric displacements produced by the Bi<sup>3+</sup> lone-pair electrons and octahedral rotations in establishing spin canting via the antisymmetric Dzyaloshinskii-Moriya interaction. Our analysis naturally explains the dramatic increase in net magnetization on cooling, and remarkably, the antiferroelectrically-induced spin canting elucidated in the high temperature magnetic phase is, to the best of our knowledge, unprecedented in perovskite systems.

- [1] C. Darie *et al.*, Solid State Sciences **12**, 660 (2010).
- [2] S. Niitaka *et al.*, Solid State Ionics **172**, 552 (2004).
- [3] A. A. Belik *et al.*, Chemistry of Materials **20**, 3765 (2008).
- [4] C. V. Colin *et al.*, Physical Review B **85**, 224103 (2012).
- [5] J. P. Cardoso *et al.*, Inorganic Chemistry **59**, 8727 (2020).

## Hidden Charge Order in an Iron Oxide Square-Lattice Compound

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Since the discovery of charge disproportionation in the FeO<sub>2</sub> square-lattice compound Sr<sub>3</sub>Fe<sub>2</sub>O<sub>7</sub> by Mößbauer spectroscopy more than fifty years ago, the spatial ordering pattern of the disproportionated charges has remained “hidden” to conventional diffraction probes, despite numerous x-ray and neutron scattering studies. We have used neutron Larmor diffraction and Fe K-edge resonant x-ray scattering to demonstrate checkerboard charge order in the FeO<sub>2</sub> planes that vanishes at a sharp second-order phase transition upon heating above 332 K. Stacking disorder of the checkerboard pattern due to frustrated interlayer interactions broadens the corresponding superstructure reflections and greatly reduces their amplitude, thus explaining the difficulty of detecting them by conventional probes.

# Field-induced spin freezing and low-temperature heat capacity of $\text{Ho}_2\text{Zr}_2\text{O}_7$

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Spin ice materials are the model systems that have a zero-point entropy as  $T \rightarrow 0$  K, owing to the frozen disordered states [1-2]. Here, we chemically alter the well-known spin ice  $\text{Ho}_2\text{Ti}_2\text{O}_7$  by replacing Ti sites with isovalent but larger Zr ion. Unlike the  $\text{Ho}_2\text{Ti}_2\text{O}_7$  which is a pyrochlore material,  $\text{Ho}_2\text{Zr}_2\text{O}_7$  crystallizes in disordered pyrochlore structure [2]. We have performed detailed structural, ac magnetic susceptibility and heat capacity studies on  $\text{Ho}_2\text{Zr}_2\text{O}_7$  to investigate the interplay of structural disorder and frustrated interactions. The zero-field ground state exhibits large magnetic susceptibility and remains dynamic down to 300 mK without showing Pauling's residual entropy. The dynamic state is suppressed continuously with the magnetic field and freezing transition evolves ( $\sim 10$  K) at a field of  $\sim 10$  kOe. We have further analyzed the low-temperature heat capacity and discussed the error arising from the estimation of nuclear contribution in Holmium based system. Our studies suggest that the alteration of chemical order and local strain in  $\text{Ho}_2\text{Ti}_2\text{O}_7$  prevents the development of spin ice state and provides a new material to study the geometrical frustration based on the structure.

## References:

- [1] A. P. Ramirez *et al.*, Nature **399**, 333 (1999).
- [2] M. J. Harris *et al.*, Phys. Rev. Lett. **79**, 2554 (1997).
- [3] Sheetal *et al.*, arXiv:2110.04555v1 (under review)

# Anomalous Hall Effect in Single-Crystals of the Noncollinear Antiferromagnet Mn<sub>3</sub>Pt

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Mn<sub>3</sub>Pt is one of the first noncollinear antiferromagnets where an intrinsic anomalous Hall effect was predicted based on the spin structure in  $k$  space [1], rather than a bulk ferromagnetism. However, experimental demonstration requires polarizing the antiferromagnetic domains, which does not appear to be possible in bulk single crystals with laboratory-achievable magnetic fields. The magnetism has been polarized in epitaxial thin films, where epitaxial strain lifts the cubic symmetry of the crystal [2], but with epitaxial strain it is not possible to perfectly release the applied strain. In the present work, we measure the anomalous Hall effect of bulk single crystals of Mn<sub>3</sub>Pt under uniaxial stress. We demonstrate that uniaxial stress induces a field-polarizable anomalous Hall effect. We show in addition that the anomalous Hall effect remains “locked-in” when the stress is released, indicating that it is a consequence of the non-collinear antiferromagnetic spin arrangement rather than a strain-induced magnetic moment.

[1] H. Chen *et al.*, Phys. Rev. Lett. **112**, 017205 (2014).

[2] Z. Liu *et al.*, Nat. Electron **1**, 172 (2018).

# Majorana-mediated spin transport in Kitaev model at finite temperatures

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Spin transport mediated by the itinerant Majorana fermions is one of the interesting phenomena realized in the Kitaev model, where the spin excitations flow in the quantum spin liquid (QSL) region without exciting local spin moments [1]. This phenomenon should be observed in the system with edges (see Figure). After the magnetic-field pulse is introduced to one of the edges, spin moments are excited in the other edge region under the magnetic field although no spin moments are induced in the middle QSL region. This nontrivial spin transport originates from the fact that the  $S=1/2$  spins are fractionalized into the itinerant and localized Majorana fermions in the Kitaev system. It is known that these Majorana fermions have distinct energy scales, leading to the double peaks in the specific heat [2]. Therefore, it is unclear how stable the Majorana-mediated spin transport in the Kitaev model is against thermal fluctuations.

In this study, we examine finite-temperature spin dynamics in the Kitaev model by means of the thermal pure quantum state method [3]. At low temperatures, the spin excitation propagates in a similar way to that for the ground state. At intermediate temperatures, larger oscillations in the spin moments are induced in the other edge, compared to the results at the ground state. At higher temperatures, excited localized Majorana fermions disturb the coherent motion of the itinerant Majorana fermions, which suppresses the spin propagation. Our results demonstrate an important role of thermal fluctuations in the Majorana-mediated spin transport [4].

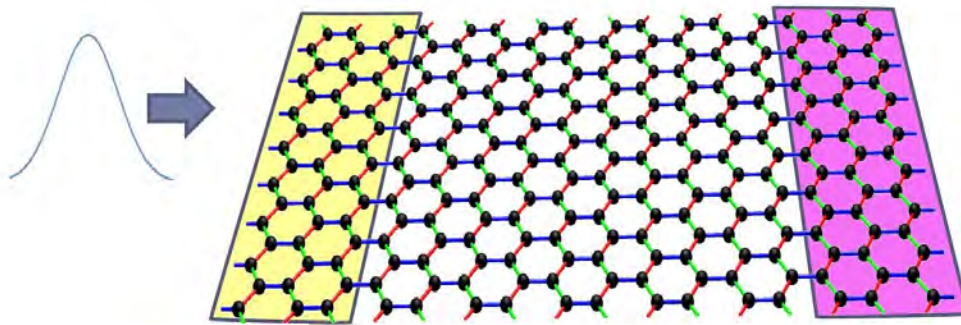


Figure: Kitaev model on the honeycomb lattice with two edges. The lattice is composed of three regions. The static magnetic field is applied in the right region. In the bulk, no magnetic field is applied. Pulsed magnetic field is introduced in the left region.

[1] T. Minakawa, Y. Murakami, A. Koga, and J. Nasu, Phys. Rev. Lett. 125, 047204 (2020).

[2] J. Nasu, M. Udagawa, and Y. Motome, Phys. Rev. B 92, 115122 (2015).

[3] S. Sugiura, and A. Shimizu, Phys. Rev. Lett. 108, 240401 (2012).

[4] H. Taguchi, Y. Murakami, and A. Koga, arXiv:2201.12517.

# Singlet ground state in the alternating spin-1/2 chain compound NaVOAsO<sub>4</sub>

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We present the synthesis and a detailed investigation of structural and magnetic properties of polycrystalline NaVOAsO<sub>4</sub> by means of x-ray diffraction (XRD), magnetization, electron spin resonance (ESR), and <sup>75</sup>As nuclear magnetic resonance (NMR) measurements as well as density-functional band structure calculations[1]. Temperature-dependent magnetic susceptibility, ESR intensity, and NMR line shift could be described well using an alternating spin-1/2 chain model[2] with the exchange coupling  $J/k_B \approx 52$  K and an alternation parameter  $\alpha \approx 0.65$ . From the high-field magnetization measured at  $T = 1.5$  K, the critical field of the gap closing is found to be  $H_C \approx 16$  T, which corresponds to the zero-field spin gap of  $\Delta_0/k_B \approx 21.4$  K. Both NMR shift and spin-lattice relaxation rate show an activated behaviour at low temperatures, further confirming the singlet ground state. The spin chains do not coincide with the structural chains, whereas the couplings between the spin chains are frustrated. Because of a relatively small spin gap, NaVOAsO<sub>4</sub> is a promising compound for further experimental studies under high magnetic fields.

[1] U. Arjun, *et al.*, Phys. Rev. B **99**, 014421 (2019).

[2] D. C. Johnston *et al.*, Phys. Rev. B **61**, 9558 (2000).

# Magnetization plateaux in the distorted triangular quantum antiferromagnet $\text{Cs}_2\text{CoBr}_4$

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Single-crystal neutron scattering experiments and low-temperature thermodynamics revealed the competition of two frustration mechanisms in the 2D quantum antiferromagnet  $\text{Cs}_2\text{CoBr}_4$ . Key actors are the alternation of single-ion planar anisotropy direction of the individual magnetic  $\text{Co}^{2+}$  ions, and their arrangement in a distorted triangular lattice fashion. In particular, uniquely oriented Ising-type anisotropy emerges from the competition of easy-plane ones, and magnetic fields applied along this axis stabilize a cascade of five ordered phases [1]. The magnetic structure of 3 of the 5 phases is identified and shown to be of purely quantum origin. Spin dynamics is further investigated through multiplexing neutron scattering.

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[1] K. Povarov, L. Facheris, *et al.*, Phys. Rev. Res. **2**, 043384 (2020).

## Anisotropic magnetic phase diagram of geometrically frustrated iridate $\text{Ca}_5\text{Ir}_3\text{O}_{12}$

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The crystal structure of iridium oxide  $\text{Ca}_5\text{Ir}_3\text{O}_{12}$  is a hexagonal with noncentrosymmetric space group of  $P-62m$  (No. 189) [1]. In the structure, 1D chains of the edge-sharing  $\text{IrO}_6$  octahedra form triangular lattices in the  $c$ -plane.  $\text{Ca}_5\text{Ir}_3\text{O}_{12}$  has a mixed valance state of  $\text{Ir}^{4+}$  ( $5d^5$ ) and  $\text{Ir}^{5+}$  ( $5d^4$ ) with the average valence of Ir ions is +4.67. This situation can lead to the geometrical frustration of charge on both the triangular lattice in  $c$ -plane and 1D chains along the  $c$ -axis.  $\text{Ca}_5\text{Ir}_3\text{O}_{12}$  shows a nonlinear conductivity along  $c$ -axis [2].  $\text{Ca}_5\text{Ir}_3\text{O}_{12}$  indicates successive second order phase transitions at  $T_N=7.8$  K and  $T_s=105$  K [1,3]. The phase transition at  $T_N$  is magnetic ordering [1-4]. The phase transition at  $T_s$  comes from electric toroidal multipole ordering belongs to the irreducible representation  $A_2$  [5]. The magnetic ordering at  $T_N$  is not clear still.

We report the magnetic phase diagram of  $\text{Ca}_5\text{Ir}_3\text{O}_{12}$  obtained by magnetization measurements on a single crystal. The magnetization perpendicular to  $c$ -axis shows a kink at magnetic order. On the other hand, the magnetization along  $c$ -axis shows upward bend at magnetic order. From these results, the magnetic phase diagram is anisotropic;  $T_N$  perpendicular to  $c$ -axis is suppressed with increasing magnetic field and  $T_N$  along  $c$ -axis continues to increase to at least 7 T. This anomalous behavior can be reported in low dimensional spin systems and magnetic field induced multipole ordering such as  $\text{CeB}_6$  and  $\text{PrPb}_3$ . We will present the results in detail and discuss the anisotropic magnetic phase diagram.

[1] M. Wakeshima *et al.*, Solid State Commun. **125**, 311 (2003).

[2] K. Matsuhira *et al.*, J. Phys. Soc. Jpn. **87**, 013703 (2018).

[3] G. Cao *et al.*, Phys. Rev. B **75**, 134402 (2007).

[4] I. Franke *et al.*, Phys. Rev. B **83**, 094416 (2011).

[5] H. Hanate *et al.*, J. Phys. Soc. Jpn. **90**, 063702 (2021).



## Pressure-tuning of $\text{Li}_2\text{IrO}_3$ Kitaev materials

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Quantum spin liquid behavior in the Kitaev honeycomb model, characterized by quantum entanglement and fractionalized excitations, is subject of extensive investigation. Here, we present magnetization measurements under pressure for honeycomb  $\alpha\text{-Li}_2\text{IrO}_3$  and hyper-honeycomb  $\beta\text{-Li}_2\text{IrO}_3$  to determine their temperature-pressure phase diagrams.

A delicate interplay between magnetism and dimerization is revealed in both compounds [1,2]. Upon applying hydrostatic pressure,  $T_N$  is slightly enhanced before it abruptly disappears at around 1.8(1.5) GPa in  $\alpha(\beta)\text{-Li}_2\text{IrO}_3$ . At around (1.2)1.4 GPa, a signature of structural dimerization—a step in the magnetic susceptibility—appears and shifts to higher temperatures upon further compression. The temperature dependence of dimerization in  $\alpha\text{-Li}_2\text{IrO}_3$  can be well reproduced on the *ab initio* level by taking into account lower phonon entropy in the nonmagnetic phase. Furthermore, our *ab initio* calculations suggest a subtle difference of the dimerization in two compounds: The dimerization in  $\alpha\text{-Li}_2\text{IrO}_3$  is complete while the one observed in  $\beta\text{-Li}_2\text{IrO}_3$  at low pressure is partial which features a fraction of magnetic  $\text{Ir}^{4+}$  sites. Our study reveals a common thread in the interplay of magnetism and dimerization in pressured Kitaev materials.

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[1] Bin Shen *et al.*, Phys. Rev. B **104**, 134426 (2021).

[2] Bin Shen *et al.*, Phys. Rev. B **105**, 054412 (2022).

# $\pi$ -orbital order coupled to the spin-1/2 pyrochlore lattice in alkali-sesquioxides

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Here we report that mixed-valence alkali sesquioxides  $A_4O_6$  ( $A =$  alkali metal) represent a novel class of compounds showing orbital degeneracy coupled to the spin-1/2 pyrochlore lattice frustration. These anionic mixed-valence compounds with a simple cubic structure at high temperatures first undergo a structural transition to the tetragonal phase just below the room temperature that is accompanied by a metal-to-insulator transition reminiscent of the Verwey transition [1,2]. The low-temperature charge-ordered phase comprises non-magnetic  $O_2^{2-}$  and magnetic  $O_2^-$  ( $S = 1/2$ ) anions, where the latter form a geometrically frustrated pyrochlore lattice. Extensive muon spin relaxation, electron paramagnetic resonance (EPR) and nuclear magnetic resonance (NMR) over broad temperature and magnetic field range show that the coupling between spin and orbital degrees of freedom dimerizes the lattice of  $Rb_4O_6$ , triggers the long-range orbital ordering and opens up a spin-gap in the excitation spectrum. The spin-gap initially decreases with increasing magnetic field but the quantum phase transition to the condensed triplet phase at the critical field of 14.2 T is absent due to the Dzyaloshinskii-Moriya interaction. Nevertheless, the quantum critical fluctuations of the spin-dimer state are clearly revealed from the nuclear spin-lattice relaxation rates in this field range [6]. The  $A_4O_6$  family thus emerges as one of the very few  $\pi$ -electron systems showing coupling of the orbital order to a geometrically frustrated spin lattice and yielding a quantum spin-dimer state.

[1] P. Adler, P. Jeglič, D. Arčon, et al., *Sci. Adv.* 4, eaap7581 (2018).

[2] T. Knaflič, D. Arčon et al., *Phys. Rev. B* 101, 024419 (2020).

[3] Ž. Gosar, D. Arčon et al., submitted (2022).

# Field-induced magnetic order and quantum spin liquid on planar triangular lattice, $\text{TlYbSe}_2$

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In classic spin-1/2 triangular-lattice antiferromagnets, the ground state is known to be a  $120^\circ$  order in the Heisenberg model [1]. For the delafossites,  $\text{NaYbCh}_2$  ( $\text{Ch} = \text{O}, \text{S}, \text{Se}$ ) have already evidenced the emergence of a quantum spin liquid (QSL) state accompanied by field-induced order [2, 3, 4, 5]. The QSL state is most probably due to complex spin-orbit entangled exchange between the nearest and next nearest Yb ions on the triangular layer. Upon the application of a magnetic field, the classical  $120^\circ$  order is recovered. Here, we present  $\text{TlYbSe}_2$  as a new member of this group of QSL materials. For  $\text{TlYbSe}_2$  polycrystalline sample, the magnetization curves up to 30 T and the specific heat at low temperatures allow to determine the magnetic phase boundaries, which are reminiscent of those of  $\text{NaYbSe}_2$  but extend to higher temperatures close to 2 K. This result implies the QSL state is more stable in  $\text{TlYbSe}_2$  than in  $\text{NaYbSe}_2$  due to the larger magnetic anisotropy. Our NMR and ESR studies revealed a large magnetic anisotropy due to the larger size of the monovalent ion Tl. For  $\text{NaYbCh}_2$ , NMR studies were performed on Na which locate at interlayer of  $\text{YbCh}_6$ . Here, we present Se-NMR data. Se is directly incorporated into the superexchange. Based on the analysis of the powder spectra, the  $H//c$  and  $H\perp c$  components could be extracted, and the relaxation rates of each component were selectively measured. These relaxation rates are rather anisotropic. Clear evidence for field-induced order is also given by Se-NMR.

[1] R. Kaneko *et al.*, J. Phys. Soc. Jpn. **83**, 093707 (2014).

[2] M. Baenitz *et al.*, Phys. Rev. B **98**, 220409(R) (2018).

[3] K. Ranjith *et al.*, Phys. Rev. B **100**, 224417 (2019).

[4] K. Ranjith *et al.*, Phys. Rev. B **99**, 180401(R) (2019).

[5] B. Schmidt *et al.*, Phys. Rev. B **103**, 214445 (2021).

# Low temperature spin dynamics in the $S = 2$ kagome magnet $\text{Fe}_4\text{Si}_2\text{Sn}_7\text{O}_{16}$ : An AC susceptibility, NMR and $\mu\text{SR}$ study

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$\text{Fe}_4\text{Si}_2\text{Sn}_7\text{O}_{16}$  displays an undistorted kagome lattice of  $\text{Fe}^{2+}$  ( $3d^6$ ,  $S = 2$ ) ions. We present results of DC-pulse-field magnetisation up to 50 T, Nuclear Magnetic Resonance (NMR), AC-susceptibility and muon-spin-resonance ( $\mu\text{SR}$ ) measurements down to 19 mK on powder sample of  $\text{Fe}_4\text{Si}_2\text{Sn}_7\text{O}_{16}$ . The magnetization measurement at 2 K excludes the presence of strong Ising anisotropies. In the temperature range of 3 K to 8 K, the maximum in the real part of AC-susceptibility shows frequency-dependent shift and indicates the presence of spin-glass-like behavior. An additional frequency-independent magnetic regime is observed below  $T = 0.7$  K. The transverse-field and zero-field  $\mu\text{SR}$  results show the onset of static magnetic correlations below 30 K. Further, below  $T = 1$  K, ZF-relaxation rate remains relatively constant which indicates the presence of persistence spin dynamics down to 19 mK. Based on the longitudinal field decoupling  $\mu\text{SR}$  studies, we discuss the coexistence of static and dynamic magnetic correlations below 250 mK. From our combined AC-susceptibility and  $\mu\text{SR}$  results, we demonstrate that in  $\text{Fe}_4\text{Si}_2\text{Sn}_7\text{O}_{16}$  the dynamic magnetic correlations increase below 250 mK and a possible gapless-spin-liquid behavior is achieved.

# Competing states in the two-dimensional Kondo-Necklace model on the triangular lattice

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The interplay between Kondo effect, indirect magnetic interaction and geometrical frustration is studied in the two-dimensional Kondo-Necklace model on the triangular lattice. Using infinite projected entangled pair states (iPEPS), we compute the ground state as a function of the antiferromagnetic local Kondo interaction  $J_K$  and the Ising-type direct spin-spin interaction  $I_z$ .

Geometrical frustration is shown to lead to an extended region in the  $J_K - I_z$  phase-diagram in between the two paradigmatic phases of the Doniach competition: (i) a disordered phase consisting of local spin-singlets at strong  $J_K$  and (ii) a magnetically ordered phase at weak  $J_K$ . This intermediate region is dominated by a strong competition of two different ground state candidates. The first candidate exhibits partial Kondo screening (PKS) which was also found in previous studies (see Ref. [1,2]). Here, one-third of the spins are screened in a local Kondo singlet while the other two-thirds form a long-range ordered antiferromagnetic state. The second candidate is an entirely new phase for heavy fermion systems. It is characterized by a strongly polarized central spin in each hexagon and its anti-parallel, weakly polarized neighbors. We name it central spin (CS) phase.

[1] Y. Motome, K. Nakamikawa, Y. Yamaji & M. Udagawa, Phys. Rev. Lett. **105**, 036403 (2010)

[2] M. Aulbach, F. Assaad & M. Potthoff, Phys. Rev. B **92**, 235131 (2015).

# Classification of anisotropic exchange interactions in momentum space toward understanding multiple- $Q$ instability

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Multiple- $Q$  magnetic states, such as a skyrmion crystal, become a source of unusual transport phenomena and dynamics [1]. Recent theoretical and experimental studies have clarified that such multiple- $Q$  states ubiquitously appear under different crystal structures [2]. One of the origins of the multiple- $Q$  states is anisotropic exchange interactions that arise from the relativistic spin-orbit coupling. The most familiar example is the *antisymmetric* Dzyaloshinskii-Moriya interaction in noncentrosymmetric materials. Meanwhile, recent studies in centrosymmetric magnets have opened up the possibility of a further variety of multiple- $Q$  states by *symmetric* anisotropic exchange interactions [3]. However, there have been few studies focusing on the symmetric anisotropic exchange interactions despite various types of them depending on the crystal symmetry. To understand the role of the anisotropic exchange interactions on the multiple- $Q$  states, it is highly desired to perform a systematic investigation for various space groups irrespective of the centrosymmetric and noncentrosymmetric crystals.

Toward a systematic understanding of the multiple- $Q$  instability in various crystal systems, we classify the symmetric and antisymmetric anisotropic exchange interactions by performing magnetic representation analysis [4]. We find six symmetry rules to obtain anisotropic exchange interactions in momentum space, which are regarded as an extension of Moriya's rule in real space. According to the rules, one can systematically construct the effective spin model in any primitive lattices, which is useful for the systematic understanding of the multiple- $Q$  instability. The foundation of the systematic understanding will stimulate further exploration of exotic multiple- $Q$  states in materials with the spin-orbit coupling.

- [1] A. Fert, V. Cros, and J. Sampaio, *Nat. Nanotechnol.* **8**, 152 (2013).
- [2] Y. Tokura and N. Kanazawa, *Chem. Rev.* **121**, 2857 (2020).
- [3] S. Hayami and Y. Motome, *J. Phys.: Condens. Matter* **33**, 443001 (2021).
- [4] R. Yambe and S. Hayami, arXiv:2202.09744 (2022).

# Unusual thermal Hall effect in the 3d cobalt Kitaev system $\text{Na}_2\text{Co}_2\text{TeO}_6$

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Kitaev physics has recently attracted attention in condensed matter for its anticipated novel quantum spin liquid state. The thermal transport measurement is crucial for probing the novel features of charge-neutral quasiparticles. In this letter, we report a significant thermal Hall effect in  $\text{Na}_2\text{Co}_2\text{TeO}_6$  (NCTO), a Kitaev spin liquid candidate, when the magnetic field is applied along the out-of-plane direction of the honeycomb plane. The thermal conductivity ( $\kappa_{xx}$ ) and thermal Hall conductivity ( $\kappa_{xy}$ ) in NCTO reveals distinct magnetic field dependences below and above the Neel temperature ( $T_N$ ) of 27 K. For  $T > T_N$ ,  $\kappa_{xx}$  has a monotonic decrease in the field dependence, while  $\kappa_{xy}$  persists up to  $T^* = 150$  K. On the other hand, both  $\kappa_{xx}$  and  $\kappa_{xy}$  exhibit complex field dependence for  $T < T_N$ . We found that the experimental  $\kappa_{xy}$  data are inconsistent with reported magnon or phonon Hall scenarios. Comparing the similar thermal properties of NCTO and  $\alpha\text{-RuCl}_3$ , we suggest that both NCTO and  $\alpha\text{-RuCl}_3$  would share the origin for thermal Hall effect.

# Engineering skyrmion crystal in centrosymmetric ferromagnetic/antiferromagnetic bilayers

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A magnetic skyrmion crystal (SkX), which is a topologically nontrivial swirling spin texture, has attracted attention as an origin of emergent electromagnetic phenomena. As a stabilization mechanism of the SkX, it was well known that the Dzyaloshinskii-Moriya (DM) interaction that is present in noncentrosymmetric systems plays a key role [1]. Indeed, the first discovery of the SkX has been achieved in the chiral magnet MnSi [2]. On the other hand, recent studies indicated other mechanisms to stabilize the SkX, such as short-range competing exchange interactions [3] and effective long-range exchange interactions mediated by itinerant electrons [4]. Since these mechanisms are applicable to centrosymmetric lattice structures without the DM interaction, they have been thought to be possible origins of the SkXs in centrosymmetric magnets, such as Gd<sub>2</sub>PdSi<sub>3</sub> [5] and GdRu<sub>2</sub>Si<sub>2</sub> [6].

In the present study, we investigate another scenario to stabilize the SkX by considering the role of the layered structure in the centrosymmetric systems. Specifically, we consider a bilayer triangular lattice system with different types of interactions: One is characterized by the ferromagnetic exchange interaction and the other is the antiferromagnetic exchange interaction. By performing the variational calculations and Monte Carlo simulations, we find that such a bilayer system can host the SkX in the ground state under an external magnetic field and an easy-axis anisotropy depending on the strength of the interlayer exchange interaction. We discuss the ground-state magnetic phase diagram by changing the temperature and the interlayer exchange interaction.

[1] N. Nagaosa and Y. Tokura, *Nat. Nanotech.* **8**, 899 (2013).

[2] S. Mühlbauer *et al.*, *Science*, **323**, 915 (2009).

[3] T. Okubo *et al.*, *Phys. Rev. Lett.* **108**, 017206 (2012).

[4] S. Hayami *et al.*, *Phys. Rev. B* **95**, 224424 (2017).

[5] T. Kurumaji *et al.*, *Science* **365**, 914 (2019).

[6] N. D. Khanh *et al.*, *Nat. Nanotechnol.* **15**, 444 (2020).



# NMR evidence against spin-nematic nature of the presaturation phase in frustrated magnet $\text{SrZnVO}(\text{PO}_4)_2$

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The spin-nematic state in frustrated magnets is an exotic state that could arise from the Bose-Einstein condensation of the two-magnon bound state. Such spin nematic states have been predicted in frustrated ferro-antiferromagnetic one- and two-dimensional spin systems close to their saturated phase [1,2]. Here, we investigate a frustrated two-dimensional ferro-antiferromagnet  $\text{SrZnVO}(\text{PO}_4)_2$ , in which a pre-saturation phase was identified recently above 13.75 T while the full saturation is observed above 14.06 T [3]. Motivated by the possibility that the pre-saturation phase in  $\text{SrZnVO}(\text{PO}_4)_2$  could be a spin-nematic one, and the fact that the corresponding magnetic field values ( $\sim 14$  T) are easily accessible, we have performed a detailed  $^{31}\text{P}$ -nuclear magnetic resonance (NMR) study of the related static (NMR spectra) and dynamic (spin-lattice relaxation rate,  $1/T_1$ ) properties. Both of these provide evidence against the spin-nematic nature of the phase, and we thereby define the two corresponding clear-cut NMR criteria [4].

More importantly, we have provided the first extensive set of  $1/T_1$  (measuring low-energy spin dynamics) data at and above the critical field, and fully explained its low-temperature behavior as a sum of the critical and the one-magnon excitation contribution. The corresponding analysis can be taken as an archetypal description for the one-magnon condensation.

- [1] N. Shannon *et al.*, Phys. Rev. Lett. **96**, 027213 (2006).
- [2] H. T. Ueda and T. Momoi, Phys. Rev. B **87**, 144417 (2017).
- [3] F. Landolt *et al.*, Phys. Rev. B **104**, 224435 (2021).
- [4] K. M. Ranjith *et al.*, arXiv:2112.12603

# Colossal spin-phonon coupling and Higgs-amplitude fluctuations in $\text{Nd}_2\text{Ru}_2\text{O}_7$

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Strongly correlated 4d pyrochlore compounds provide exceptional platforms to realize a multitude of different states of matter, which are governed by an intimate interplay of orbital, spin, and lattice degrees of freedom [1]. Critical phenomena and dynamical fluctuations arise in the vicinity where two different states of matter meet. Recently, we succeeded in growing for the first time sizable single crystals of  $\text{Nd}_2\text{Ru}_2\text{O}_7$ , a member of the pyrochlore ruthenates. At  $T_N = 147$  K,  $\text{Nd}_2\text{Ru}_2\text{O}_7$  orders magnetically as evidenced by magnetic susceptibility and specific heat. Our temperature- and polarization-resolved Raman spectroscopic study unveils dramatic phonon anomalies associated with this transition, pointing to colossal spin-phonon coupling. In addition, a regime of significant fluctuations marked by quasi-elastic scattering exists within the ordered phase. A new low-energy mode emerges out of these fluctuations at  $T^* = 100$  K, alluding to Higgs-type amplitude fluctuations of the magnetic moment. The two-fold symmetry of this amplitude mode, incompatible with the underlying crystal structure, hints towards nematic order in  $\text{Nd}_2\text{Ru}_2\text{O}_7$ , which is corroborated by the observation of concomitant lattice instabilities.

[1] Gao *et al.*, *Front. Phys.* **15(6)**, 63201 (2020).

# Exchange anisotropy and field-induced magnetic order of the triangular-lattice delafossites $\text{NaYbCh}_2$ ( $\text{Ch} = \text{O}, \text{S}, \text{Se}$ )

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The Yb-based delafossites  $\text{NaYbCh}_2$  ( $\text{Ch} = \text{O}, \text{S}, \text{Se}$ ) are planar triangular-lattice spin liquids with a trigonal crystal structure (space group  $R\bar{3}m$ ). In these compounds, a strong spin-orbit coupling combined with crystalline-electric-field effects leads to a pronounced magnetic anisotropy and a pseudospin-1/2 spin-liquid ground state of the  $\text{Yb}^{3+}$  ions at low temperatures. The chalcogen series provides the possibility for tuning the interlayer distance and the associated exchange couplings by changing the chemical composition. The absence of magnetic long-range order at zero field down to lowest temperatures is strongly suggestive of a quantum spin-liquid ground state. Relaxation measurements by means of  $\mu\text{SR}$  and NMR have shown persistent strong quantum fluctuations down to 100 mK at low magnetic fields. Based on specific-heat and magnetization experiments, we have observed magnetic order for applied fields exceeding 2 T perpendicular to  $c$  for all three compounds. This is confirmed microscopically by  $^{23}\text{Na}$  NMR. For in-plane fields of several tesla, a plateau-like feature in the magnetization indicates an up-up-down spin arrangement [1-3]. Furthermore, our measurements up to fields of 30 T allow to probe the saturation fields and polarized moments and, thus, the determination of the anisotropic exchange couplings [4].

[1] M. Baenitz *et al.*, Phys. Rev. B **98**, 220409(R) (2018)

[2] K. M. Ranjith *et al.*, Phys. Rev. B **99**, 180401(R) (2019)

[3] K. M. Ranjith *et al.*, Phys. Rev. B **100**, 224417 (2019)

[4] B. Schmidt *et al.*, Phys. Rev. B **103**, 214445 (2021)

## Magnetic field induced magnetic disorder in honeycomb lattice, $Tb_5Si_3$

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The magnetism of  $Tb_5Si_3$ , a hexagonal  $Mn_5Si_3$ -type compound, has been shown to be exotic more than a decade ago due to a huge positive magnetoresistance at a critical field, in the magnetically ordered state below 69 K [1]. To understand this anomaly, a neutron diffraction study of  $Tb_5Si_3$  was carried out in external magnetic fields ( $H$ ).

We find that, as the sample is cooled towards 69 K, magnetic peaks appear at  $\sim 100$  K without any well-defined phase transition and the magnetic structure could be explained in terms of an antiferromagnetic commensurate propagation vector  $k(0, 0, 1/4)$  with moments lying in the  $ab$ -plane. As the temperature is further decreased, a strong antiferromagnetic peak appears due to the presence of an incommensurate  $k = (0, 0, \pm\sim 0.47)$  which persists down to 2K. With increasing  $H$  at 2K, the magnetic structure remains incommensurate till up to  $H \sim 40$  kOe. However, at 60 kOe, just above the critical field, the magnetic structure could be described in terms of multiple propagation vectors (i.e., magnetic disorder) comprised of weakened incommensurate component and additional commensurate components. Viewing together these results with the suppression of magnetic features in magnetic susceptibility and heat-capacity at high-fields, this honeycomb lattice could be the first example of Kitaev-like spin-liquid behaviour among rare-earths and RKKY controlled magnetic systems. This magnetic disorder explains the positive magnetoresistance [1].

[1] S. N. Jammalamadaka *et al.*, Phys. Rev. B **79**, 060403(R) (2009); N. Mohapatra *et al.*, Solid State Commun. **151**, 1340 – 1343 (2011); K. Mukherjee *et al.*, J. Phys. Condens. Matter **23**, 206002 (2011).

# Quantum Monte Carlo simulations of generalized Kitaev models: applications to $\alpha$ -RuCl<sub>3</sub>

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We introduce a phase pinning approach in the realm of the auxiliary field quantum Monte Carlo (QMC) algorithm that mitigates the severity of the negative sign problem inherent to Monte Carlo methods of frustrated spin systems [1]. This allows us to access high-temperature thermodynamic and dynamical properties of the aforementioned systems and, for instance, carry out exact QMC simulations in a window of temperatures relevant to experiments for various frustrated magnets. The generalized Kitaev models describe frustrated spin systems which, among other spin orders, support a  $Z_2$  spin-liquid phase. It is of present interest due to its relation to layered iridates and  $\alpha$ -RuCl<sub>3</sub>. We use our method to carry out extensive simulations of thermodynamic properties under magnetic fields in generalized Kitaev models describing  $\alpha$ -RuCl<sub>3</sub>, and discuss the characteristic feature in the field-angle dependence of the magnetic susceptibility, the specific heat as well as the magnetotropic coefficient. Our numerical results are of experimental relevance and allow for comparison with recent measurements of the magnetotropic coefficient for  $\alpha$ -RuCl<sub>3</sub> [2].

[1] T. Sato and F. F. Assaad, Phys. Rev. B. 104, L081106 (2021).

[2] K. A. Modic et al., Nat. Phys. 17, 240-244 (2021).

# Angle-resolved magnetoresistance in strongly anisotropic quantum magnet $\text{TmB}_4$

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Precise angle-resolved magneto-resistance (ARMR) measurements in various magnetic fields enabled to create illustrative distributions of  $\Delta\rho/\rho(\varphi, H)$  in  $\text{TmB}_4$ , where  $\varphi$  is the angle between the samples  $c$  axis and applied magnetic field  $H$ . These distributions reveal the charge transport anisotropy in this strongly Ising anisotropic quantum antiferromagnet with a geometrically frustrated Shastry-Sutherland lattice exhibiting fractional magnetization plateaus [1]. While in the paramagnetic region  $\Delta\rho/\rho(\varphi, H)$  reaches its maxima for  $H \perp c$ , below Néel temperature  $T_N = 11.7$  K is the situation different. Here the main MR features appear for  $H \parallel c$ , i.e. along the easy axis of magnetic anisotropy, and correspond to magnetic phases [2] and phase transitions between them. Expressive are above all the features (maxima) related with the scattering of conduction electrons on spin magnetic structure related with fractional magnetization plateaus. With increasing  $\varphi$  MR anomalies shift to higher fields. Above the field of magnetic saturation, moreover, significant MR maxima have been observed at certain angles which correspond to specific directions in the crystal lattice, what is pointing to field directions in which the scattering of conduction electrons on the magnetic structure is the highest. Thus, ARMR appears to be a sensitive experimental tool reflecting the angular dependence of the interplay between charge carriers and magnetic structure as a function of temperature and applied magnetic field.

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[1] K. Siemensmeyer *et al.*, Phys. Rev. Lett. **101**, 177201 (2008).

[2] S. Gabani *et al.*, Acta Phys. Pol. A **113**, 227 (2008).

# Magnetic field-temperature phase diagrams and spin excitation spectra for topological multiple- $Q$ magnetic orders

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Multiple- $Q$  magnetic orders are magnetically ordered states composed of superpositions of multiple spin helices or spin density waves, as represented by two-dimensional skyrmion lattices and three-dimensional hedgehog lattices. Such magnetic orders have been observed in various substances in recent years, and attracted much attention due to their unique magnetic, transport, and optical properties associated with topology and emergent electromagnetic fields of noncoplanar spin textures. However, it is not fully understood yet how such multiple- $Q$  magnetic orders are stabilized under keen competition with other magnetic orders. To address this issue, we investigate the magnetic field-temperature phase diagrams by the exact method of the steepest descent [1] and the spin excitation spectra by the standard linear spin-wave theory [2] for effective spin models with long-range interactions mediated by conduction electrons. The phase diagrams show drastic changes depending on the form of the interactions and the direction of the external magnetic field, in which for example we find triple- $Q$  and sextuple- $Q$  orders appear only at finite temperature. Moreover, the excitation spectra tell that uniaxial anisotropy in the interactions manifests itself in the dynamical spin structure factor: a strong intensity in the transverse components to the characteristic wave number of the spin helix appears only when the helical wave vector and the corresponding easy axis are perpendicular to each other. Our findings could be useful not only to deduce the stabilization mechanism but also to understand the phase transitions and related quantum phenomena in the magnetic metals hosting multiple- $Q$  magnetic orders.

[1] Y. Kato and Y. Motome, arXiv:2202.04407 (2022).

[2] Y. Kato, S. Hayami, and Y. Motome, Phys. Rev. B **104**, 224405 (2021).

# Engineering antiferromagnetic skyrmions and antiskyrmions at metallic interfaces

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We identify a mechanism to convert skyrmions and antiskyrmions into their antiferromagnetic (AFM) counterparts via interface engineering. The key idea is to combine properties of an antiferromagnet and a spin-orbit (SO) coupled metal. Utilizing hybrid Monte Carlo (HMC) simulations for a generic microscopic electronic Hamiltonian for the interfacial layers, we explicitly show the emergence of AFM skyrmions and AFM antiskyrmions. We further show that an effective spin Hamiltonian provides a simpler understanding of the results. We discuss the role of electronic itinerancy in determining the nature of magnetic textures, and demonstrate that the mechanism also allows for a tuning of antiskyrmion size without changing the SO coupling. The derived effective spin Hamiltonian from Dresselhaus SOC modified double exchange model is given by,

$$H_{\text{eff}} = - \sum_{\langle ij \rangle} D_{ij}^{x(y)} f_{ij}^{x(y)} + J_{\text{AF}} \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - h_z \sum_i S_i^z,$$
$$f_{ij}^{x(y)} = \frac{1}{\sqrt{2}} \left[ t_{x(y)}^2 \{1 + \mathbf{S}_i \cdot \mathbf{S}_j\} - (+) 2t\lambda \hat{x}(\hat{y}) \cdot \{\mathbf{S}_i \times \mathbf{S}_j\} + \lambda^2 \{1 - \mathbf{S}_i \cdot \mathbf{S}_j + 2\{\hat{x}(\hat{y}) \cdot \mathbf{S}_i\}\{\hat{x}(\hat{y}) \cdot \mathbf{S}_j\}\} \right]^{1/2}.$$

$J_{\text{AF}}$  denotes the AFM coupling between localized moments. While  $D_{ij}^{x(y)}$  can, in principle, be  $ij$  and electronic filling ( $n_e$ ) dependent, it has been shown that  $D_{ij}^{x(y)} \equiv D_0$  is a very good approximation to study the magnetic phase diagrams.

[1] D. S. Kathyat, A. Mukherjee, and S. Kumar, Phys. Rev. B 104, 184434 (2021).

[2] A. Mukherjee, D. S. Kathyat, and S. Kumar, Phys. Rev. B 105, 075102 (2022).



# From quantum spin liquid to long range order in the distorted kagome compound, $Y_3Cu_9(OH)_{18}OCl_8$

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Quantum spin liquids are novel magnetic states of matter characterized by the absence of phase transition down to  $T=0$  K, macroscopic entanglement and emergent fractionalized excitations. The quest for materials realizing such states recently yielded a new family of interesting kagome compounds resulting from the substitution of  $Zn^{2+}$  by  $Y^{3+}$  in the archetypal herbertsmithite  $ZnCu_3(OH)_6Cl_2$ . The initial aim was to charge dope a quantum spin liquid and to reduce the possibility of exchange with the magnetic  $Cu^{2+}$  ions. While charge doping is not successful, the new materials  $YCu_3(OH)_6O_xCl_{3-x}$  ( $x = 0, 1/3$ ), sometimes coined Y-kapellasite, do not show measurable dilution of the magnetic lattice and provide us with new variations of the kagome structure. The  $x = 0$  compound features a perfect kagome geometry and a strong Dzyaloshinskii-Moriya anisotropy which drives a  $q = 0$  long range order below 15 K [1]. Here, we present a detailed study using NMR,  $\mu$ SR and neutron scattering techniques of the  $x = 1/3$  counterpart which materializes an original anisotropic kagome lattice with 3 different nearest neighbor interactions.

NMR and neutron diffraction studies demonstrate the occurrence of a definite structural transition at  $\sim 33$  K and a weaker one at  $\sim 15$  K. These transitions occur at very small scale (change in structure factor  $\sim 9\%$ ) due to change in only hydrogen positions in the crystals.

Further, our results provide clear evidence for a magnetic transition at  $\sim 2.1$  K from complementary experimental methods in contrast to the dynamical ground state reported for powder samples [2] but in line with the theoretical prediction of a  $(1/3,1/3)$  long range order [3]. From  $\mu$ SR, the ground state in Y-Kapellasite ( $x = 1/3$ ) appears to be rather short range ordered with a low frozen moment value.

[1] A Zorko et al , Physical Review B, **99** (21), 214441 (2019)

[2] Quentin. et al , Phys. Rev. Materials, **3** (7), 074401 (2019)

[3] Hering et al , npj Comput Mater **8**, 10 (2022).

## Quantum magnetism of ferromagnetic spin dimers in $\alpha$ -KVOPO<sub>4</sub>

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Magnetism of the spin-1/2  $\alpha$ -KVOPO<sub>4</sub> is studied by thermodynamic measurements, <sup>31</sup>P nuclear magnetic resonance, neutron diffraction, and density-functional band-structure calculations [1]. Ferromagnetic Curie-Weiss temperature of  $\theta_{\text{CW}} \approx 15.9$  K and the saturation field of  $\mu_0 H_s \approx 11.3$  T suggest the predominant ferromagnetic coupling augmented by a weaker antiferromagnetic exchange that leads to a short-range order below 5 K and the long-range antiferromagnetic order below  $T_N \approx 2.7$  K in zero field. Magnetic structure with the propagation vector  $\mathbf{k} = (0, 1/2, 0)$  and the ordered magnetic moment of  $0.58 \mu_B$  at 1.5 K exposes a non-trivial spin lattice where strong ferromagnetic dimers are coupled antiferromagnetically [2]. The reduction in the ordered magnetic moment with respect to the classical value ( $1 \mu_B$ ) indicates sizable quantum fluctuations in this setting, despite the predominance of ferromagnetic exchange. We interpret this tendency toward ferromagnetism as arising from the effective orbital order in the folded chains of the VO<sub>6</sub> octahedra.

[1] P. K. Mukharjee, K. Somesh, K. M. Ranjith, M. Baenitz, Y. Skourski, D. T. Adroja, D. Khalyavin, A. A. Tsirlin, and R. Nath, *Phys. Rev. B* **104**, 224409 (2021).

[2] F. Sapiña, J. R. guez Carvajal, M. J. Sanchis, R. I. nez, A. Beltrán, and D. Beltrán, *Solid State Comm.* **74**, 779 (1990).

## Revealing the Impact of Interchain Exchange Interactions on the Magnetic Quasiparticles in a Tomonaga-Luttinger Liquid

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The quasi-one-dimensional spin- $\frac{1}{2}$  magnet  $\text{SrCo}_2\text{V}_2\text{O}_8$  is a rare testbed for studying the Tomonaga-Luttinger liquid (TLL) spin dynamics inherent in the one-dimensional quantum Heisenberg-Ising XXZ model [1, 2]. Current understanding on the complex TLL modes in this system, including the psinon-psinons, psinon-antipsinons and Bethe strings, is based on a simplified theory which only takes into account the intrachain exchange interactions [1]. The interchain exchange interactions, on the other hand, are neglected because they are considered to be ‘perturbative’.

Recently, we have reported that the psinon-antipsinon excitations in the magnetic-field-induced TLL state of  $\text{SrCo}_2\text{V}_2\text{O}_8$  exhibit a strong in-plane dispersion [3], contradicting the hypothesis that the interchain exchange is negligible. In order to understand these observations, we have performed a systematic inelastic neutron scattering investigation on the psinon-antipsinons as a function of magnetic field, temperature and momentum transfer. When the temperature increases, the psinon-antipsinons at the antiferromagnetic zone centers are profoundly softened and damped, while those at the ferromagnetic zone centers only get damped. Moreover, the damping is stronger at the ferromagnetic zone centers at fields probed. In this talk, we will present and discuss these observations, which firmly confirm the critical impact of interchain exchange interactions on the magnetic quasiparticles in the TLL state.

[1] A. K. Bera *et al.*, Nat. Phys. 16, 625 (2020).

[2] L. Shen *et al.*, New J. Phys. 21, 073014 (2019).

[3] L. Shen *et al.*, Phys. Rev. Research 4, 013111 (2022).

# Crystal structure, electronic properties, and unusual antiferromagnetism in tetragonal CeLiBi<sub>2</sub>

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We report the discovery of CeLiBi<sub>2</sub> and investigate its magnetic and electronic properties with bulk single crystal measurements and elastic neutron powder diffraction. CeLiBi<sub>2</sub> crystallizes in the  $P4/nmm$  space group and is the first example of a crystal in the CeTX<sub>2</sub> ( $T$  = transition metal,  $X$  = pnictogen) family with an alkali cation replacing the transition metal  $T$ . In this family, the magnetic ground state is closely linked to the crystalline electric field ground state derived from splitting the  $J = 5/2$  Ce<sup>3+</sup> spin orbit coupled manifold and have shown exciting phenomena such as quantum criticality [1-2], successive metamagnetic transitions [3], and nematic order [4]. From anisotropic magnetic susceptibility measurements on CeLiBi<sub>2</sub>, we show that the local Ce moment contains a  $\Gamma_6$  crystalline electric field ground state doublet and exhibits long range magnetic order below  $T_N = 3.4$  K. Antiferromagnetism combined with a  $\Gamma_6$  doublet is unusual for the CeTX<sub>2</sub> materials family as all of the other  $\Gamma_6$  doublet materials are ferromagnetic [5]. We further find a subtle hard axis metamagnetic transition at 2 T in thermal expansion, magnetization, and resistivity measurement along with quantum oscillations comprised of light 0.05  $m_e$  carriers that extend to around  $T = 30$  K. The complex interplay of magnetic order and electronic character are tracked with field-dependent resistivity, magnetization, and thermal expansion measurements.

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[1] S. Araki, N. Metoki, A. Galatanu, E. Yamamoto, A. Thamizhavel, Y. Ōnuki, *Phys. Rev. B*, **69**, 024408 (2003).

[2] L. Balicas, S. Nakatsuji, H. Lee, P. Schlottmann, T.P. Murphy, Z. Fisk, *Phys. Rev. B*, **72**, 064422 (2005).

[3] S.M. Thomas, P.F.S. Rosa, S.B. Lee, S.A. Parameswaran, Z. Fisk, J. Xia, *Phys. Rev. B*, **93**, 075149 (2016).

[4] S. Seo, X. Wang, S.M. Thomas, M.C. Rahn, D. Carmo, F. Ronning, E.D. Bauer, R.D. dos Reis, M. Janoschek, J.D. Thompson, R.M. Fernandes, P.F.S. Rosa, *Phys. Rev. X*, **10**, 011035 (2020).

[5] K.E. Avers, P.A. Maksimov, P.F.S. Rosa, S.M. Thomas, J.D. Thompson, W.P. Halperin, R. Movshovich, A.L. Chernyshev, *Phys. Rev. B*, **103**, L180406 (2021).

## Magnetic ground state in semiconducting Yb-based compounds with a zigzag-chain structure

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Ce and Yb compounds were recently identified as effective spin-1/2 antiferromagnets when the spin and orbital degeneracy of the Ce<sup>3+</sup> and Yb<sup>3+</sup> ions is lifted to the Kramers doublets. Eventually the low-temperature behaviors of the compounds can be regarded as arising from the effective spin-1/2 ground state. YbCuS<sub>2</sub> is one of such Yb-based compounds. YbCuS<sub>2</sub> is a magnetic semiconductor with Yb zigzag chains along the *a*-axis [1]. From the magnetic susceptibility, the first excited state was shown to be well separated from the crystalline electric field ground state by an energy gap of  $\Delta \sim 300$  K [3]. At zero magnetic field  $H = 0$ , the specific heat exhibits a sharp peak at  $T_0 = 0.95$  K, suggesting a phase transition [2, 3]. Since  $T_0$  is much lower than the Weiss temperature and the peculiar magnetic anomalies are observed under magnetic fields, the non-trivial ground state induced by the frustration effect is anticipated [3]. To investigate low-temperature magnetic state, we performed the <sup>63/65</sup>Cu-nuclear quadrupole resonance (NQR) measurements, and found metallic-like excitation at low temperatures, which cannot be explained by conventional magnetic semiconductors [4,5].

To investigate the origin and properties of the novel gapless excitation observed in YbCuS<sub>2</sub>, we have studied a related compound YbAgSe<sub>2</sub>, which has the same structure as YbCuS<sub>2</sub> [6] and shows a similar *H-T* phase diagram [7]. We have performed <sup>77</sup>Se-NMR on YbAgSe<sub>2</sub> down to low temperatures.

In this presentation, we show the NMR results on YbAgSe<sub>2</sub> and discuss the unique properties of the Yb zigzag-chain systems.

[1] L. D. Gulay and I. D. Olekseyuk, *J. Alloys Compd.* **402**, 89 (2005).

[2] Y. Ohmagari *et al.*, *JPS Conf. Proc.* **30**, 011167 (2020).

[3] Y. Ohmagari *et al.*, *J. Phys. Soc. Jpn.* **89**, 093701 (2020).

[4] F. Hori *et al.*, arXiv:2201.07563, (2022).

[5] F. Hori *et al.*, *J. Phys.: Conf. Ser.*, in press.

[6] M. Julien-Pouzol and M. Guittard, *Ann. Chim.* **8**, 139 (1973).

[7] S. Mizutani *et al.*, *J. Phys.: Conf. Ser.*, in press.

# Collinear order in the spin-5/2 triangular-lattice antiferromagnet $\text{Na}_3\text{Fe}(\text{PO}_4)_2$

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We set forth the structural and magnetic properties of the frustrated spin-5/2 triangle lattice antiferromagnet  $\text{Na}_3\text{Fe}(\text{PO}_4)_2$  examined via x-ray diffraction, magnetization, heat capacity, and neutron diffraction measurements on the polycrystalline sample [1]. No structural distortion was detected from the temperature-dependent x-ray diffraction down to 12.5 K, except a systematic lattice contraction. The magnetic susceptibility at high temperatures agrees well with the high-temperature series expansion for a spin-5/2 isotropic triangular lattice antiferromagnet with an average exchange coupling of  $J/k_B \simeq 1.8$  K rather than a one-dimensional spin-5/2 chain model. This value of the exchange coupling is consistently reproduced by the saturation field of the pulse field magnetization data. It undergoes a magnetic long-range order at  $T_N \simeq 10.4$  K. Neutron diffraction experiments elucidate a collinear antiferromagnetic ordering below  $T_N$  with the propagation vector  $k = (1, 0, 0)$ . An intermediate value of frustration ration ( $f \simeq 3.6$ ) reflects moderate frustration in the compound which is corroborated by a reduced magnetic moment  $\sim 1.52 \mu_B$  at 1.6 K, compared to its classical value ( $5 \mu_B$ ). Magnetic isotherms exhibit a change of slope envisaging a field induced spin-flop transition at  $H_{SF} \simeq 3.2$  T. The magnetic field vs temperature phase diagram clearly unfold three distinct phase regimes, reminiscent of a frustrated magnet with in-plane (XY-type) anisotropy.

[1] Sebin J. Sebastian *et al.*, Phys. Rev. B **105**, 104425 (2022).

# Field-angle anisotropy of magnon specific heat in proximate Kitaev systems under an in-plane magnetic field

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The magnetic phase transition of the best Kitaev material  $\alpha$ -RuCl<sub>3</sub> under the magnetic field has recently drawn much attention because of putative intermediate spin liquid phase. Its magnetic ground state changes from the antiferromagnetic zigzag order to the polarized phase through the intermediate phase (IP) under the magnetic field. The non-Abelian spin liquid (NASL) phase has been proposed as promising IP candidate because of observed half-integer plateau of thermal Hall conductivity and field-angle anisotropy of specific heat under the magnetic field.

In this study [1], we have investigated the field-angle anisotropy of magnetic excitations under an in-plane magnetic field for proximate Kitaev systems. By employing the exact diagonalization method and the linear spin wave theory, we have shown that the magnetic excitation gap in the polarized phase is determined by the magnon excitation at M points and has a strong anisotropy with respect to the field direction near the critical field limit. The specific heat from this magnon excitation bears qualitatively the same anisotropic behaviors as the expected one for the NASL phase in the Kitaev model and the experimentally observed one of the IPs in  $\alpha$ -RuCl<sub>3</sub>

[1] B. H. Kim, Phys. Rev. Res. **3**, 043032 (2021)

## Thermodynamic Signatures of the Soliton Lattice in Single-Crystal TbFeO<sub>3</sub>

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The properties of the orthorhombic perovskite TbFeO<sub>3</sub> originate from the interplay of a Tb and Fe magnetic sublattices, resulting in a complex magnetic phase diagram. Perhaps most remarkable, at low temperatures, a complex and anharmonic magnetic structure, a so-called magnetic soliton lattice, was identified by means of neutron scattering under magnetic fields up to 4T [1], while thermodynamic information has been missing. Here, we report the single-crystal growth of TbFeO<sub>3</sub> using a combination of a solid-state reactions and optical float-zoning. X-ray powder diffraction as a function of temperature reveals an anomaly in the thermal expansion at the onset of canted antiferromagnetic ordering of the iron spins at  $T_N = 688$  K. Measurements of the magnetic ac susceptibility and the specific heat between 2 K and 300 K are characteristic of strong easy-plane magnetic anisotropy with two prominent magnetic phase transitions in zero magnetic field. Below 8 K, canted antiferromagnetic order of the Tb spin emerges and below 3 K the two magnetic sublattices are subject to a reorientation, consistent with the literature [1,2,3]. By combining transverse-field ac susceptibility and transverse-field specific heat measurements using bespoke setups with neutron scattering, we have determined the magnetic phase diagram for fields applied along the major crystallographic axes. When magnetic field is applied along the hard magnetic c axis, the soliton lattice may be traced up to 12 T, the highest field studied.

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[1] S. Artyukhin *et al.*, *Nature Materials*, **11**, 694-699 (2012)

[2] O. Nikolov *et al.*, *J. Phys. Condens. Matter*, **6**, 3793 (1994)

[3] K. P. Belov *et al.*, *Sov. Phys. JETP*, **49**, 557 (1979)



# Effects of electron-phonon coupling on the interfacial carriers in Al<sub>2</sub>O<sub>3</sub>/TiO<sub>2</sub> heterostructure

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Recently, a novel 2-dimensional electron system was discovered: Al<sub>2</sub>O<sub>3</sub>/TiO<sub>2</sub> thin films heterostructure [1]. Al<sub>2</sub>O<sub>3</sub> slightly reduces the TiO<sub>2</sub> surface as to generate interfacial electron carriers. It is well known that the electron states in TiO<sub>2</sub> are strongly coupled with the phonons (i.e. polarons). Thus, the generated Ti  $d^1$  states (Ti<sup>3+</sup>) should be affected by the polaronic effect as well. Ti L<sub>3</sub>-edge resonant inelastic x-ray scattering study [2] clearly showed that there emerges a low energy loss feature (< 1eV, LEL), which can be attributed to the multi-phonon energy loss process, thereby manifesting the strong electron-phonon coupling effect. Furthermore, the TiO<sub>2</sub> thickness dependence of the LELs suggests that they are originated mostly at the interface. The near-total-reflection hard x-ray photoemission further demonstrates the depth profile of the quasiparticle states, which confirms that the effects of the electron-phonon coupling are indeed enhanced at the interface [3].

[1] T. J. Seok *et al.*, ACS Nano **12**, 10403 (2018).

[2] Y.-C. Shao *et al.*, Advanced Functional Materials **31**, 2104430 (2021).

[3] Y. Kim *et al.*, in preparation.

# Thermoelectric properties of topological chains coupled to a quantum dot

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Topological one-dimensional superconductors can sustain in their extremities zero energy modes that are protected by different kinds of symmetries. The observation of these excitations in the form of Majorana fermions is one of the most intensive quests in condensed matter physics. Their study is not only interesting in itself, but also because they have promising applications in the area of quantum computation. In this work we are interested in another class of one dimensional topological systems, namely topological insulators. These also present symmetry protected end modes with robust properties and do not require the low temperatures necessary for topological superconductivity. We consider the simplest kind of topological insulators, namely chains of atoms with hybridized sp orbitals. We study the transport properties of these chains in the trivial, non-trivial topological phases and at the quantum topological transition. We use a simple device consisting of two semi-infinite hybridized sp-chains connected to a quantum dot and obtain the thermoelectric properties of this system as a function of temperature and distance to the topological transition. We show that the electrical conductance and the Wiedemann-Franz ratio of the device at the topological transition have universal values at very low temperatures. The thermopower gives direct evidence of fractional charges in these systems.

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# Magnetic-Field Controlled Cascade of Soliton Layers in Epitaxial MnSi

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We have charted the phase diagram of epitaxial MnSi films grown on Si(111) by magnetometry, differential susceptibility, planar Hall, polarised neutron reflectometry and small-angle neutron scattering data. Our experimental results are supported by micromagnetic simulations, which jointly reveal a magnetic phase diagram dominated by a field-induced cascade of single-Q soliton layers. The soliton layers are stabilized through the applied field which modifies a zero-field, out-of-plane propagating helix with  $\lambda = 11.5$  nm. Field and temperature history provide specific routes for the nucleation of the distinct soliton phases, comprising of four-, three-, two-, and single-soliton layers depending on the field strength. At low temperatures ( $T < 10$  K) a discrete phase regime can be discerned unambiguously in the susceptibility, which may be attributed to the irreversibility of the two-soliton and single-soliton regimes. These observations provide insights into the integral role of magnetic anisotropy and dimensionality on the low-temperature phase diagram of thin film MnSi.

## Observation of giant spin pumping in Ferromagnet – organic semiconductor heterostructures

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In spintronics, the Injection of pure spin current into nonmagnetic materials plays a key role in transmitting, processing and storing information. A pure spin current is a flow of electron spin angular momentum without a simultaneous flow of charge current. It has been studied in many Inorganic metals, semiconductors and insulators, but not yet in organic semiconductors (OSC). OSCs have low spin-orbit coupling, large spin diffusion length and long spin relaxation time. Here, we explore the spin pumping mechanism i.e. the injection of pure spin current at electrochemically deposited Naphthalene Dimide (1-NAPH-D) and electron beam evaporated permalloy (Py) heterostructures based OSC interface by employing ferromagnetic resonance spectroscopy. The dependence of the net spin-current transportation on Py layer thickness, from 5 to 25 nm, and the enhancement of the net effective gilbert damping are observed. The experimental data have been analysed to deduce the interfacial spin mixing conductance and change in line-width broadening. The damping constant is found to be  $1.70 (\pm 0.03) \times 10^{-2}$  in the Naph/Py sample corresponding to an  $\sim 89\%$  enhancement of the original Gilbert damping  $0.90 (\pm 0.01) \times 10^{-2}$  in the bare Py thin film.

### References:-

1. Angela Wittman et.al. , [Phys. Rev. Lett. 124,027204 \(2020\)](#).
2. Yaroslav Tserkovnyak, Arne Bratass et. al. , [Phys. Rev. Lett. 88,117601 \(2002\)](#).
3. Talluri Manoj et.al. , [RSC Adv, 2021, 11, 35567](#).
4. Shun watanabe et.al., [Nature Physics.10 308-313\(2014\)](#)

# Scanning SQUID microscopy studies of ferromagnetism in $\text{LaMnO}_3$ thin films grown on $\text{SrTiO}_3$

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While  $\text{LaMnO}_3$  (LMO) is an antiferromagnet in the bulk, thin films deposited on  $\text{SrTiO}_3$  (STO) usually exhibit ferromagnetism with a Curie temperature of  $\sim 115$  K, accompanied by electrically insulating behaviour [1]. The thickness of the LMO plays a significant role in the emergence of the ferromagnetic behaviour in LMO/STO heterostructures [2]. A critical minimum thickness for ferromagnetic behaviour of 6 unit cells was observed. This effect was clearly visible using a scanning SQUID microscope (SSM), where a SQUID chip is scanned along the surface of a sample. This is a powerful tool to image the ferromagnetism with a micrometer scale resolution [3].

We now report the use of the SSM to study the emergence and disappearance of the ferromagnetism in different metal/LMO/STO structures. We show that sputtering metallic layers on LMO thin films affects their ferromagnetic behaviour. In partially metal-covered LMO surfaces, the SSM is able to provide a clear picture of the effect of adding a metal/LMO interface. While Au does not significantly influence the ferromagnetic order of the underlying LMO film, a thin Ti capping layer induces a dramatic change in the magnetic signal. These results could enable a local control of the ferromagnetism in LMO for potential applications in oxide electronics.

[1] A. Gupta *et al.*, Appl. Phys. Lett. **67**, 3494 (1995).

[2] X. Renshaw Wang *et al.*, Science **349**, 716 (2015).

[3] P. Reith *et al.*, Rev. Sci. Instrum. **88**, 123706 (2017).

# First-principles study of momentum-forbidden excitons in bulk 2H-MoX<sub>2</sub> (X= S, Se)

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Coulomb-bound electron-hole pairs (excitons) dominate the optical response of atomically thin transition metal dichalcogenide (TMD) semiconductors. While Mo-based TMDs monolayers have a direct gap, bulk MoS<sub>2</sub> and MoSe<sub>2</sub> possess an indirect gap [1], with momentum-forbidden lowest energy excitonic transitions. Here we study how the effects of translational symmetry breaking by thermal phonons and in scanning spectroscopies [2,3] can lead to a violation of the usual optical selection rules.

[1] A. Molina-Sánchez, L. Wirtz, Physical Review B (2011)

[2] F. Hu et al. Nature Photonics (2017)

[3] T. Low et al. Nature Materials (2017)

# Multi-level operation in vanadium dioxide-based resistive switching devices

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Vanadium dioxide (VO<sub>2</sub>) is widely studied for its prominent insulator-metal transition (IMT) near room temperature, with potential applications in novel memory devices and brain-inspired neuromorphic computing. In previous work of our group, Rana et al. observed multiple intermediate stable resistive states between the insulating and metallic states in VO<sub>2</sub> films by tailored temperature sweeps. [1] The existence of these intermediate resistive states is particularly attractive for reconfigurable electronic circuitry.

In this work, we fabricated planar bridge-structure devices from VO<sub>2</sub> thin films. Under voltage/current sweeps, Joule heating in the device triggers the IMT. Furthermore, intermediate steps can happen during the reset when tuning the voltage under a high compliance current. This unique measurement can allow multistate memory within one VO<sub>2</sub>-based memory cell (in our demonstration 3 bits per cell) and reliable multilevel operation. [2]

In order to exploit these intermediate states, we also fabricated devices with two identical parallel VO<sub>2</sub> bridges with varying bridge-to-bridge distances. Depending on the bridge distance, we obtain a higher degree of control for the intermediate states. The switching behavior of these bridges depend ultimately on heat dissipation effects. To develop optimum device designs, we carried out nanoscale thermal mapping of in operando devices with varying bridge-to-bridge distances using Scanning Thermal Microscopy (SThM). The concept can readily be extended to more parallel channels and complex network configurations. Moreover, one may further use multilayering to stack bridges in the vertical direction and provide a further dimension for multibit operations.

[1] A. Rana, C. Li, G. Koster, and H. Hilgenkamp, *Sci. Rep.* **10**, 2 (2020).

[2] X. Gao, C. M. M. Rosário, and H. Hilgenkamp, *AIP Adv.* **12**, 015218 (2022).

# Relation between anomalous gap dependence of high harmonic generation and extremely strong light-matter coupling

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Recent developments in laser technology have led to substantial progress in strong field physics. Especially, high harmonic generation (HHG) has been observed in various systems such as atomic gases[1], solid state systems[2], and strongly correlated electron systems[3]. HHG attracts much attention because of its non-perturbative physics and its great potential to probe ultrafast electron dynamics in materials. Theoretically, HHG has been understood based mainly on a semiclassical picture, the three-step model[4]. On the other hand, experimentally, it has been observed that the HHG intensity in a Mott insulator  $\text{Ca}_2\text{RuO}_4$  is enhanced exponentially as the band gap is increased[3]. This anomalous gap dependence cannot be explained by the three-step model, because the model is based on a picture that the HHG is caused by tunneling electrons through the band gap.

In this work, we focus on the gap dependence of HHG in two-level systems and semiconductors. We numerically calculate the HHG in these systems considering diabatic transition processes of electrons. As a result, we find that there are some parameter regions where the HHG intensity exponentially grows as the band gap is increased. In this presentation, we discuss the relation of this gap dependence and parameters such as the relaxation time of electrons and the electric field intensity.

[1] M. Ferray et al., *J. Phys. B* **21**, L31–L35 (1988).

[2] S. Ghimire et al., *Nat. Phys.* **7** 138 (2011).

[3] K. Uchida et al., *Phys. Rev. Lett.* **128**, 127401 (2022).

[4] P. B. Corkum, *Phys. Rev. Lett.* **71**, 1994 (1993).



# Hole transporting conductor designed by polarizability encouraged strongly correlated oxide

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Hole transporting conductor (HTC) is one of the most critical components in electronic/optoelectronic devices not only for delivering but also for injecting hole carriers.[1-3] We report the polarizability encouraged strongly correlated oxide of NiWO<sub>4</sub> as a new HTC candidate with high hole carrier mobility as well as deep work function level. By partial substitution of Ni sites with Cu in NiWO<sub>4</sub>, drastic increase of electrical conductivity by  $\sim 10^8$  times could be observed as exhibiting band-like hole carrier conduction behavior. From optical, magnetic, dielectric studies assisted by density functional theory calculations confirm that the emergence of large Flöhlich polaronic conduction along deep-lying valence band maximum under a sustained correlation strength in Cu-substituted NiWO<sub>4</sub>. By applying Cu-substituted NiWO<sub>4</sub> as a hole transporting layer on CdSe quantum dot light emitting device, record-high green luminescence and efficiency of 16258 cd/m<sup>2</sup> and 8.67 cd/A could be attained, respectively, without any additional blocking layer. It strongly suggests that our approach is well operated toward an ideal hole deliverer in practical device applications.

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[1] X. Yu, T. J. Marks, and A. Facchetti, *Nat. Mater.* **15**, 383 (2016).

[2] M. T. Greiner *et al.*, *Nat. Mater.* **11**, 76 (2011).

[3] N. B. Kotadiya *et al.*, *Nat. Mater.* **17**, 329 (2018).

# Thin-film deposition of Cu-substituted NiWO<sub>4</sub> by electron beam evaporation and its device application

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Nickel tungstate (NiWO<sub>4</sub>) is one of correlated oxide candidates that is anticipated for exhibiting high hole carrier conductivity. We report the physical properties of Cu-substituted NiWO<sub>4</sub> (Cu-NiWO<sub>4</sub>) thin-film deposited by electron beam (E-beam) evaporation process, and its feasibility on the practical diode application.

NiO, CuO, and WO<sub>3</sub> powders were mixed in a molar ratio of 2.25:0.25:1, then heated at 950 °C for 24 hours in a furnace to produce Cu-NiWO<sub>4</sub> powder source. To encourage homogeneity, we repeated pelletizing, annealing, and pulverizing the sample two more times, thus it enables us to prepare high purity Cu-NiWO<sub>4</sub> E-beam source in powder form. We deposited 100 nm-thick Cu-NiWO<sub>4</sub> thin-films on n-Si and glass substrates by E-beam evaporation in the fixed deposition rate of ~0.5 Å/s under various substrate temperatures. (RT ~ 300 °C)

The crystalline quality and atomic composition of the deposited thin-film were identified through X-ray diffraction (XRD) and X-ray fluorescence (XRF) analysis, respectively. The vibrational modes were studied by Raman spectroscopy, and inter-band transition properties were investigated by UV-visible transmittance measurement. Electrical properties were measured using the 4-point probe measurement. We applied our Cu-NiWO<sub>4</sub> thin-film as p-type layer on n-Si substrate for fabricating p/n junction diode device. It exhibited the highest on-state current and on/off current ratio up to ~19.36 A/cm<sup>2</sup> and ~1E5, respectively, when we deposited Cu-NiWO<sub>4</sub> p-type layer at 300 °C condition. It suggests that Cu-NiWO<sub>4</sub> can be utilized as a new correlated functional oxide toward practical device applications.

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# Large polaronic conduction in strongly correlated Cu-substituted NiWO<sub>4</sub>

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The electrical properties of transition metal-based oxides under a strong correlation have been limited by a poor carrier mobility, because their conduction mechanisms mainly originate from an inefficient small polaron hopping.[1-2] We report the occurrence of large polaronic conduction in strongly correlated Cu-substituted NiWO<sub>4</sub> evidenced by the band-like negative temperature dependence of hole mobility.

Cu-substituted NiWO<sub>4</sub> (Ni<sub>1-x</sub>Cu<sub>x</sub>WO<sub>4</sub> where 0.00 ≤ x ≤ 0.20) samples without any secondary phase were synthesized with NiO, CuO, WO<sub>3</sub> powders by a solid state reaction method. We analyzed structural and vibrational characteristics by X-ray diffraction (XRD) and Raman spectroscopy, respectively. And atomic composition ratio of synthesized samples were evaluated by Rietveld refinement and inductively coupled plasma (ICP) experiment. Their electrical properties such as resistivity, carrier concentration, and mobility were examined by Hall-effect measurement system. As x value increases, resistivity was significantly decreased from 3.69 × 10<sup>12</sup> to 3.28 × 10<sup>3</sup> Ω·cm at room temperature. The most conductive Ni<sub>0.8</sub>Cu<sub>0.2</sub>WO<sub>4</sub> sample exhibited a high hole mobility up to 2.81 cm<sup>2</sup>/V·s at 160 K. Impedance spectroscopy results confirmed that dielectric permeability increased with increasing x value, leading to weakening of electron-phonon coupling in which the large Fröhlich polaron state becomes favorable.[2]

From these results, we propose Cu-substituted NiWO<sub>4</sub> as an efficient hole transporting conductor based on strongly correlated system.

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[1] I. G. Austin and N. F. Mott, *Adv. Phys.* **18**, 41 (1969)

[2] C. Franchini, M. Reticcioli, M. Setvin, and U. Diebold, *Nat. Rev. Mater.* **6**, 560 (2021)

# **NbSe<sub>2</sub>-Based van der Waals Heterostructure Josephson Junction**

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NbSe<sub>2</sub> is an intrinsic 2D superconductor down to the single-layer limit [1]. At lower layer counts the critical temperature depends on the layer thickness. Here, we explore the physics behind the Josephson Junction built by stacking two separate NbSe<sub>2</sub> flakes on top of each other. For this, several devices were fabricated from mechanical exfoliated NbSe<sub>2</sub> flakes by the fast dry transfer technique. Charge transport measurements were first performed on individual flakes with various thicknesses to characterize their superconducting ordering. Two flakes with similar thickness were used to build the junction. The devices are built without any heat treatment to avoid excessive oxidation. The junctions were then characterized by the critical current oscillation under an in-plane magnetic field. The data obtained shows clear Josephson tunnelling characteristics, exhibiting high supercurrent transparency. The critical current oscillation periods in magnetic fields, however, yield very small London penetration depths (nm range). This directly contradicts current literature values [2], suggesting a more complex interface and supercurrent path than expected. Furthermore, Focused Ion Beam milling is used to pattern the stacking junctions, demonstrating further opportunities to understand van der Waals heterostructure Josephson Junctions.

[1] Wang, H., Huang, X., Lin, J. et al. Nat Commun 8, 394 (2017)

[2] James J. Finley, Bascom S. Deaver. Solid State Communications 36, 493 (1980)

# Nanocalorimetry of Quantum Materials

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New strongly correlated quantum materials not yet available as large single crystals as well as designer heterostructures grown by thin film techniques are central to many condensed matter research programmes. Thermodynamic measurements can give clear information about excitations and phase transitions but the low thermal mass of these materials precludes direct study by conventional specific heat experiments.

Here we report the development of a calorimeter for the measurement of specific heat of single crystals smaller than  $100\mu\text{m}^3$  at temperatures in the mK regime and high magnetic fields. Core of the design are Coulomb Blockade Thermometers [1] suspended on 200nm thick SiN membranes using nanofabrication techniques for Al/Al<sub>2</sub>O<sub>3</sub>/Al tunnel junctions. These thermometers are self-calibrating via a primary measurement mode and field independent, largely removing the requirement of time and resource consuming calibration runs. We successfully evaluated the calorimeter's performance on a microcrystal of Sr<sub>3</sub>Ru<sub>2</sub>O<sub>7</sub> with  $6.4 \times 10^{-8}$  mol-Ru reproducing previous results on the field dependent specific heat using a thousand times larger sample mass [2]. Current target materials include micrometre sized crystals of spin liquid candidates unavailable in larger dimensions as well as thin films of heavy fermion compounds.

[1] J. P. Kauppinen *et al.*, *Rev. Sci. Instrum.*, **69**, 4166 (1998)

[2] A. W. Rost *et al.*, *Science*, **325**, 1360 (2009)

## **A spatially resolved optical method to measure thermal diffusivity**

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We introduce an optical method to directly measure thermal diffusivity. Two laser beams are used, one as a source to locally modulate the temperature at the sample surface, and the other as a probe of the sample reflectivity, which is a function of the modulated temperature. Thermal diffusivity can be obtained from the phase delay between source and probe signals. Combining this technique with a microscope setup allows us to measure thermal diffusivity with a micron-scale spatial resolution, especially valuable when studying multidomain samples. We use the setup to study the diffusivity in a single polar domain of the bilayer ruthenate  $\text{Ca}_3\text{Ru}_2\text{O}_7$ , uncovering a  $\sim 25\%$  in-plane anisotropy of the diffusivity at 300 K and it becomes less anisotropic with the decreasing of temperature. Overall temperature dependence of the diffusivity suggests phonon-mediated thermal transport. To confirm, we also study the Ti-doped  $\text{Ca}_3\text{Ru}_2\text{O}_7$ , which holds a metal-to-insulator transition at around 100 K (depends on the doping level). Spatial resolution helped because of inherent disorder, and we recognize the surface inhomogeneity of the diffusivity in doped compound. More broadly, combining the spatial resolution with other probes of symmetry breaking (birefringence, Kerr rotation, second harmonic generation, *etc.*) will allow us to explore and visualize thermal properties across a range of phase transitions in correlated materials.

## MGML.eu - Material Growth & Measurement Laboratory

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Material growth and measurement laboratory (MGML) [1] is the newly established research infrastructure in Prague, Czech Republic. MGML offers open access for external users to the instrument suite dedicated to measurements of a rich spectrum of physical properties of materials in a wide range of temperatures (down to 10 mK), magnetic fields (up to 19.5 T), and hydrostatic and uniaxial pressures. The MGML technology facilities are enabling controlled preparation and characterization of high-quality samples (single crystals and polycrystals) of materials of various types which is available to users who do not have their own well-characterized samples needed for measurements.

Because the facility is open to all scientists, we want to present it to the strongly correlated electron systems community. In addition to our wide instrument suite, we will present our recent scientific highlights. Our users have identified the electric quadrupoles that maintain their degrees of freedom without ordering at a magnetic vortex arrangement in UNi<sub>4</sub>B [2], another group constructed an extremely complex 3D phase diagram of UTe<sub>2</sub> with a complete reshuffling of the magnetic anisotropy [3] and our in-house research shed light on how the transition between the 3D and quasi-2D system affects magnetic interactions in the VI<sub>3</sub> van der Waals ferromagnet [4].

[1] P. Javorský et al. MGML - Czech open access research infrastructure, accessed 20 April 2022

<<https://youtu.be/Ppt0Z2xUoIw>>

[2] J. Willwater et al. Phys. Rev. B **103**, 184426 (2021).

[3] M. Vališka et al. Phys. Rev. B **104**, 214507 (2021).

[4] J. Valenta et al. Phys. Rev. B **103**, 054424 (2021).

## **Fine details of sixfold Dirac fermions in a pyrite-structured PdSb<sub>2</sub>**

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We report detailed angle-resolved photoemission measurements on the electronic structure of an unconventional multi-fold Dirac fermionic semimetal PdSb<sub>2</sub> with a pyrite structure. By exploiting the photon energy and polarization dependence of the matrix element in photoemission intensity and by comparing photoemission data with ab-initio band calculations, we experimentally identify the exact structure including the orbital characters of the electron pockets at the R point in the Brillouin zone of PdSb<sub>2</sub>. Each electron pocket and hole pocket-like structure consists of three doubly degenerate parabolic bands respectively, which cross one another at the R point, forming a sixfold Dirac fermion. The overall electronic structure is consistent with the band calculation results, but the gap size between two sextuple points is very sensitive to the Wyckoff position of Sb atoms.

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# Uniaxial strain effects on the magnetoresistance and Fermi surface of the Dirac nodal-line semimetal ZrSiS

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Dirac nodal line semi-metals (DNLSMs) are materials in which the Dirac band crossing takes place along a one-dimensional line or loop in momentum space in contrast to Weyl- and Dirac semimetals, which are characterized by singular points where the valence and conduction band touch each other in the Brillouin zone. DNLSMs are not only ideal systems with which to investigate the properties of charge carriers with a linear dispersion relation, they also have the potential to create a platform for research on topological correlated matter demonstrated by recent theoretical predictions and experimental observations in ZrSiS [1,2] and ZrSiSe [3].

To search for correlation effects in these materials, tuning the Fermi level is of fundamental importance since it has been predicted that correlation effects manifest themselves when the density of states is very low [1]. In this case, uniaxial strain as a tuning parameter preserves the symmetry that protects the topology, allowing us to solely tune possible correlation effects.

In this work, we investigated single crystalline samples of ZrSiS by means of elasto-magnetoresistance (EMR) in high magnetic fields up to 30 T motivated also by recent theoretical predictions for applying strain on the compound [4]. We present our experimental technique using the Razorbill CS100 strain cell. Acquired data shows significant changes in EMR with varying uniaxial strain. Further analysis aims to determine the changes in the Fermi surface probed by means of the Shubnikov-de Haas effect.

[1] Y. Huh, E.-G. Moon and Y.-B. Kim, *Phys. Rev. B* **93**, 035138 (2016).

[2] S. Pezzini *et al.*, *Nat. Phys.* **14**, 178 (2018).

[3] Y. Shao *et al.*, *Nat. Phys* **16**, 636–641 (2020).

[4] W. Zhou *et al.*, *Adv. Elec. Mat.* **6**, 1900860 (2020).

# Transport and magnetic properties of the topological (Weyl) semimetal: Hexagonal - $(\text{Mn}_{1-\alpha}\text{Fe}_\alpha)_3\text{Ge}$ ( $\alpha = 0 - 0.3$ )

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Hexagonal- $\text{Mn}_3\text{Ge}$ , displays a large anomalous Hall effect (AHE) near room temperature, which originates from the topologically protected Weyl nodes. The Weyl parameters- location and separation of the Weyl nodes- determine the strength of AHE and chiral anomaly present in the system. These parameters can be controlled by the suitable dopants of the parent Weyl semimetal. Therefore, we have explored the electrical transport and magnetic properties of the single crystal  $(\text{Mn}_{1-\alpha}\text{Fe}_\alpha)_3\text{Ge}$ . Clear signatures of the AHE and chiral anomaly were observed for samples up to  $\alpha = 0.22$ , in a certain temperature regime. However, the strength of AHE and chiral anomaly weakens drastically with an increase in Fe doping and vanishes beyond  $\alpha = 0.22$ . Furthermore, the ground state magnetic structure of  $\alpha = 0.22$  was determined using single-crystal (polarized and unpolarized) neutron diffraction techniques. We observed that the magnetic structure of the doped sample remains the same as that of the parent compound only in the temperature regime where AHE and the chiral anomaly were observed. These observations led us to two main conclusions: (i) the Weyl nodes are very likely to be present in the doped samples, and (ii) the characteristics of the Weyl nodes can be tuned significantly by suitable doping of the Weyl semimetals.

# ***The Phase puzzle of $\nu = 0$ (charge neutrality) Graphene***

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The true ground state of  $\nu = 0$  (charge neutrality) monolayer graphene quantum Hall has long been debated. Famously the symmetry of the monolayer graphene at  $\nu = 0$  (charge neutrality) was analyzed by J. Alicea and P. A. Fisher [1], and canted anti-ferromagnet (CAF) was predicted by I. F. Herbut [2]. However, the complete picture of the Hamiltonian was missing until the seminal paper by M. Kharitonov [3] which predicts a phase transition from a vanilla insulator (CAF) to a topological insulator Ferromagnetic phase (F) as one changes the Zeeman coupling keeping the cyclotron energy fixed. This was later confirmed in the experiment by A. F. Young et. al. [4]. However recent local measurement experiments [5-7] find evidence against the proposed bulk ground states. In the light of these experiments, we revisit this phase diagram and present a resolution to this ambiguity. We show that, generically, in the regime of interest there is a region of coexistence between magnetic and bond orders in the phase diagram. We demonstrate this result both in continuum and lattice models and argue that the coexistence phase naturally provides an explanation for unreconciled experimental observations on the quantum Hall effect in graphene.

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- [1] J. Alicea and P. A. Fisher , PRB 74, 075422 (2006)
- [2] I. F. Herbut, PRB 75, 165411 (2007)
- [3] M. Kharitonov, PRB 85, 155439 (2012)
- [4] A. F. Young et. al., Nature 505, 528 (2014)
- [5] L. He et. al. PRB 100, 085437 (2019)
- [6] X. Liu et. al. Science abm3770 (2021)
- [7] A. Coissard arXiv:2110.02811

## The origin of the second transition in the Weyl semimetal $\text{Co}_3\text{Sn}_2\text{S}_2$

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Recent discovery of topologically non-trivial behavior in  $\text{Co}_3\text{Sn}_2\text{S}_2$  [1,2] stimulated a notable interest in this itinerant ferromagnet ( $T_c = 174$  K). The exact magnetic state remains ambiguous, with several reports indicating the existence of a second transition in the range 125 – 130 K, with antiferromagnetic and glassy phases proposed to coexist with the ferromagnetic phase [3,4]. Using detailed angle-dependent DC and AC magnetization measurements on large, high-quality single crystals we reveal a highly anisotropic behavior of both static and dynamic response of  $\text{Co}_3\text{Sn}_2\text{S}_2$ . It is established that many observations related to sharp magnetization changes when  $B \parallel c$  are influenced by the demagnetization factor of a sample. On the other hand, a genuine transition has been found at  $T_p = 128$  K, with the magnetic response being strictly perpendicular to the  $c$ -axis and several orders of magnitude smaller than for  $B \parallel c$ . Calculations using density-functional theory indicate that the ground state magnetic structure consist of magnetic moments canted away from the  $c$ -axis by a small angle ( $\sim 1.5^\circ$ ). We argue that the second transition originates from a small additional canting of moments within the kagome plane, with two equivalent orientations for each spin.

- [1] E. Liu et al., Nat. Phys. 14, 1125 (2018)
- [2] D. F. Liu et al., Science 365, 1282 (2019)
- [3] M. A. Kassem et al., Phys. Rev. B 96, 014429 (2017)
- [4] E. Lachman et al., Nat. Commun. 11, 560 (2020)

# Berry paramagnetism in the Dirac semimetal ZrTe<sub>5</sub>

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Dirac matters have attracted a lot of interest due to their unique band structure with linear band dispersions, which have great potential for technological applications. Recently, three-dimensional Dirac and Weyl semimetals have invoked distinctive phenomena originating from a non-trivial Berry phase. The nontrivial  $\pi$  Berry's phase plays an important role in the unconventional phenomena, especially in transport properties. However, magnetic properties associated with a nontrivial  $\pi$  Berry's phase have rarely been reported. The recent studies on Weyl semimetals, such as NbAs and TaAs [1,2], show that they can display unconventional paramagnetic and diamagnetic contributions due to the magnetic field-independent 0<sup>th</sup> Landau level, unlike conventional materials with a parabolic band.

In this study, we prepare single crystals of Ti<sub>x</sub>Zr<sub>1-x</sub>Te<sub>5</sub> using a chemical vapor transport method [3]. Our detailed electrical transport measurements reveal that the crystals show the Lifshitz transition and the Ti doping induces a band shift. The quantum oscillation analyses demonstrate that the Ti<sub>x</sub>Zr<sub>1-x</sub>Te<sub>5</sub> crystals are 3D Dirac semimetals with a nontrivial  $\pi$  Berry phase and an additional phase shift of 1/8. In further studies on the magnetic properties, we observe a minimum temperature-dependent magnetic susceptibility, which is close to a peak position of electrical resistivity. This observation is interpreted in terms of the Berry paramagnetism. Our finding paves the way to determine a band topology by magnetism and also provides a platform to apply the Berry magnetism to Dirac semimetals.

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[1] P. J. W. Moll et al., Nat. Commun. 7, 12492 (2016).

[2] C.-L. Zhang et al., Nat. Commun. 10, 1028 (2019).

[3] S. Ji et al., Commun. Phys. 4, 265 (2021).

# Network of topological charges in the electronic structure of CoSi

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The discovery of multifold-fermions [1] and symmetry-enforced topological band crossings that are generically located at the Fermi level and may be switched on and off by an applied magnetic field [2] in non-symmorphic B20 compounds has recently generated tremendous interest. However, the putative relationship between all topological charges remained unexplored up to now. We report the experimental identification of symmetry-enforced topological nodal planes in CoSi which together with multifold point degeneracies and Weyl points form a network of band crossings that satisfies the Nielsen-Ninomiya no-go theorem. In our study [3], we combined measurements of Shubnikov-de Haas oscillations with material-specific first-principle electronic structure calculations, a symmetry analysis of space group 198, in which CoSi crystallizes, as well as a direct calculation of the topological charges from the DFT wave functions. The observation of two nearly dispersionless Shubnikov-de Haas frequency branches is shown to provide clear evidence of four distinct Fermi surface sheets around the R point and of the symmetry-enforced orthogonality of the wave functions at the intersections with the nodal planes on the Brillouin zone (BZ) boundary. These results in combination with our symmetry analysis show that the sum of topological charges in the interior of the BZ must be odd and therefore needs to be compensated by the topological charge of the nodal planes. Taken together, the identification of topological band crossings in the electronic structure of CoSi we report represents a showcase of an entire network of topological charges including nodal planes in this class of materials.

[1] P. Tang, *et al.*, Phys. Rev. Lett. **119**, 206402 (2017); Z. Rao, *et al.*, Nature **567**, 496 (2019); D.S. Sanchez, *et al.*, Nature **567**, 500 (2019); Q.-Q. Yuan, *et al.*, Sci. Adv. **5**, aaw9485 (2019); N. Schröter, *et al.*, Science **369**, 179 (2020).

[2] M. Wilde, *et al.*, Nature **594**, 374 (2021).

[3] N. Huber *et al.*, arXiv:2107.02820 (2021).

# Nodal-line driven anomalous susceptibility in ZrSiS

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We demonstrate a unique approach to test the signature of the nodal-line physics by thermodynamic methods. By measuring magnetic susceptibility in ZrSiS we found an intriguing step-like temperature-driven transition from dia- to paramagnetic behavior. ZrSiS is one of the most studied nodal-line Dirac semimetal with indication of correlation effects. We show that the anomalous behavior represents a real thermodynamic signature of the underlying nodal-line physics through the means of chemical pressure (isovalent substitution of Zr for Hf), quantum oscillations, and theoretical modeling. The anomalous part of the susceptibility is orbital by nature, and it arises due to the vicinity of the Fermi level to a degeneracy point created by the crossing of two nodal lines. Furthermore, an unexpected Lifshitz topological transition at the degeneracy point is revealed by tuning the Fermi level.

The present findings in ZrSiS give a new and attractive starting point for various nodal-line physics-related phenomena to be tested by thermodynamic methods in other related materials.

## *Quantum oscillations in $Zr_{1-x}Hf_xSiS$*

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Dirac matter is a class of materials where the low-energy excitation spectrum can be described by the Dirac equation. They share a property of forming symmetry protected Dirac nodes (or lines) on valence and conductive bands crossings, with bands linear in close vicinity of nodes [1]. When magnetic field is applied to a system of free charged fermions, their energy states quantize into Landau levels. In a quantum oscillation experiment, the external magnetic field is varied, which causes Landau levels to pass over the Fermi surface. This in turn results in oscillations of the electronic density of states at the Fermi level, resulting in oscillations in various properties [2].

Using different angles of external field, we explored anisotropy of Dirac nodal line semimetal  $Zr_{1-x}Hf_xSiS$ . Material is solid solution of ZrSiS and HfSiS and we managed to grow quality single crystals that show quantum oscillations. Here we present Shubnikov-de Haas and de Haas-van Alphen oscillations for external field along [001] for several  $x$  in  $Zr_{1-x}Hf_xSiS$ . Knowing the frequency of recorded quantum oscillations, as well as direction of applied field, we were able to reconstruct parts of Fermi surface for ZrSiS and HfSiS.

[1] T.O. Wehling, A.M. Black-Schaffer & A.V. Balatsky (2014) Dirac materials, *Advances in Physics*, 63:1, 1-76

[2] Shoenberg, D. (1984). *Magnetic Oscillations in Metals* (Cambridge Monographs on Physics).



# **Analyse of Anti-symmetric component in the magnetoresistance in Sb-doped tellurium using Fourier analysis**

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Tellurium is a van-der-Waals Weyl-semiconductor with a chiral crystal structure and an enormous potential for future applications, stemming from the strong spin-orbit coupling, from which emerges a peculiar spin-texture and non-trivial magnetoelectric physics of the material. Here, we present an experimental angle-dependent AC-magneto transport study of Sb-doped and chemically pure needle-shaped tellurium single crystals, where the current flows along the chiral screw axis, while the direction of the external magnetic field is varied. Our Fourier analysis of the acquired fixed-field rotator scan data reveals interesting features, which we relate to the Weyl nature of the material. The observations are consistent with the chiral anomaly and topologically induced effects due the peculiar spin texture of the system. Specifically, our data demonstrates the connection between the current-induced changes in the electronic structure and the therewith induced magnetism.

# Signatures of a magnetic field induced Lifshitz transition in the ultra-quantum limit of the topological semi-metal ZrTe<sub>5</sub>

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The ultra-quantum-limit (UQL), realized at strong magnetic fields, has long been proposed to host a wealth of strongly correlated states of matter. Electronic states in the UQL are for example quasi one-dimensional (1D), which implies perfectly nested Fermi surfaces. Whereas the UQL typically requires unreachably strong magnetic fields, the topological semi-metal ZrTe<sub>5</sub> has been shown to reach the UQL at fields of only a few Tesla [1, 2].

Here, we characterize the UQL of ZrTe<sub>5</sub> at fields up to 65 T by a combination of electric transport and ultrasound measurements. We find that the Zeeman effect in ZrTe<sub>5</sub> enables an efficient tuning of the quasi-1D Landau band structure with magnetic field. This allows to reach a Lifshitz transition towards a 1D Weyl regime in which perfect charge neutrality can be achieved. Because no instability-driven phase transitions destabilize the quasi-one-dimensional electron liquid for the investigated field strengths and temperatures, our analysis establishes ZrTe<sub>5</sub> as a thoroughly understood platform the study of more exotic interaction-driven phases at lower temperatures. In addition, our results corroborate the strong topological insulating nature of the ZrTe<sub>5</sub> ground state[3].

[1] Tang, F. *et al.* Nature 569, 537–541 (2019).

[2] Galeski, S. *et al.* Nat. Commun. 2021 121 12, 1–8 (2020).

[3] Weng, H., Dai, X. & Fang, Z. Phys. Rev. X 4, 011002 (2014).

## Thermal and electrical transport in $\text{Ce}_3\text{Bi}_4\text{Pd}_3$

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The non-centrosymmetric and non-magnetic compound  $\text{Ce}_3\text{Bi}_4\text{Pd}_3$  is known as the first representative of the recently introduced materials class of Weyl-Kondo semimetals [1-3]. In these materials the Kondo interaction causes the appearance of Weyl nodes close to the Fermi energy. They manifest in a giant spontaneous Hall effect [3]. To deepen our understanding of this intriguing phenomenon, we study its angular dependence as well as its thermal equivalent.

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[1] S. Dzsaber *et al.*, Phys. Rev. Lett., **118**, 246601 (2017).

[2] H.-H. Lai *et al.*, Proc. Natl. Acad. Sci. U.S.A., **115**, 93 (2018).

[3] S. Dzsaber *et al.*, Proc. Natl. Acad. Sci. U.S.A., **118**, e2013386118 (2021).

# Thermodynamic and transport properties of $\text{EuZn}_2\text{As}_2$ single crystals

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In recent years, there has been much interest in the prediction and experimental exploration of new topological materials due to their intriguing physical behavior and potential applications. In particular, magnetic Weyl semimetals exhibit physical properties such as chiral magnetic anomaly and large anomalous Hall effect, which can be exploited in spintronics [1]. Eu-based topological materials are particularly promising because  $\text{Eu}^{2+}$  ion has a large spin-only magnetic moment.

In this context, the trigonal compound  $\text{EuCd}_2\text{As}_2$  has been intensively studied using various experimental techniques and identified as a possible antiferromagnetic (AFM) Dirac semimetal with a single Dirac cone located near the Fermi level when its in-plane three-fold symmetry is preserved [2]. However, the experimentally determined AFM structure is of A-type, and this spin arrangement breaks the rotational symmetry, causing opening of an energy gap and thus destruction of the Dirac point [3]. This feature poses a serious issue for the use of this material in spin-based devices.

In the present work we studied the compound  $\text{EuZn}_2\text{As}_2$ , isostructural to  $\text{EuCd}_2\text{As}_2$ , which is also antiferromagnetic, but its A-type AFM ground state can be easily switched to gapless ferromagnetic ordering along the hexagonal  $c$ -axis that may give rise to the emergence of a single pair of Weyl nodes [4]. Here, we report on magnetic susceptibility, magnetization, heat capacity, resistivity and magnetoresistance measurements, performed on high-quality single crystals of  $\text{EuZn}_2\text{As}_2$  over wide ranges of temperature and magnetic field strength.

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[1] B. Yan and C. Felser, *Ann. Rev. Condens. Matter Phys.* **8**, 337 (2017).

[2] G. Hua, et al., *Phys. Rev. B* **98**, 201116(R) (2018).

[3] M. C. Rahn, et al., *Phys. Rev. B* **97**, 214422 (2018).

[4] J.-R. Soh, et al., *Phys. Rev. B* **100**, 201102(R) (2019).

# Ultrasound propagation in candidate material for electron hydrodynamics, Weyl semimetal WTe<sub>2</sub>

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Interactions between electrons might lead to the appearance of a regime where the dominating time-scale is defined by momentum-conserving processes. This is manifested by electron liquid exhibiting features characteristic for classical liquids, like Poiseuille flow, resulting in non-Ohmic, sample-width-dependent resistivity. This was recently observed in a two-dimensional metal PdCoO<sub>2</sub> and two Weyl semimetals[1-3]. Neither of the observations was accounted for with complete microscopic description. For WTe<sub>2</sub> there was proposed a mechanism based on the electron-electron scattering process involving a virtual phonon[3].

The predictions of the mentioned model, based on *ab-initio* calculations are in good agreement with the results of scanning probe study of temperature dependence of the electrical current profile throughout the sample width[3].

Additional insight into the validity of presented claims might be gained from examination of ultrasound propagation in the mentioned material. This course of investigation provides invaluable possibility to observe variation of speed of sound and its attenuation giving the opportunity of looking at the phenomena from both thermodynamic and transport point of view.

Here we report results of such a study performed on WTe<sub>2</sub> Weyl semimetal. We have analyzed temperature and field dependence of propagation of longitudinal and two transverse modes of different polarization propagating along the *a* crystallographic directions. The data shows anomalous decrease in speed of the longitudinal mode below 10 K and non-monotonous *T*-dependence of its attenuation. Moreover, quantum oscillations observed in all six measured quantities reveal the details of coupling between measured phonon modes and different parts of systems Fermi surface.

[1] Moll, P. J. W., Kushwaha, P., Nandi, N., Schmidt, B. & Mackenzie, A. P. Evidence for hydrodynamic electron flow in PdCoO<sub>2</sub>. *Science* **351**, 1061–1064 (2016).

[2] Gooth, J. et al. Thermal and electrical signatures of a hydrodynamic electron fluid in tungsten diphosphide. *Nat. Commun.* **9**, 4093 (2018).

[3] Vool, U., Hamo, A., Varnavides, G. et al. Imaging phonon-mediated hydrodynamic flow in WTe<sub>2</sub>. *Nat. Phys.* **17**, 1216–1220 (2021).

# Structural and superconducting properties of PdTe<sub>2</sub> under high pressure

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The transition metal dichalcogenide PdTe<sub>2</sub> has attractive features based on its classification as a type-II Dirac semimetal and the occurrence of type-I superconductivity. At ambient pressure, the bulk superconducting transition temperature ( $T_c$ ) is 1.64 K [1]. Our previous study focusing on pressures below 2.5 GPa revealed that the pressure dependence of  $T_c$  shows a maximum of  $\sim 1.9$  K at around 1 GPa [2], which is inconsistent with the theoretical calculation [3]. Meanwhile, the carrier density varies monotonically without any anomalies at around 1 GPa, and its variation cannot explain the variation of  $T_c$ . Then, powder x-ray diffraction studies were carried out up to 8 GPa at room temperature to investigate the contribution of structure. We performed normalized pressure-strain analysis utilizing lattice constants. The results indicate that the compressibility changes around 1 GPa, suggesting that a Lifshitz transition occurs.

Furthermore, the topological transition from type-II to I Dirac semimetal was theoretically predicted between 4.7 and 6.1 GPa [3]. To reveal the effect of the transition on superconductivity, we investigated the pressure variation of  $T_c$  by electrical resistivity measurements up to 8 GPa. As a result, no indications related to the transition were observed in resistivity measurements; namely,  $T_c$  shows a monotonic decrease at pressures beyond 1 GPa, and there is no anomalous behavior in the temperature dependence of the resistivity.

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[1] H. Leng *et al.*, Phys. Rev. B **96**, 220506(R) (2017).

[2] H. Leng *et al.*, J. Phys.: Condens. Mat. **32**, 025603 (2020).

[3] R. C. Xiao *et al.*, Phys. Rev. B **96**, 705101 (2017).

# Superconductivity and Charge Density Wave in the Extended Fermi-Hubbard Model with Disorder

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The study of simple models of strongly correlated systems provides clues for the understanding of macroscopic quantum phenomena. One of the most attractive and active fields in this matter is high-temperature superconductivity (HTSC) and the search for mechanisms that strengthen the superconductivity (SC) in quantum materials. One possible avenue for this enhancement is to weaken competing electronic phases, among which charge density waves (CDW) rise as feasible candidates [1], as these seem to be ubiquitous in the phase diagrams of, for example, high-temperature superconductors and transition metal dichalcogenides.

From the theoretical perspective, the Extended Fermi-Hubbard model (EFH) is one of the simplest models that exhibits the physics of this interplay. Recent simulations based on the Density Matrix Renormalization Group algorithm (DMRG) and others based on mean-field calculations [2,3] suggest that by introducing a moderate amount of disorder in the interaction parameters of the Hamiltonian, it is possible to strengthen SC. Here, we propose to study the interplay of SC and CDW by disordering the coupling parameters of the EFH Hamiltonian, in a way that closely resembles the variations generated by chemical substitution in real experiments. For this end, we use the DMRG algorithm to calculate ground states and perform calculations of correlations and Luttinger parameters to characterize the phases. Here we show preliminary results for doping one parameter of the Hamiltonian and the appearance of domains of CDW when the doping is strong enough.

\*This work is supported by the Program Committee.

[1] Li, L., Deng, X., Wang, Z. *et al.*, npj Quan Mater **2**, **11** (2017).

[2] Glocke, S., Klümper, A., and Sirker, J., Phys. Rev. B. **76**, 155121 (2007).

[3] Banerjee, A., Garg, A., and Ghosal, A. Phys. Rev. B. **98**, 104206 (2018).

# Resonant inelastic x-ray scattering of hematite Fe<sub>2</sub>O<sub>3</sub>: LDA+DMFT analysis

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Hematite Fe<sub>2</sub>O<sub>3</sub> is a typical antiferromagnetic Mott insulator with a large spin  $S = 5/2$ . Its spin properties, such as a weak in-plane magnetic anisotropy and low spin dissipation, make it a promising candidate material for spintronics.

In this work, we study magnetic excitations as well as orbital ( $dd$ ) and charge excitations in Fe<sub>2</sub>O<sub>3</sub> using the high-resolution resonant inelastic x-ray scattering (RIXS) at the Fe  $L_3$ -edge. The experimental spectra are analyzed by means of the local density approximation (LDA) + dynamical mean-field theory (DMFT) method which was introduced recently to simulate the RIXS spectra of strongly correlated materials [1,2]. The momentum dependence in the RIXS spectra is simulated within a linear spin-wave theory.

From a fitting analysis of  $dd$  and charge excitations in the high-resolution Fe  $L_3$ -edge RIXS data, we obtain the lattice model of Fe<sub>2</sub>O<sub>3</sub>. The low-energy RIXS intensities are computed by the Anderson impurity model build on the LDA+DMFT solution to the lattice model. Our theoretical and experimental spectra reveal multiple spin excitations that appear at sequential energies, i.e., 97meV, 188meV, 286meV, 376meV and 478meV, and are attributed to  $\Delta S_z = 1$  to 5 spin-flip excitations on the antiferromagnetic ground state. In this talk, we examine the dispersive behavior of these spin excitations, and discuss how these multiple spin excitations take place in the RIXS optical process.

\*This work is supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences, Early Career Award Program and KAKENHI.

[1] A. Hariki *et al.*, Phys. Rev. B **101**, 115130 (2020).

[2] A. Hariki *et al.*, Phys. Rev. Lett. **121**, 126403 (2018).



# Can we kill a hole quasiparticle in an Ising antiferromagnet on a Bethe lattice?

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We show that the density of states of the  $t$ - $J_z$  model on a Bethe lattice, regardless of lattice dimension, is equivalent to the spectral function of a non-interacting fermionic chain in an external potential. We investigate this correspondence and are able to understand the well-known  $t$ - $J_z$  density of states from a different perspective, whose advantage is a very natural interpretation of quasiparticle peaks as bound states in a potential well. Moreover, this setting allows us to observe the appearance and disappearance of quasiparticles by slightly modifying the  $t$ - $J_z$  model.

# Physics of strong-electron correlations: $\text{CoTiO}_3$ , $\text{Ba}_2\text{YMoO}_6$ and $\text{CeRh}_2\text{Si}_2$

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$\text{CoTiO}_3$  is suggested as candidate to Quantum Spin Liquid state ( $T_N=37$  K).  $\text{CeRh}_2\text{Si}_2$  is regarded as Kondo-insulator antiferromagnet ( $T_N=35$  K). By analysis of magnetic and electronic properties we have derived the low-energy discrete electronic structure which turns out to be associated with on-site localized states of strongly-correlated  $\text{Co}^{2+}(3d^7)$ ,  $\text{Mo}^{5+}(4d^1)$ ,  $\text{Ce}^{3+}(4f^1)$  ions. Derived states turn out to be predominantly described by crystal-field (CEF) and the relativistic spin-orbit interactions. The crystal field, produced by charge-ionic surroundings, can drastically change the atomic-scale magnetic moment, like it happens in case of  $\text{LaCoO}_3$ [1], in which the Co ion becomes nonmagnetic.

We conclude that predominant strong-electron correlations in transition-metal compounds, i.e. compounds containing 3d/4f/5f/4d/5d atoms, are predominantly on-site correlations, with a minor role of intersite correlations needed for realization of the magnetically-ordered state, which is obviously a collective state. CEF, via the multipolar electrostatic interactions, produces orbital order of spin-orbital states in the crystal. In the simplest case the tetragonal symmetry alone align electronic orbitals, and associated with them magnetic moment, along or perpendicular to the tetragonal axis.

Our atomistic approach allows for unification description of all open-shell transition-metal compounds, including heavy-fermion systems. In our view the observed large low-temperature specific heat originates from difficulties in the removal of the ionic Kramers-doublet ground state causing an opening of the on-site spin gap at low temperatures, even so low as 70mK as is in  $\text{YbRh}_2\text{Si}_2$ . According to us heavy-fermion excitations are spin-like charge-neutral low-energy excitations,  $<0.2\text{meV}$ , in contrary to charge excitations expected by the hybridization Fermi-liquid mechanism.

\*This work is supported by the Program Committee.

[1] Z. Ropka and R. J. Radwanski, Phys. Rev. B **67**, 172401 (2003).

[2] R. J. Radwanski, Z. Ropka, and D. M. Nalecz, Mater. Chem. Phys. **252**, 301 (2019).

# Inverse Hamiltonian design by automatic differentiation

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An ultimate goal of materials science is to deliver materials with desired properties at will. In the theoretical study, a standard approach consists of constructing a Hamiltonian based on phenomenology or first principles, calculating physical observables, and improving the Hamiltonian through feedback. However, there is also an approach that bypasses such a cumbersome procedure, namely, to obtain an appropriate Hamiltonian directly from the desired properties. Solving the inverse problem has the potential to reach qualitatively different principles [1], but most research to date has been limited to quantitative determination of parameters within known models [2–4].

To address these issues, we develop a general framework that can automatically design a Hamiltonian with desired physical properties by using automatic differentiation. In the presentation, by applying it to the quantum anomalous Hall effect, we show that our framework can not only rediscover the Haldane model but also automatically generate a new Hamiltonian that exhibits a six-times larger anomalous Hall effect. In addition, the application to the photovoltaic effect [5] gives an optimal Hamiltonian for electrons moving on a noncoplanar spin texture, which can generate  $\sim 900$  A/m<sup>2</sup> under solar radiation [6].

Since automatic differentiation is a versatile technique, our framework has a wide range of the applicability, such as strongly correlated electron systems, quantum spin systems, and interacting bosonic systems. In addition, it is applicable to a wide range of physical properties to be optimized. Thus, our finding will open up new directions to explore new models and principles in materials science.

[1] E. Lander *et al.*, *Materials Genome Initiative Strategic Plan* (National Science and Technology Council, 2021). [2] G. L. W. Hart *et al.*, *Nature Materials* **4**, 391 (2005). [3] R. Tamura and K. Hukushima, *Phys. Rev. B* **95**, 064407 (2017). [4] H. Fujita *et al.*, *Phys. Rev. B* **97**, 075114 (2018). [5] R.C.Miller, *Phys. Rev.* **134**, A1313 (1964). [6] K. Inui and Y. Motome, arXiv:2203.07157 (2022).

## Seeking for conditions that could improve the thermoelectric efficiency in quantum dots systems

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Employing universal relations obtained recently for the Onsager coefficients in the linear regime at the symmetric point of the single impurity Anderson model [1], and using the Mahan-Sofo parameter [2], we obtain conditions for the quantum scattering phase shift associated with the asymptotic Carnot's limit for the thermoelectric efficiency. We show that with a single quantum dot at the Kondo regime is impossible to achieve the conditions that causes the improving of the thermoelectric efficiency.

We study a system of two coupled identical quantum dots, without inter-dot correlations and preserving one dot in the electron-hole symmetric point; employing analogies between this system -similar to a quantum dot in the electron-hole symmetric point, immersed in a non ballistic quantum wire- and the original system -a quantum dot at the symmetric electron-hole point, immersed in a ballistic quantum wire-; we shows that is possible to obtain conditions for the quantum phase shift -linked to charge fluctuations in one of the quantum dots- that satisfy the conditions associated with enhance the thermoelectric efficiency in this system.

We discuss possible temperature values and conditions that would be linked with the experimental research of our theoretical results.

[1] D. F. Aranguren-Quintero *et al.*, Phys. Rev. B **103**, 085112 (2021).

[2] G. D. Mahan and J. O. Sofo, Proc. Natl. Acad. Sci. USA **93**, 7436-7439 (1996).

## Universality of Transport in Holographic Lattices

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The study of densely entangled systems has long been a challenge, as perturbative methods fail to describe the strong-coupling physics involved. Using the Holographic Duality, we can use black hole physics to study the generic properties of densely entangled systems. In particular, using sophisticated numerical techniques we are able to break translational symmetry in two dimensions. We study a range of AC and DC (magneto)transport properties, which produce some very intriguing results.

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## Holographic quasinormal modes and cuprates physics

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High  $T_c$  cuprates and other bad metals show an emerging mid-IR peak in the optical conductivity when temperature increase much above 200K. Inspired by computations in holographic strange metals using the AdS/CFT correspondence, we show a model that can explain this phenomenon. Assuming that bad metal transport is hydrodynamic, lattice effects can cause an interaction between the conventional Drude hydrodynamic pole and an unklapped charge-diffusion mode. This interaction causes the observed emergent mid IR peak.

# Sine-square deformed mean-field theory and its application to spin-orbit coupled systems

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We propose an efficient protocol that can accurately evaluate quantum states with large-scale emergent structures. There is a growing demand to understand such phases including magnetic skyrmions [1], twisted bilayer graphene [2], and high-Tc cuprates with doping [3]. However, an accurate description of these phases in theory was very difficult. All known methods require a priori knowledge of their structure or period, and the results often depend on the numerical conditions.

Our protocol, sine-square deformed mean-field theory, overcomes this issue [4]. We spatially deform a real-space mean-field Hamiltonian on a finite-size cluster using a sine-squared envelop function, which is known to keep the nature of the system unchanged and suppressing the boundary and finite-size effects. The obtained quantum state is insensitive to the mismatch of the order and lattice, and the result for the thermodynamic limit is already obtained for a relatively small size without bias. We demonstrate the usefulness of our proposed method by applying it to hole-doped and spin-orbit coupled Mott insulators. In particular, we elucidate the nature of very long-period spin-density waves induced by the interplay between strong electron correlation and Rashba spin-orbit coupling. Using the obtained results and the SU(2) gauge field description of spin-orbit coupling, we also show the deep connection between SU(2) gauge-invariant quantities and the magnetic ordering.

[1] U. K. Rößler *et al.*, *Nature* **442**, 797 (2006), S. Mühlbauer *et al.*, *Science* **323**, 915 (2009), X. Z. Yu *et al.*, *Nature* **465**, 901 (2010), S. Heinze *et al.*, *Nat. Phys.* **7**, 713 (2011).

[2] Y. Cao *et al.*, *Nature* **556**, 43 (2018).

[3] J. G. Bednorz and K. A. Müller, *Z. Phys. B* **64**, 189 (1986), T. Wu *et al.*, *Nature* **477**, 191 (2011).

[4] M. Kawano and C. Hotta, *Phys. Rev. Research* **4**, L012033 (2022).

# Tensor network algorithms for 3D quantum systems with applications to the Shastry-Sutherland model

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Tensor network algorithms have proven to be very competitive methods for the study of one- and two-dimensional strongly correlated systems. An important advantage of these techniques is that they allow for the study of fermionic and frustrated models, which are notoriously hard to simulate using quantum Monte Carlo algorithms due to the negative sign problem. Applications to three-dimensional systems, however, are a lot more limited because of the rapid increase in computational cost for most algorithms.

In this talk, I will present some of our progress in the development of tensor network algorithms to simulate 3D quantum models directly in the thermodynamic limit. I will discuss several contraction methods and show benchmarking results for the 3D Heisenberg and 3D Bose-Hubbard models. I will then switch focus to a technique designed for layered 2D systems. This technique will be applied to study the effect of an interlayer coupling on the phase diagram of the Shastry-Sutherland model, which is an effective model of the layered compound  $\text{SrCu}_2(\text{BO}_3)_2$ , that, as a function of pressure, exhibits a phase transition from a dimer phase into a non-magnetic plaquette phase, followed by a transition into an antiferromagnetic phase.



## **Tight-binding models coupled to quantum light**

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The study of theoretical models to describe the interaction between light and matter from fundamental principles has become a central issue in the last years, following the detection [1] and subsequent [2] resolution of gauge ambiguities in fundamental models of Quantum Optics.

It was then revealed that studying regimes of interaction in which the coupling strength is comparable to the frequencies of the system requires the addition of the photonic field to arbitrary order in the Hamiltonian. In the case of tight-binding models for strongly correlated electrons, this can be achieved through the so-called Peierls substitution, a dressing of the hopping amplitudes proportional to the exponential of the photonic operators.

In this work [3], we propose an analytical approach to the highly-nonlinear Peierls Hamiltonian through an expansion in the basis of number of photons, which allows to truncate it to one-photon processes without incurring in the trivial linearization of the light-matter coupling. For the fermionic system, we consider the case of the well-known SSH chain, a canonical example of topological insulators, as a test ground of our results.

We find that our approach reproduces very nicely the exact results for the photon dynamics and how they are influenced by the interaction. Similarly, the truncated model captures the change in the properties of the electronic system and the topological phase transitions it undergoes due to the coupling with the photons. We investigate the consequences for both open and periodic boundary conditions.

[1] Phys. Rev. A 98, 053819 (2018)

[2] Nature Physics 15, 803 (2019)

[3] Soon on the arxiv

# Anderson localization in fractional quantum Hall effect at $\nu = n/(2n + 1)$

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The interplay between interaction and disorder-induced localization is of fundamental interest. This article addresses localization physics in the fractional quantum Hall state, where both interaction and disorder have nonperturbative consequences. We provide compelling theoretical evidence that the localization of a single quasiparticle of the fractional quantum Hall state at filling factor  $\nu=n/(2n+1)$  has a striking quantitative correspondence to the localization of a single electron in the  $(n+1)$ th Landau level [1]. By analogy to the dramatic experimental manifestations of Anderson localization in integer quantum Hall effect, this leads to predictions in the fractional quantum Hall regime regarding the existence of extended states at a critical energy, and the nature of the divergence of the localization length as this energy is approached. Within a mean field approximation these results can be extended to situations where a finite density of quasiparticles is present.

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[1] Songyang Pu, G. J. Sreejith, and J. K. Jain, to be published on Phys. Rev. Lett (2022)

# Quantum Kibble-Zurek mechanism and incommensurate-commensurate phase transitions in chains of Rydberg atoms

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Rydberg atoms have become an ideal platform for studying isolated quantum many-body systems. By controlling the laser detuning and the inter-atomic distance, one can realize a wide variety of critical phenomena, in particular, the commensurate-incommensurate quantum phase transitions. We address this problem numerically by simulating the critical real-time dynamics in isolated non-equilibrium chains of Rydberg atoms. Using the time-evolving block decimation algorithm, we explore the nature of the commensurate-incommensurate phase transition through the Kibble-Zureck mechanism. We study the isolated conformal points surrounded by the new types of chiral quantum phase transition in a way that maximally resembles the actual experimental protocol. The implication of the finite-size effect will be briefly discussed.

# Critical Properties of 1-dim Bose-Hubbard model with a Limited Amount of Entanglement

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Entanglement is a convenient tool to quantify quantum correlations in quantum critical systems. Diverging correlation lengths near criticality are accompanied by a sharp increase in entanglement. How critical properties are modified by a limited amount of entanglement is an interesting question. In this work, we study the critical properties of the Mott-insulator-to-superfluid transition in the ground state of the one-dimensional Bose-Hubbard model, represented by the matrix-product states, where the size of matrices,  $\chi$ , characterize how much entanglement is included.

A finite amount of entanglement certainly introduces a length scale defining the range of quantum correlations. However, we find that the sharp signal of the transition rather remains than blurred by the finite length scale, contrary to the common scenario formulated for finite-size scaling. This occurs through a first-order transition. The transition also occurs from the insulating to a mean-field-like conducting phase, followed by a more strongly entangled state. The entanglement spectrum shows the behavior of the universal distribution predicted by the conformal field theory at the critical points whose positions are shifted significantly depending on  $\chi$ . Some numerical estimates of numbers, such as exponents and transition points, are discussed.

# Critical dielectric susceptibility at a magnetic BEC quantum critical point

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We report on the latest developments on the unique physics displayed by the frustrated quantum magnet  $\text{Rb}_2\text{Cu}_2\text{Mo}_3\text{O}_{12}$ . Much has been argued about the magnetic and dielectric properties of this quasi-one-dimensional magnet, including the existence of ferroelectricity driven by exotic spin-chiral order [1,2]. However, the lack of single-crystal samples was a patent problem, hampering further understanding of the underlying relevant physical mechanisms.

We succeeded in growing macroscopic crystalline samples of  $\text{Rb}_2\text{Cu}_2\text{Mo}_3\text{O}_{12}$ , which brought along a number of important breakthroughs [3,4], including key insight on its ferroelectric behaviour. Of particular interest are the results regarding the magnetic-field-tuned BEC of magnons. The significant magnetoelectric coupling in this material allowed to directly measure channel the critical susceptibility at a BEC transition from the dielectric, a quantity that is usually experimentally inaccessible or even nonphysical. The observed power-law behaviour is in very good agreement with theoretical expectations for three-dimensional BEC transitions [5]. Additionally, magnetic presaturation phases are revealed in this compound, which may feature exotic order with unconventional broken symmetries.

[1] Y. Yasui, *et al.*, J. Appl. Phys. **113**, 17D910 (2013).

[2] H. Ueda, *et al.*, Phys. Rev. B **101**, 140408(R) (2020).

[3] S. Hayashida, *et al.*, Phys. Rev. B **100**, 134427 (2020).

[4] D. Flavián, *et al.*, Phys. Rev. B **101**, 224408 (2020).

[5] S. Hayashida, *et al.*, Phys. Rev. Research **3**, 033053 (2021).

## ***Spin-liquid of 2 Kondo impurities driven by RKKY coupling with or without frustration***

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The phase diagram of the conventional 2-impurity Kondo model and its relevance to correlated lattice models have been a subject of a long debate. It features Jones-Varma quantum phase transition (QPT) between the Kondo and the RKKY phase, which is unstable against particle-hole asymmetry in the presence of inter-impurity charge transfer. I will present results obtained for a modified 2-impurity model, where each of the impurities is coupled to a different host, and the hosts (not impurities) are directly coupled by spin-spin exchange. The model exhibits Jones-Varma QPT even away from the particle-hole symmetry point. Even more importantly, a second QPT occurs upon tuning the same inter-host coupling to even higher values, where the system forms 2-impurity version of a Kondo-stabilized spin-liquid, a state with large, but not complete spin-spin correlations and non-universal impurity spectral density.

Further evolution of the phase diagram in the presence of frustration shall be also explained. This includes emergence of the phase exhibiting ferromagnetic correlations and stability of the spin-liquid regime. I will also discuss the possibilities for direct realization of these scenarios in quantum-dot structures and their relevance for heavy-fermion materials through dynamical mean-field theory mapping.

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[1] K. P. Wójcik, J. Kroha, arXiv:2106.07519 (2021).

## Electronuclear quantum criticality

J. Banda<sup>1</sup>, D. Hafner<sup>1</sup>, J. Landaeta<sup>1</sup>, E. Hassinger<sup>1,2</sup>, K. Mitsumoto<sup>3</sup>, M. Giovannini<sup>4</sup>,  
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We present here a rare example of electronuclear quantum criticality in a metal. The compound  $\text{YCu}_{4.6}\text{Au}_{0.4}$  is located at an unconventional quantum critical point (QCP). In this material the relevant Kondo and RKKY exchange interactions are very weak, of the order of 1 K. Furthermore, there is a strong competition between antiferromagnetic and ferromagnetic correlations, possibly due to geometrical frustration within the fcc Yb sublattice. This causes strong spin fluctuations which prevent the system to order magnetically. Because of the very low Kondo temperature the  $\text{Yb}^{3+}$  4f-electrons couple weakly with the conduction electrons allowing the coupling to the nuclear moments of the  $^{171}\text{Yb}$  and  $^{173}\text{Yb}$  isotopes to become important. Thus, the quantum critical fluctuations observed at the QCP derive not from purely electronic states but from entangled 'electronuclear' states. This is evidenced in the anomalous temperature and field dependence of the specific heat at very low temperatures [1].

[1] J. Banda *et al.*, to be published.

# Quantum critical fluctuations in the non-Fermi liquid system CeRh<sub>4</sub>Al<sub>15</sub> investigated using muon spin relaxation

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**Abstract:** We studied the spin dynamics of a non-Fermi-liquid (NFL) system CeRh<sub>4</sub>Al<sub>15</sub>, using zero-field (ZF) and longitudinal-field (LF) muon spin relaxation ( $\mu$ SR) measurements. ZF- $\mu$ SR measurements do not reveal any sign of long-range magnetic ordering down to 70 mK. The electronic relaxation rate ( $\lambda$ ) below 0.5 K increases rapidly and shows a thermal activation-like characteristic [ $T^* \ln(T) \sim T$ ] over the entire measured temperature range up to 4 K, indicating the presence of low energy spin fluctuations in CeRh<sub>4</sub>Al<sub>15</sub>. LF- $\mu$ SR measurement shows a time-field ( $t/H^n$ ) scaling of the  $\mu$ SR asymmetry indicating a quantum critical behaviour of this compound, consistent with the logarithmic divergence of the heat capacity ( $C_p/T \sim -\ln T$ ) and magnetic susceptibility ( $\chi \sim -\ln T$ ) and  $T$ -linear resistivity ( $\rho - \rho_0 \sim T^n$  with  $n = 0.92$ ) at low temperature observed by S. Nesterenko et al [1]. These features collectively confirm that CeRh<sub>4</sub>Al<sub>15</sub> exhibits NFL behaviour close to a  $T \rightarrow 0$  K quantum critical point (QCP).

[1] S. Nesterenko, V. Avzuragova, A. Tursina and A.M. Strydom, J. Alloys and Comp. **792**, 1061 (2019)



# The effect of next-neighbor interactions on the ground-state of Bose-Fermi mixtures

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We investigate a mixture composed of two-color fermions and scalar bosons in the hard-core limit, considering local interspecies and intraspecies interactions as well as the next-neighbor interactions between fermions or bosons. It is well known that the interplay between commensurability and local repulsive interactions generates diverse Mott insulator states in Bose-Fermi mixtures [1,2,3]. Also in the absence of bosons, the ground state of two-color fermions with local and next-neighbor interactions exhibit a rich phase diagram.

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[1] R. Avella, J. J. Mendoza-Arenas, R. Franco, J. Silva-Valencia, Phys. Rev. A **100**, 063620 (2019).

[2] R. Avella, J. J. Mendoza-Arenas, R. Franco, J. Silva-Valencia, Phys. Rev. A **102**, 033341 (2020).

[3] R. Guerrero-Suarez, J. J. Mendoza-Arenas, R. Franco, J. Silva-Valencia, Phys. Rev. A **103**, 023304 (2021).

## Isotopically pure YbRh<sub>2</sub>Si<sub>2</sub> single crystals with <sup>171</sup>Yb, <sup>173</sup>Yb, and <sup>174</sup>Yb

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A central question in strongly correlated electron systems concerns the interplay between quantum criticality and unconventional superconductivity. This interplay was extensively studied in Ce-based heavy-fermion systems. Superconductivity was also discovered in the Yb-based quantum-critical material YbRh<sub>2</sub>Si<sub>2</sub> at 2 mK [1]. The superconducting transition is accompanied by nuclear magnetic order of Yb, however, the interplay between electronic and nuclear moments and its impact on the superconductivity is not settled. Recently, pronounced differences were observed in the temperature-magnetic field phase diagrams for a <sup>174</sup>YbRh<sub>2</sub>Si<sub>2</sub> crystal in comparison to a crystal with a natural mixture of Yb-isotopes (70% of the Yb-isotopes do not carry a nuclear spin) [2]. For that reason, it is essential to further investigate YbRh<sub>2</sub>Si<sub>2</sub> crystals with well-defined Yb nuclear moments.

In this contribution, we present the successful growth of single crystals with three different nuclear spins I, <sup>171</sup>Yb (I = 1/2), <sup>173</sup>Yb (I = 5/2), and <sup>174</sup>Yb (I = 0). One crucial step towards isotope-pure crystals was the development of a metallothermic-reduction experiment, as the isotope pure Yb is only available as oxide. Subsequently, the single crystals were grown using the established high-temperature indium-flux method [3]. We determined the precise isotopic composition in the different crystals using the LA-ICPMS technique and confirmed an isotopic enrichment of 95.5%, 92.6%, and 99.2% for <sup>171</sup>Yb, <sup>173</sup>Yb, and <sup>174</sup>Yb, respectively. Heat-capacity measurements down to 20 mK with field along the c-direction were performed, to study the suppression of the electronic magnetic transition and the occurrence of quantum-critical behavior for the three different crystals.

[1] E. Schuberth *et al.*, *Science* **351**, 485 (2016).

[2] D. H. Nguyen *et al.*, *Nat. Commun.* **12**, 4341 (2021).

[3] C. Krellner *et al.*, *Philos. Magazine* **92**, 2508 (2012).

# Lock-in Behavior of the Partially Frustrated Order in CePdAl

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CePdAl is one of the few systems that combines a metallic ground state with geometrical frustration. Its distorted kagome structure gives rise to an incommensurate antiferromagnetic order in which 1/3 of the Ce magnetic moments remain frustrated down to at least 20 mK. If this order is suppressed by hydrostatic pressure, unusual quantum criticality with spin-liquid properties emerges [1,2]. Surprisingly, the propagation vector of the partially frustrated antiferromagnetic phase exhibits a pronounced temperature dependence below its phase transition at  $T_N \approx 2.7$  K in zero magnetic field. At temperatures below  $T_L \approx 1.9$  K, the magnetic structure locks in to a propagation vector with still an incommensurate component along the  $c$  axis [3]. We use thermal expansion and magnetostriction measurements on a high-quality single crystal to track this lock-in transition to higher magnetic fields and construct the resulting magnetic phase diagram. The anisotropy of the uniaxial stress and strain dependences of  $T_L$  are estimated. The nature of the lock-in transition is discussed in terms of geometrical frustration and glass transition physics.

[1] H. Zhao *et al.*, Nature Physics **15**, 1261 (2019)

[2] M. Majumder *et al.*, arXiv:2202.11975 [cond-mat.str-el] (2022)

[3] L. Keller *et al.*, Appl. Phys. A **74** [Suppl.], 686 (2002)

# Effects of Kondo Fluctuations on the Néel Quantum Phase Transition

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The universal quantum critical behavior of the Néel transition in the presence of conduction electrons is studied by renormalization group analysis. We first consider the case of a small Fermi surface where the Néel vector cannot connect two points on it. By integrating out the fermions we obtain a nonlinear sigma model (NLSM) with an additional Kondo-induced vertex. Near the lower critical dimension, this vertex is irrelevant at the Néel quantum critical point. The system exhibits a multi-critical fixed point at finite coupling with broken Lorentz invariance.

We then consider a quantum antiferromagnet coupled to Dirac electrons on the honeycomb lattice. In this case it is not possible to integrate out the fermionic degrees of freedom. We analyze the universal critical behavior using a Gross-Neveu-Yukawa (GNY) type low energy theory that describes a Landau-damped NLSM coupled to gapless Dirac fermion excitations.

# Effects of disorder on quantum phase transitions of two-dimensional Dirac semimetals

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We consider the effects of weak quenched fermionic disorder on the quantum-phase transition between the Dirac semimetal and charge density wave insulator in two spatial dimensions. The symmetry breaking transition is described by the Gross-Neveu-Yukawa (GNY) theory of Dirac fermions coupled to an Ising order parameter field. Treating the disorder using the replica method, we consider chemical potential, vector potential (gauge), and random mass disorders, which all arise from nonmagnetic charged impurities. We self-consistently account for the Landau damping of long-wavelength order-parameter fluctuations by using the nonperturbative RPA resummation of fermion loops and compute the renormalization-group (RG) flow to leading order in the disorder strength and  $1/N$  ( $N$  the number of Dirac fermion flavors). We find two fixed points, the clean GNY critical point, which is stable against weak disorder, and a dirty GNY multicritical point, at which the chemical potential disorder is finite and the other forms of disorder are irrelevant. We investigate the scaling of physical observables at this finite-disorder multicritical point which breaks Lorentz invariance and gives rise to distinct non-Fermi liquid behavior.

The work presented here was first published in Ref. [1].

[1] M. D. Uryszek *et al.*, Phys. Rev. B **105**, 075143 (2022).

# Tuning the Van Hove singularity in $\text{Sr}_3\text{Ru}_2\text{O}_7$

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$\text{Sr}_3\text{Ru}_2\text{O}_7$  is a prime example of a strongly correlated oxide, displaying phenomena associated with a quantum critical end point and the formation of complex electronic and magnetic phases [1,2]. The physics of this material is associated with an underlying Van Hove singularity in the band structure [3] and tuning its properties has been pursued through various strategies including magnetic field, pressure, uniaxial strain and doping.

Here we utilise isovalent Ba doping on the Sr sites as a chemical pathway to expand the lattice and increase the tolerance factor. This larger ionic radius is driving the system closer to the aristotype tetragonal structure with no octahedral rotation, as realized in the single layer compound  $\text{Sr}_2\text{RuO}_4$ . Ba being an out-of-plane dopant it is expected to effectively tune the band dispersion with minimal impurity scattering / broadening. We present high resolution neutron diffraction, magnetisation and specific heat measurements of the series  $(\text{Sr}_{1-x}\text{Ba}_x)_3\text{Ru}_2\text{O}_7$  for  $x \leq 0.1$ . Our thermodynamic data suggest the Van Hove singularity shifting towards the Fermi energy and crossing it at approximately  $x = 0.08$ , with a subsequent sharp decrease in the density of states. The specific heat with doping can be well understood within the phase diagram of the multicritical Lifshitz point in this material [4]. Combining this data with our recent high resolution magnetostriction experiments detecting quantum oscillations, we will discuss an experimental pathway to increasing the strength of the Van Hove singularity on the physics of  $\text{Sr}_3\text{Ru}_2\text{O}_7$  while simultaneously moving it towards the chemical potential.

\*This work is supported by the EPSRC grants EP/P024564/1 and EP/T011130/1.

[1] A. P. Mackenzie *et al.*, *Physica C* **481**, 207 (2012)

[2] C. Lester *et al.*, *Nature Communications* **12**, 5798 (2021)

[3] A. Tamai *et al.*, *Physical Review Letters* **101**, 026407 (2008)

[4] D.V. Efremov *et al.*, *Physical Review Letters* **123**, 207202 (2019)

# Electrical transport in MBE-grown $\text{YbRh}_2\text{Si}_2$ thin films at mK temperatures

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$\text{YbRh}_2\text{Si}_2$  is a “strange metal” heavy fermion compound that exhibits linear-in-temperature electrical resistivity over 3.5 orders of magnitude in temperature [1]. Recently, first thin films of this compound were successfully grown by molecular beam epitaxy (MBE) [2]. This allowed to perform THz time-domain transmission spectroscopy experiments down to 1.4 K, the low-temperature limit of that setup, revealing energy-over-temperature scaling of the optical conductivity [2]. A second generation of MBE films was grown by a modified growth technique, using Knudsen cells for all elements instead of the previously used e-beam evaporation system for Rh and Si [3]. These new films were used in a very recent shot noise experiment, down to temperatures of a few K [4]. To investigate how properties that can only be studied in thin films change upon tuning the material across its quantum critical point, measurements in the mili-Kelvin range are needed. Here, we report on our efforts towards this goal. We have developed a new sample holder and thermal anchoring technique as well as an advanced high-resolution resistivity measurement setup. We report measurements down to 10 mK.

[1] D. H. Nguyen, A. Sidorenko, M. Taupin, G. Knebel, G. Lapertot, E. Schuberth, S. Paschen, Superconductivity in an extreme strange metal, *Nat. Commun.* **12**, 4341(2021).

[2] L. Prochaska, X. Li, D.C. MacFarland, A. M. Andrews, M. Bonta, E. F. Bianco, S. Yazdi, W. Schrenk, H. Detz, A. Limbeck, Q. Si, E. Ringe, G. Strasser, J. Kono, S. Paschen, Singular charge fluctuation at a magnetic quantum critical point, *Science* **367**, 6475 (2020).

[3] E. Bakali, W. Artner, M. Beiser, J. Bernardi, H. Detz, G. Eguchi, M. Giparakis, C. Herzig, A. Limbeck, H. Nguyen, L. Prochaska, A. Prokofiev, S. Schwarz, W. Schrenk, G. Strasser, R. Svagera, M. Taupin, A. S. Thirsfeld, M. Waas, X. Yan, D. A. Zocco, A. M. Andrews, S. Paschen, A Knudsen cell approach for the molecular beam epitaxy of the heavy fermion compound  $\text{YbRh}_2\text{Si}_2$ , *J. Cryst. Growth* (submitted, 2021).

[4] L. Chen, D. T. Lowder, E. Bakali, A. M. Andrews, W. Schrenk, M. Waas, R. Svagera, G. Eguchi, L. Prochaska, Qimiao Si, S. Paschen, and Douglas Natelson, Shot noise indicates the lack of quasiparticles in a strange metal (submitted, 2022).

# Tunneling spectroscopy through the magnetic phases of $\text{Ce}(\text{Ru}_{0.92}\text{Rh}_{0.08})_2\text{Si}_2$

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$\text{CeRu}_2\text{Si}_2$  is an archetypical heavy fermion compound with a large electronic specific heat at low temperatures and no magnetic order. Application of a magnetic field produces a polarized phase through a metamagnetic transition at 8 T.  $\text{CeRh}_2\text{Si}_2$  presents AFM order below about 36 K.  $\text{Ce}(\text{Ru}_{0.92}\text{Rh}_{0.08})_2\text{Si}_2$  presents an antiferromagnetic phase (AFM) below 5 K. At very low temperatures, AFM vanishes above 2.5 T, and one finds a correlated paramagnetic phase. When further increasing the magnetic field, the latter becomes, above 5.5 T, a field induced polarized magnetic phase. The electronic properties of  $\text{Ce}(\text{Ru}_{0.92}\text{Rh}_{0.08})_2\text{Si}_2$  are highly susceptible to a magnetic field, as shown by a strong magnetic field dependent specific heat and a thermopower that changes sign with field. However, the actual magnetic field dependence of the electronic band structure is still debated. Here we present atomically resolved tunneling spectroscopy studies in a millikelvin Scanning Tunneling Microscope across the magnetic phase diagram. We discuss Kondo hybridization as a function of the atomic position and of the magnetic field as well as the influence of the Zeeman splitting on the electronic density of states.



# Correlation between Antiferromagnetic and Charge-Density-Wave Order in $\text{UPt}_2\text{Si}_2$ Studied by Resonant X-Ray Scattering

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The intermetallic uranium compound  $\text{UPt}_2\text{Si}_2$  crystallizes in the tetragonal  $\text{CaBe}_2\text{Ge}_2$ -type structure (space group:  $P4/nmm$ ,  $D_{4h}^7$ , No. 129) [1]. This crystal structure is characterized by an inversion-symmetric pair of two U ions, both of which are located at the locally inversion-symmetry broken site of the unit cell. It shows antiferromagnetic (AFM) ordering at  $T_N \sim 35$  K with the propagation vector  $\mathbf{Q} = 0$ , where magnetic moments ( $\sim 1.7 \mu_B \parallel c$ ) of the U pair are coupled antiferromagnetically [2,3]. This AFM ordering breaks global inversion-symmetry of the system. Moreover, recent polarized neutron diffraction measurement revealed that the charge-density-wave (CDW) order occurs at  $T_{\text{CDW}} \sim 320$  K and it coexists with the AFM order below  $T_N$  [4]. However, the relationship between these two-types of order has not been investigated yet. In the present study, we performed resonant X-ray scattering experiments at KEK PF BL-11B using synchrotron X-rays of 3.72 keV (U  $M_4$ -edge) and 3.02 keV (Pt  $M_2$ -edge) and observed signals suggesting that the magnetic structure is modulated by the CDW order. We will report the details of our experiments and discuss the correlation between the CDW and AFM order in this system.

[1] H. Ptasiwicz-Bąk *et al.*, Solid State Commun. **55**, 601 (1985).

[2] R. A. Steeman *et al.*, J. Phys.: Condens. Matter **2**, 4059 (1990).

[3] S. Süllow *et al.*, J. Phys. Soc. Jpn. **77**, 024708 (2008).

[4] J. Lee *et al.*, Phys. Rev. B **102**, 041112 (2020).

## Observation of current-induced magnetization in the antiferromagnetic state of $\text{UPt}_2\text{Si}_2$

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$\text{UPt}_2\text{Si}_2$  has a primitive tetragonal  $\text{CaBe}_2\text{Ge}_2$ -type structure with space group  $P4/nmm$  ( $D_{4h}^7$ , No. 129) and exhibits charge-density-wave (CDW) [1] and antiferromagnetic (AF) orders [2] at  $\sim 320$  K ( $\equiv T_{\text{CDW}}$ ) and  $\sim 35$  K ( $\equiv T_{\text{N}}$ ), respectively. This system has two U ions in the unit cell, which occupy the  $2c$  site ( $2mm, C_{4v}$ ) with no local inversion symmetry. On the other hand, there is an inversion center at the midpoint of the bond connecting both U ions, and the entire crystal has global inversion symmetry in the paramagnetic phase, if the effect of CDW can be ignored. Interestingly, in the AF ordered phase, the 5f magnetic moments of the two U ions align antiparallel along the  $c$  axis (corresponding to the ordering wave vector of  $\mathbf{Q} = 0$ ), resulting in a spontaneous breaking of the global inversion symmetry of the system. This situation can effectively be regarded as a uniform order of odd-parity augmented magnetic multipoles (monopoles and quadrupoles) [3,4], which is expected to manifest cross-correlation responses associated with the AF order in a metal as found in  $\text{UNi}_4\text{B}$  [5,6]. We performed magnetization measurements on a single-crystalline sample of  $\text{UPt}_2\text{Si}_2$  under electric currents and observed that static magnetization is induced by applying electric currents below  $T_{\text{N}}$ . Details of the experimental results and a discussion of the obtained magnetoelectric tensor will be presented.

[1] J. Lee *et al.*, Phys. Rev. B **102**, 041112(R) (2020).

[2] R. A. Steeman *et al.*, J. Phys.: Condens. Matter **2**, 4059 (1990).

[3] S. Hayami and H. Kusunose, J. Phys. Soc. Jpn. **87**, 033709 (2018).

[4] H. Watanabe and Y. Yanase, Phys. Rev. B **98**, 245129 (2018).

[5] S. Hayami, H. Kusunose, and Y. Motome, Phys. Rev. B **90**, 024432 (2014).

[6] H. Saito *et al.*, J. Phys. Soc. Jpn. **87**, 033702 (2018).

## Properties of UPd<sub>2</sub>Si<sub>2</sub> close to putative Lifshitz point

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UPd<sub>2</sub>Si<sub>2</sub> crystallizes with a tetragonal unit cell of the ThCr<sub>2</sub>Si<sub>2</sub> type. It exhibits complex magnetic phase diagram, constructed for magnetic field  $H$  applied parallel to the tetragonal  $c$  axis. It comprises three ordered phases, namely incommensurate longitudinal spin wave (ICLSW), ferrimagnetic (FiM) and simple antiferromagnetic (AFM) [1]. It is worth noting that the magnetic phase diagrams of UPd<sub>2</sub>Si<sub>2</sub> reported in the literature show some discrepancies [1,2], most probably because of small differences in crystal stoichiometry. However, in each case, paramagnetic (P), FiM and ICLSW phases tend to merge in high magnetic fields at a single point, that might be a bicritical Lifshitz point (LP), whose “critical behavior is strikingly different from any other” [2,3]. It should be added, that to date the existence of magnetic LP has been unambiguously confirmed solely for MnP [4].

In order to verify the hypothesis of the existence of LP in UPd<sub>2</sub>Si<sub>2</sub>, we prepared several single crystals of the compound, and characterized their properties by means of thermodynamic and electrical transport measurements. As a result, three types of magnetic phase diagrams were constructed, two of them being consistent with those reported in the literature [1,2]. Regardless the confirmed small differences, the boundaries between P, FiM and ICLSW phases were found to merge in high magnetic fields. In this contribution, we will analyze the magnetization, electrical resistivity, specific heat and thermal expansion data collected close to the putative Lifshitz point.

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[1] T. Honma, H. Amitsuka, S. Yasunami, K. Tenya, T. Sakakibara, H. Mitamura, T. Goto, G. Kido, S. Kawarazaki, Y. Miyako, K. Sugiyama, M. Date, *J. Phys. Soc. Japan* **67**, 1017 (1998).

[2] T. Plackowski, D. Kaczorowski, J. Sznajd, *Phys. Rev. B* **83**, 174443 (2011).

[3] R. M. Hornreich, M. Luban, S. Shtrikman, *Phys. Rev. Lett.* **35**, 1678 (1975).

[4] Y. Shapira, C. C. Becerra, N. F. Oliveira, T. S. Chang, *Phys. Rev. B* **24**, 2780 (1981).

# Metal-insulator transition in A-site ordered perovskite oxides $ACu_3Fe_4O_{12}$

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A-site ordered perovskite oxides with chemical formula  $AA'_3B_4O_{12}$  show a rich variety of physical properties. In this material class, electronic and magnetic interactions between two transition metal ions sitting on the A' and B-site trigger new phenomena which are absent or structurally forbidden in simple  $ABO_3$  perovskites. In particular,  $ACu_3Fe_4O_{12}$  (A=Ca, La, Pr-Nd, Sm-Lu) family exhibits two distinct metal-insulator transitions (MITs) accompanied by 1) a charge disproportionation between the Fe ions or 2) a charge transfer between the Cu and Fe ions [1,2].

To understand the driving mechanism of the MITs in  $ACu_3Fe_4O_{12}$ , we perform a computational study using local density approximation (LDA)+ $U$  and +dynamical mean-field theory (DMFT) methods. We identify two instabilities inherent in  $ACu_3Fe_4O_{12}$  to opening the charge gap: Peierls instability (for A=Ca) and magnetic instability (A=La, Pr-Nd, Sm-Tb). The leading instability can be switched by an electron doping, achieved by substituting the A-site ion with a different valence state. The spin correlation function calculated by the LDA+DMFT method reveals the characteristic spin dynamics in  $CaCu_3Fe_4O_{12}$  and  $LaCu_3Fe_4O_{12}$ . In the former, the Fe spin moment is largely screened by the ligand holes, whereas in the latter, the ligand holes couple to the Cu spin dominantly, forming the so-called Zhang-Rice singlet on the  $CuO_4$  plaquette.

With those numerical results, we explain the role of the structural distortion, magnetic ordering, and electronic correlation effect on the MITs. We also discuss the A-site dependence of the magnetic ordering in the  $Ln^{3+}Cu_3Fe_4O_{12}$  series (Ln=lanthanide).

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[1] I. Yamada, J. Ceram. Soc. Jpn. **122**, 846 (2014).

[2] Y. Shimakawa, J. Phys. D: Appl. Phys. **49**, 119601 (2016).

# Optical signature of strain-induced ferromagnetism in LaCoO<sub>3</sub> thin film

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We have performed spectroscopic ellipsometry measurements on a 22 nm LaCoO<sub>3</sub> film on LSAT substrate between 7-300 K using Woollam VASE and IR-VASE ellipsometers. The obtained differential optical conductivity,  $ds_1 = s_1(T) - s_1(T=7 \text{ K})$ , demonstrates that while the spectral weight  $N_{eff} = 2mV/\pi e^2 \int \sigma_1(\omega) d\omega$  below 3.5 eV decreases with decreasing temperature in the paramagnetic phase, it starts increasing in the ferromagnetic phase below the transition temperature  $T_c = 80 \text{ K}$ . This observation is indicative of stabilization of the high-spin state in the ferromagnetic phase.

# Ca<sub>3</sub>Ru<sub>2</sub>O<sub>7</sub>: Interplay among degrees of freedom and role of the exchange and correlation

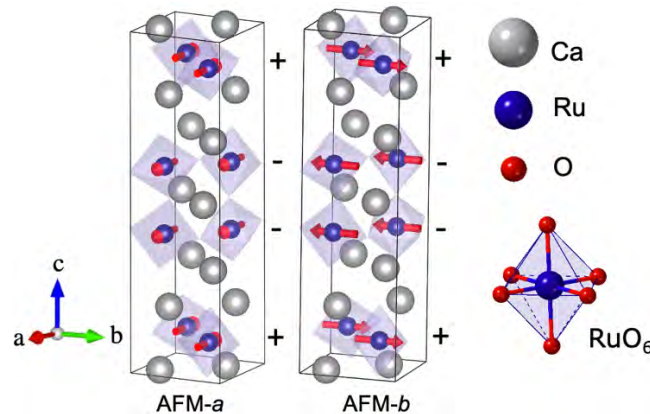
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Ca<sub>3</sub>Ru<sub>2</sub>O<sub>7</sub> is an antiferromagnetic (AFM) polar metal and is considered a fascinating material because it displays a wide range of remarkable electronic phenomena such as colossal magnetoresistance, spin-wave and multiple phase transitions, among others. Understanding these phenomena has been a hard task due to several discrepancies among experiments and between experiment and theory [1]. Recent studies have been given new perspectives about the origin of their phase transitions, evidencing that the wealth of the physical properties is governed by spin-orbit interactions (SOI), strong correlations and structural distortions. However, the role of fundamental interactions such as Coulomb and SOI has not been clarified yet [1-2]. In this research we study the electronic structure of Ca<sub>3</sub>Ru<sub>2</sub>O<sub>7</sub> through ab-initio calculations, and we discuss the interplay among magnetism, Coulomb interaction, spin-orbit coupling and the lattice degrees of freedom using different exchange and correlation approximations. Besides, we explore new paths to manipulate their electronic and magnetic states (see Fig.1) through lattice deformation.



**Figure 1:** Ca<sub>3</sub>Ru<sub>2</sub>O<sub>7</sub> in two antiferromagnetic phases, AFM-a and AFM-b, with ferromagnetic coupling within the layers and antiferromagnetic coupling between the bilayers. The +/- signs represent the relative orientation of the Ru in-plane magnetic moments.

[1] Igor Marković, *et al.* Proceedings of the National Academy of Sciences, 117(27):15524–15529, 2020.

[2] Danilo Puggioni, *et al.* Physical Review Research, 2(2):023141, 2020

# Development of vanadium zigzag chains in layered LiVSe<sub>2</sub> under high pressure

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Electronic instabilities in transition metal compounds often lead to the complex arrangement of orbital molecules in a spin-singlet state at low temperatures. In such systems, a regular and symmetric lattice is expected to be recovered at high temperatures. However, recent local structure studies using the pair distribution function (PDF) have revealed the appearance of local nematic states with local lattice symmetry reduction [1]. These properties appear in layered LiVS<sub>2</sub>, which exhibits a metal-insulator transition at 314 K [2] and forms a V-trimer structure at low temperatures [3]. Although vanadium was thought to form a regular triangular lattice at high temperatures, our PDF analysis reveals that a zigzag chain structure appears locally. In addition, STEM measurements have been used to observe the in-plane short-range ordered structure, revealing that the orientation of the zigzag chains exhibits dynamics that change on the order of seconds [4].

In this study, we have performed synchrotron X-ray structural studies of LiVSe<sub>2</sub>, a selenide analogue of LiVS<sub>2</sub>. LiVSe<sub>2</sub> exhibits metallic behavior over the entire temperature range and shows no phase transition as the temperature decreases. In the electronic phase diagram, the high-temperature metallic phase of LiVSe<sub>2</sub> and the high-temperature phase of LiVS<sub>2</sub> with zigzag chains are connected, and thus the appearance of zigzag chains with dynamics in LiVSe<sub>2</sub> is expected. We have synthesized powder samples of LiVSe<sub>2</sub> and performed synchrotron X-ray diffraction experiments. We found a zigzag chain structure as an average structure and revealed that the zigzag chain structure develops with increasing pressure.

[1] E.S. Bozin *et al.*, Nat. Commun. **10**, 3638 (2019) and more.

[2] N. Katayama *et al.*, Phys. Rev. Lett. **103**, 146405 (2009).

[3] K. Kojima *et al.*, Phys. Rev. B **100**, 235120 (2019).

[4] N. Katayama, K. Kojima *et al.*, npj Quantum Mater. **6**, 16 (2021).

# Photo-induced insulator-to-metal transition and coherent acoustic phonon propagation in $\text{LaCoO}_3$ explored by femtosecond ellipsometry

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We have studied [1] ultrafast dynamics of thin films of  $\text{LaCoO}_3$  and  $\text{La}_{0.5}\text{Sr}_{0.5}\text{CoO}_3$  with femtosecond pump-probe ellipsometry in the energy range of 1.6-3.4 eV. We have observed a large pump-induced transfer of spectral weight in  $\text{LaCoO}_3$  that corresponds to an insulator-to-metal transition. The photo-induced metallic state initially relaxes via a fast process with a decay constant of about 200 fs. Both  $\text{LaCoO}_3$  and  $\text{La}_{0.5}\text{Sr}_{0.5}\text{CoO}_3$  exhibit a significant secondary peak in the 1-30 ps range. Results of measurements on films with different thicknesses demonstrate that it corresponds to a propagation of an acoustic strain pulse. On timescales longer than 100 ps, heat diffusion to the substrate takes place that can be modelled with a bi-exponential decay.

[1] M. Zahradník *et al.*, [arXiv: 2201.02525](https://arxiv.org/abs/2201.02525).



# ***Dynamical mean-field study of collective modes in antiferromagnetically ordered systems***

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We investigate antiferromagnetically ordered systems from weak to strong coupling, focusing on the evolution of collective modes in the crossover between a Slater and a Heisenberg/Mott antiferromagnet. To this aim, we consider the antiferromagnetic phase of the half-filled Hubbard model solved by means of Dynamical Mean Field Theory (DMFT), as this technique is applicable also in the intermediate-to-strong coupling regime, where perturbative methods fail. In particular, we extend the work by Sangiovanni et. al [1], where the difference between static and dynamic mean-field theory for strongly-coupled antiferromagnets was investigated at the one-particle level only, by systematically comparing two-particle dynamical spectra calculated using Random Phase Approximation (RPA) and DMFT in different parameter regimes. Beyond the fundamental understanding of the effects of local correlations of increasing magnitude onto the properties of the Goldstone and Higgs collective modes in the antiferromagnetic phase, our DMFT results will provide the essential building block for a future inclusion of the nonlocal correlations effects in the ordered phase (cfr. L. Del Re et al. [2]) via diagrammatic extensions of DMFT.

\*This work is supported from Operational Programme Research, Development and Education – “Project Internal Grant Agency of Masaryk University” (No. CZ.02.2.69 / 0.0 / 19\_073 / 0016943).

[1] G. Sangiovanni *et. al.*, Phys. Rev. B **76**, 159905 (2007).

[2] L. Del Re and A. Toschi, Phys. Rev. B **104**, 085120 (2021).

## Investigation of role of disorder in pristine cage compound FeGa<sub>3</sub>

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The cage compound FeGa<sub>3</sub> calls attention as a thermoelectric material and as a candidate of half-metallic ferromagnetism for spintronic application. The crystal structure of FeGa<sub>3</sub> is tetragonal P4<sub>2</sub>/mmn, where Fe atoms are surrounded by Ga atoms in a manner that it resembles other semiconductors with a type-cage structure. A small energy gap ( $\Delta$ ) opens at the Fermi energy level ( $E_F$ ) ( $\Delta \approx 0.4$  eV) suggesting that strong electronic correlations disturb the Fe-3d-Ga-4p hybridization, Coulomb repulsion, and  $E_F$ . The competition between these low-lying energy scales sets the ground state of FeGa<sub>3</sub> as a Kondo-insulator-like semiconductor with a diamagnetic ground state [1]. Such an intriguing ground state can be tuned towards an insulator-metal-transition by pressure-induced disruption of the local environment of Fe-Fe dimers [2]. Recent calculations show that a tiny amount of disorder can induce magnetic polarization, and complex structure of in-gap states, together with disruptions of conduction and valence band edges [3].

By the combination of arc-melting furnace, mechanical milling, uniaxial compression, and timely x-ray analysis we managed to quantify deviations of the occupancy number of Fe and Ga sites from those expected in the pristine compound and thus tuning the disorder.

Besides that, our electrical transport and magnetization measurements reveal that hierarchy in Fe and Ga site disorder tunes the ground state of FeGa<sub>3</sub> from semiconducting to a metal arising with a weak ferromagnetism. We discuss these findings inside the framework of Mott-Anderson variable range hopping.

Our results show a new route to reach correlated ground states under elegant controlled disorder.

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[1] Y. Zhang *et al.*, Proc. Natl. Acad. Sci. U.S.A, **115**, 3273 (2018).

[2] G.R Hearne *et al.*, Phys. Rev. B **98**, 020101(R) (2018).

[3] Alvarez-Quiceno, *et al.*, Phys. Rev. B, **102**, 094110 (2020).

# Charge disproportionation and “Hund’s insulating” behavior in different transition metal oxides by DFT+DMFT

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Several materials such as the rare earth nickelates  $RNiO_3$  or the alkaline earth ferrate  $CaFeO_3$  exhibit a metal-insulator transition (MIT) involving a charge-disproportionation of the transition metal cation, resulting in inequivalent crystallographic sites with different nominal cation valence. The MIT coincides with a structural transition involving a “breathing”, i.e. an expansion or contraction, of the oxygen octahedra surrounding the inequivalent cation sites.

Calculations for purely electronic multiband Hubbard models indicate that a charge-disproportionated insulating phase can be stabilized if the Hund’s coupling is relatively strong and the Hubbard interaction is strongly screened [1,2,3]. Nevertheless, coupling to structural degrees of freedom is crucial to stabilize the insulating phase for realistic parameters [1,3,4].

We explore the coupling between charge disproportionation, MIT, and structural distortions using density functional theory in combination with dynamical mean-field theory (DFT+DMFT) for  $RNiO_3$ ,  $CaFeO_3$ , and  $SrCrO_3$ , which map to effective two-orbital, five-orbital, and three-orbital models, respectively. We discuss the relevance of a small or negative charge transfer energy, by comparing a description using an effective  $d$ -only basis with a more extended picture including also the oxygen  $p$  states for the case of  $CaFeO_3$ . This allows us to quantify the occupation in terms of “ligand-holes” and to assess the equivalence of the two different pictures.

This presentation results from collaborations with Maximilian Merkel, Alberto Carta (ETH Zurich), Alexander Hampel, Antoine Georges (Flatiron Institute), and Oleg Peil (Materials Center Leoben).

[1] A. Subedi, O. E. Peil, and A. Georges., Phys. Rev. B **91**, 075128 (2015).

[2] A. Isidori *et al.*, Phys. Rev. Lett. **122**, 186401 (2019).

[3] M. E. Merkel and C. Ederer, Phys. Rev. B **104**, 165135 (2021).

[4] O. E. Peil, A. Hampel, C. Ederer, and A. Georges., Phys. Rev. B **99**, 245127 (2019).

## Modified orbital occupancy induced phase transition of VO<sub>2</sub>

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Vanadium dioxide (VO<sub>2</sub>) has received much attention due to its near room temperature (RT) metal-insulator phase transition. Even though the phase transition mechanism is still controversial scientifically, near RT phase transition offers many potential applications. Therefore, obtaining the controllability of phase transition characteristics such as temperature (T<sub>c</sub>) and transition slope (dp/dT), and resistivity variation (Δρ) are crucial.

In this presentation, we showed the transition characteristics modification of VO<sub>2</sub> via varying film thickness. By carefully examining the structural and chemical variations, we found that the correlation between the asymmetric octahedral structure, orbital occupancy, and the IMT temperature of monoclinic VO<sub>2</sub> films with different in-plane compressive strains are the origin of the transition characteristic variations. As a result, the octahedral structure with low asymmetry, caused by the in-plane compressive strain, increased the splitting between  $d_{||}$  and  $d_{||}^*$  orbitals and the bandwidth of  $\pi^*$ . The modified orbitals suppressed the hybridization of V 3d - O 2p and subsequently increased interdimer hopping energy, lowering the energy barrier for IMT. As a result, the VO<sub>2</sub> with the low asymmetric octahedral structure has a lower IMT temperature than the VO<sub>2</sub> with a high asymmetric one. These results provide the role of octahedral symmetry in tuning the IMT temperature of VO<sub>2</sub>.

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[1] D. Lee & S. Park *et al.*, Journal of Physical Chemistry Letters, 2022, 13(1), 75-82

# Ionic based gate control of quantum phase transitions on $\text{ZrS}_2$

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Exotic physical phenomena can be observed and exploited by tuning the charge carrier density of materials. Traditional chemical doping has limited application in the context of two-dimensional materials, here the use of electrostatic gating, in particular ionic liquid gating, provides a highly efficient doping alternative [1].

Transitional metal dichalcogenides (TMDCs) have emerged as a potential two-dimensional replacement for silicon in many technological applications, however their carrier mobility needs to be vastly increased. Ionic liquid gating enables carrier concentrations of the order of  $10^{14}$  carriers per  $\text{cm}^2$  in certain TMDCs [2], this, in turn, allows for the emergence of unique physical phenomena, being gate induced superconductivity [3] the one that gathers the most attention.

Here, an overview of the ionic liquid gating technique is given, including device fabrication and characterization methods, focusing on the transition metal dichalcogenides,  $\text{ZrS}_2$  and  $\text{ZrSe}_2$ . Being  $\text{ZrSe}_2$  an oxygen sensitive material, a method of estimating its thickness by its optical image is discussed. Furthermore, experimental efforts reporting how ionic liquid gating can be used to tune the phase of  $\text{ZrS}_2$  are presented.

[1] D. Jena *et al.*, Phys. Rev. Lett., **98**,136805 (2007).

[2] H. Zhang *et al.*, Nano Letters **19**, 8836 (2019).

[3] J. T. Ye *et al.*, Science, **338**, 1193 (2012).

**large-gap insulating phase induced by magnetic ordering in the  
two-dimensional material  $\text{Si}(111)(\sqrt{3} \times \sqrt{3})R30^\circ\text{-Sn}$  at low  
temperature**

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It has been suggested that a class of surface crystals, called  $\alpha$ -phase, consisting in a low dense single-layer of tetravalent metal atoms (Pb or Sn) grown on tetravalent semiconducting substrates like Si(111) or Ge(111) form a very promising system to study Mott physics in two dimensions [1,2,3]. The atoms are organized in a triangular lattice forming a  $\sqrt{3} \times \sqrt{3}$   $R30^\circ$  surface reconstruction in the high-temperature metallic phase. Each metal atom leaves a free electron leading to a single half-filled electronic band confined at the surface and isolated from bulk bands. The strong electronic repulsion comes from the large nearest-neighbor distance  $\approx 7$  Å between the metal atoms. In the Sn/Si(111) phase, previous experimental studies reported an insulating gap at temperatures well below 100 K [4,5] which has been attributed to a Mott insulating state induced by strong on-site electronic interactions. Spin-resolved photoemission experiments suggested that a  $(2\sqrt{3} \times \sqrt{3})$  magnetic ordering develops at low-temperature with a row-wise anti-ferromagnetic order [6].

In the present study we revisit and extend very much previous experimental and theoretical studies of the Sn/Si(111) phase. By measuring the local density-of-states at 4 K we demonstrate that this material undergoes a large insulating gap of the order of 1 eV. Our advanced DFT+U calculations do not enable explaining such a large gap taking into account only strong on-site Coulomb interaction. Instead, taking into account the additional exchange interaction between Sn adatoms and substrate Si atoms, enables rationalizing the experimental results. Our results suggests that this system is in fact a magnetic insulator with a row-wise anti-ferromagnetic order induced by non-local exchange interactions but is not a Mott insulator as reported previously by experimental and numerical studies [3,4,5,6].

[1] G. Santoro, S. Scandolo and E. Tosatti, *Phys. Rev. B* **59**, 1891 (1999)

[2] G.Profeta and E. Tosatti, *et al*, *Phys. Rev. Lett.* **98**, 086401 (2007)

[3] P. Hansmann *et al*, *Phys. Rev. Lett.* **110**, 166401 (2013)

[4] S. Modesti *et al*, *Phys. Rev. Lett.* **98**, 126401 (2007)

[5] F. Ming *et al*, *Phys. Rev. Lett.* **119**, 266802 (2017)

[6] M. J'ager *et al*, *Phys. Rev. B.* **98**, 165422 (2018)

# High-mobility surface conduction in FeSi at low temperatures

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FeSi is a correlated small-gap semiconductor in which an unexpected metallization at high temperatures has attracted great interest for decades. We report a study of a series of single-crystal FeSi with slightly different Fe content, revealing a saturation of the resistivity below temperatures of a few Kelvin. The magnetic field dependence of the electrical transport properties provides strong evidence of a high-mobility surface conduction channel, that is insensitive to the additional presence of an impurity band in the bulk [1, 2]. The mobility of the surface conduction channel is quantitatively similar to typical topological insulators, but displays a striking lack of sensitivity to the presence of ferromagnetic impurities as studied by means of a series of single crystals with slightly different starting compositions. High-resolution tunneling spectroscopy on single-crystal surfaces provides evidence of two in-gap states in the low-temperature regime [3], consistent with the transport model proposed. Here, we report measurements of the specific heat and the magnetic torque of high-quality single crystals of FeSi with slightly different Fe content in order to shed further light on the nature of the high-mobility surface conduction at low temperatures.

[1] M. Wagner, PhD thesis, Technical University of Munich (2014)

[2] Y. Fang, et al., Proc.Natl. Acad. Sci., (USA) **115**, 8558 (2018)

[3] B. Yang, M. Uphoff, Y. Zhang, J. Reichert, A. P. Seitsonen, A. Bauer, C. Pfleiderer, and J. V. Barth, Proc. Natl. Acad. Sci. (USA) **118**, e2021203118 (2021).

# Gate-tunable insulator-metal transition and weak antilocalization in two-dimensional tellurium

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Charge carrier density control is a key factor to modify the electronic functionality of materials. The ability to induce high charge carrier density into various two-dimensional materials has led to exotic phenomena such as insulator-metal transition and superconductivity [1, 2]. So far, different techniques have been used to achieve this. Meanwhile, electric double layer transistors (EDLTs), which is a special case of field effect transistors (FETs) using liquid electrolytes instead of solid dielectrics, is a highly promising platform as it can provide the charge carrier density of up to  $10^{15} \text{ cm}^{-2}$  in its channel material. This is two orders of magnitude larger than that in the conventional solid-gate FETs [3]. First, I will give a short overview on the EDLTs, then I will present our recent experimental results of ionic liquid gated two-dimensional tellurium (Te). Our results show the possibility of gate tuning insulator-metal phase transition and the gate and temperature-dependent weak-antilocalization in p-type Te films.

- [1] AM. Goldman , Annual Review of Materials Research **44**, 45-63 (2014).
- [2] D. Costanzo *et al.*, Nature nanotechnology **13**, 483-488 (2018).
- [3] K. Ueno *et al.*, Journal of the Physical Society of Japan **83**, 3200 (2014).



## Electron spin resonance on FeSi crystals

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The correlated  $d$ -electron compound FeSi has been the focus of intense research due to its unusual electrical and magnetic properties, which are not well understood. Recently, electrical resistivity measurements [1,2] showed, below 19 K, a cross-over from semiconducting to metallic behavior, which was attributed to the emergence of a surface state, suggesting that FeSi could be a topological insulator [1]. In this work, we explore the  $T$  dependence of the electron spin resonance (ESR), magnetic susceptibility  $\chi(T)$ , and specific heat  $C_p(T)$  of the FeSi crystals. The crystals were grown by the metal flux method using Sn as flux. The X-ray diffraction data indicate that the FeSi crystallizes in the cubic structure with space group  $P2_13a$  ( $B20$ -type) in accordance with [3]. The  $T$  dependence of the  $\chi(T)$  for FeSi is consistent with a weak Pauli paramagnet with a gap opening below  $T \sim 200$  K. At very low- $T$ , small Curie-Weiss tails indicate the presence of  $\text{Fe}^{3+}$  magnetic impurities.

These  $\text{Fe}^{3+}$  magnetic impurities allow us to perform the ESR experiments taken in the temperature range  $4 \leq T \leq 300$  K. The ESR data show a single  $g \sim 2$  line for which the ESR linewidth follows the  $\chi(T)$  in the entire  $T$ -range, while the  $g$  value is  $T$  independent. These results suggest that the spin dynamics of the  $\text{Fe}^{3+}$  magnetic impurities are capturing the intrinsic behavior of  $d$ -conduction electrons of this material. We will interpret our results considering the opening of a hybridization gap and the presence of non-trivial electronic states in this material.

[1] Y. Fang *et al.*, *Proc. Natl. Acad. Sci. U.S.A.* **115**, 8558 (2018).

[2] A. Breindel *et al.*, arXiv:2203.12839v1 (2022)

[3] A. E. Petrova *et al.*, *Physical Review B* **82** (2010)

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# Universal size-dependent nonlinear charge transport in single crystals of the Mott insulator $\text{Ca}_2\text{RuO}_4$

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The surprisingly low current density required for inducing the insulator to metal transition has made  $\text{Ca}_2\text{RuO}_4$  an attractive candidate material for developing Mott-based electronics devices. The mechanism driving the resistive switching, however, remains a controversial topic in the field of strongly correlated electron systems. Here we probe an uncovered region of phase space by studying high-purity  $\text{Ca}_2\text{RuO}_4$  single crystals, using the sample size as principal tuning parameter. Upon reducing the crystal size, we find a four orders of magnitude increase in the current density required for driving  $\text{Ca}_2\text{RuO}_4$  out of the insulating state into a non-equilibrium (also called metastable) phase, which is the precursor to the fully metallic phase.

By integrating a microscopic platinum thermometer and performing thermal simulations, we gain insight into the local temperature during simultaneous application of current and establish that the size dependence is not a result of Joule heating. The findings suggest an inhomogeneous current distribution in the nominally homogeneous crystal. Our study calls for a reexamination of the interplay between sample size, charge current, and temperature in driving  $\text{Ca}_2\text{RuO}_4$  towards the Mott insulator to metal transition.

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# Universal properties of dissipative Tomonaga-Luttinger liquids: A case study of a non-Hermitian XXZ spin chain

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In recent years, open quantum systems have been actively studied both experimentally and theoretically, as exemplified by driven-dissipative systems and non-Hermitian (NH) quantum systems. In this talk, we demonstrate the universal properties of dissipative Tomonaga-Luttinger (TL) liquids by calculating correlation functions and performing finite-size scaling analysis of a non-Hermitian XXZ spin chain as a prototypical model in one-dimensional open quantum many-body systems [1]. Our analytic calculation is based on an effective field theory with bosonization, a finite-size scaling approach in conformal field theory, and the Bethe-ansatz solution. We also perform numerical calculations based on the density-matrix renormalization group analysis generalized to non-Hermitian systems (NH-DMRG). We uncover that the model in the massless regime with weak dissipation belongs to the universality class characterized by the complex-valued TL parameter, which is related to the complex generalization of the  $c = 1$  conformal field theory. As the dissipation strength increases, the values of the TL parameter obtained by the NH-DMRG and the Bethe-ansatz analysis start to deviate from each other, indicating that the model becomes massive for strong dissipation. Our results can be tested with ultracold atoms by introducing two-body loss to the two-component Bose-Hubbard system [2].

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[1] K. Yamamoto *et al.*, arXiv:2112.12467 (to be published).

[2] T. Tomita, S. Nakajima, I. Danshita, Y. Takasu, and Y. Takahashi, *Sci. Adv.* **3**, e1701513 (2017).

# Current induced hysteresis phenomena in resistivity of spin-orbit coupled iridate $\text{Ca}_5\text{Ir}_3\text{O}_{12}$

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The spin-orbit coupled iridate  $\text{Ca}_5\text{Ir}_3\text{O}_{12}$  with non-centrosymmetric hexagonal ( $P\bar{6}2m$ , #189,  $D_{3h}^3$ ) shows a semiconducting electrical conductivity [1]. As one crystallographic site for the Ir ion, the mixed valance state of  $\text{Ir}^{4+}$  ( $5d^5$ ) and  $\text{Ir}^{5+}$  ( $5d^4$ ) is confirmed by Mössbauer measurement for  $^{193}\text{Ir}$  nuclei [2].  $\text{Ca}_5\text{Ir}_3\text{O}_{12}$  indicates successive second order phase transitions at  $T_N = 7.8$  K and  $T_s = 105$  K [1,3]; antiferromagnetic ordering at 7.8 K [1-4] and a non-magnetic second-order phase transition at 105 K [1,3,6]. The phase transition at 105 K comes from an electric toroidal multipole order belonging to the  $A_2$  irreducible representation of the order-disorder type [6]. Furthermore,  $\text{Ca}_5\text{Ir}_3\text{O}_{12}$  shows nonlinear electrical conductivity in the  $c$ -axis direction even in the disordered state [3], and the electrical resistance decreases with increasing current density in the current-voltage characteristic; the origin of nonlinear conductivity is not still clear.

In this study, the electrical resistance of  $\text{Ca}_5\text{Ir}_3\text{O}_{12}$  in the nonlinear region was investigated in detail using the pulsed current method. Interestingly, hysteresis phenomena in resistivity was discovered. Furthermore, in order to observe current-induced structural change, Raman spectra under applying current were measured. As the result, a slight change due to the application of current in Raman spectra is confirmed. This change means an atomic position changed by applying current. In this presentation, we will report on the hysteresis phenomena in resistivity and Raman spectra under applying current.

[1] M. Wakeshima *et al.*, Solid State Commun., **125**, 311 (2003).

[2] S. Tsutsui *et al.*, J. Phys. Soc. Jpn. **90**, 083701 (2021).

[3] K. Matsuhira *et al.*, J. Phys. Soc. Jpn. **87**, 013703 (2018).

[4] G. Cao *et al.*, Phys. Rev. B, **75**, 134402 (2007).

[5] I. Franke *et al.*, Phys. Rev. B, **83**, 094416 (2011).

[6] H. Hanate *et al.*, J. Phys. Soc. Jpn. **90**, 063702 (2021).

## Diffusion of photo-excited holes in viscous electron fluid

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We address our investigation to the diffusion processes which take place in the hydrodynamic regime in a high-mobility mesoscopic GaAs channel, where strongly correlated electrons reveal hydrodynamic behavior [1,2]. In particular, we report on a photocurrent study of diffusion of the photo-generated holes within a viscous electron fluid. Scanning PC microscopy was performed at the 3.7 K in a multi-terminal Hall bar structure with the 5  $\mu\text{m}$  width and 100  $\mu\text{m}$  length of the channel area, fabricated using a 14 nm thick GaAs/AlGaAs quantum well. The sheet electron density and the mobility measured at 1.4 K were  $9.1 \cdot 10^{11} \text{ cm}^{-2}$  and  $2.0 \cdot 10^6 \text{ cm}^2/\text{Vs}$ , respectively. It was shown that the observed diffusion is due to the photo-generated heavy and light holes. The effective viscosity of the electron-hole system was determined. The presented results differ from the hydrodynamic effects observed so far in viscous electron systems, since in the reported case the diffusion of holes occurs within a mixture consisting of the hydrodynamic electrons and the injected photo holes.

[1] D. Levin, G. M. Gusev, E. V. Levinson, Z. D. Kwon, and A. K. Bakarov, *Phys. Rev. B* **97**, 245308 (2018).

[2] G. M. Gusev, A. D. Levin, E. V. Levinson, and A. K. Bakarov, *Phys. Rev. B* **98**, 161303(R), (2018).

# Nonequilibrium Seebeck coefficient of a correlated molecular junction

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Thermoelectric properties of nanostructures, including molecules, nanowires or quantum dots, have been under rigorous research. This interest primarily stems from the enhanced thermoelectric efficiency expected in low-dimensional systems and possible applications in energy harvesting. Besides, thermoelectric coefficients provide additional means to study and understand more fundamental aspects of nanoscale systems. In particular, sign changes of thermopower have been used as signatures to indicate the onset of Kondo correlations. Nevertheless, most of investigations dealing with strong correlations have been focused on the linear response regime, as the analysis of thermoelectric transport in far-from-equilibrium conditions, with accurate treatment of Kondo phenomena, still poses a great challenge.

Therefore, in this communication, we address this problem focusing particularly on the case of a molecule embedded in an asymmetric tunnel junction. To accurately describe the strongly coupled part of the system we use the numerical renormalization group method, while the weakly coupled part of the system is treated perturbatively, allowing us to determine the conductance and thermopower of the system in out-of-equilibrium conditions while treating the relevant correlations exactly. The nonequilibrium thermoelectric effects can be estimated through different Seebeck coefficients, namely the non-linear and the differential Seebeck effects. We provide a thorough analysis of the dependence of these thermopowers on the dot energy level, capacitance of the couplings, finite bias and temperature gradients across the system. This work provides new insight into the thermoelectric transport in correlated nanostructures, which is important for various experimental investigations.

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# Cascade of charge density wave transitions in selenium doped 1T-TaS<sub>2</sub> probed with optics

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1T-TaS<sub>2</sub> is a unique material among the transition metal dichalcogenides (TMDC) in the sense that it undergoes several distinct charge density wave (CDW) transitions and ends in what has been suggested to be a strongly correlated phase at low temperature. In 1T-TaS<sub>2</sub> a light induced meta-stable state has previously been observed. We recently discovered that close to the Se concentration where the low-temperature strongly correlated phase gives way to superconductivity ( $x \approx 0.8$  in 1T-TaS<sub>2-x</sub>Se<sub>x</sub>), a meta-stable charge density wave state (MS-CDW) can be reached by fast cooling through the low temperature CDW phase transition [1]. Our optical experiments indicate that this low temperature phase strongly resembles the CCDW phase of 1T-TaS<sub>2</sub>, but a detailed study of the electronic properties is called for.

We have used bulk sensitive FT-IR spectroscopy to collect optical spectra of single crystalline 1T-TaS<sub>2-x</sub>Se<sub>x</sub> (with  $x \approx 0.8$  and  $x \approx 1.0$ ) between 10 K and 400 K and over the photon energy range of 4 meV to 4 eV, which allows us to observe a series of different CDW phase transitions during cooling and warming cycles. We observe significant differences between the MS-CDW state, reached after cooling from 400 K and the normal CCDW that can be reached by subsequent heating and re-cooling.

I will present an analysis of the infrared active optical phonons and the different spectral signatures of the various CDW phases. By comparing the  $x \approx 0.8$  and  $x \approx 1.0$  crystals, more insight in this meta stable state will be provided.

[1] Nevill, Aimee, et al. "Novel hysteresis effects in the charge density wave compound 1T-TaS<sub>2-x</sub>Se<sub>x</sub>." Bulletin of the American Physical Society (2022).

# Recombination of Weyl points in periodically driven Dirac semimetals

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Topological electronic states induced by periodic external fields such as laser light have attracted much attention [1, 2]. Recently, it has been theoretically predicted that the time-reversal symmetry is broken by irradiating the three-dimensional Dirac semimetal with a circularly polarized laser, and Weyl points appear due to the chiral gauge field [3]. This is called the Floquet Weyl semimetal state. It is well known that the Weyl semimetals can show anomalous Hall effect originating from finite Berry curvature between the two Weyl points with opposite chirality. However, the topological natures and transport properties in the Floquet Weyl semimetal state have not been detailed in a periodically driven system.

In this work, we study an effective model for paramagnetic Dirac semimetals hosting two spin-degenerated Dirac cones near the Fermi level and investigate the consequence of the periodically driven system by using Floquet theory. We clarify that when the spin-orbit coupling is finite, the Floquet Weyl semimetal state can be realized by splitting the Dirac points into two Weyl point pairs by circularly polarized irradiation. Furthermore, we find several topological phase transitions with realignments of the Weyl points by varying strength, frequency, and direction of the incident laser. We also calculate the optical conductivity by linear response theory, assuming distribution functions close to an equilibrium system. As a result, we show that the anomalous Hall conductivity drastically changes amplitude and sign through the phase transitions with the recombination of the Weyl points.

\*This work is supported by JST CREST (No. JPMJCR19T3).

[1] T. Oka and H. Aoki, *Phys. Rev. B* **79**, 081406(R) (2009).

[2] J. W. McIver *et al.*, *Nat. Phys.* **16**, 38 (2020).

[3] S. Ebihara, K. Fukushima, and T. Oka, *Phys. Rev. B* **79**, 155107 (2016).



# Thermal Hall response: violation of gravitational analogues

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The response of solids to temperature gradients is often described in terms of a gravitational analogue: the effect of a space-dependent temperature is modeled using a space dependent metric [1]. We investigate the validity of this approach in describing the bulk response of quantum Hall states and other gapped chiral topological states. To this end, we consider the prototypical Haldane model in two different cases of (i) a space-dependent electrostatic potential and gravitational potential (i.e. metric) and (ii) a space-dependent temperature and chemical potential imprinted by a weak coupling to non-interacting electron baths or phonons. Each case may be realized by different physical setups, e.g., (i) a distorted lattice with space dependent hoppings and (ii) a focused laser beam to locally heat the system by phonon. We find that the thermal analogue is invalid; while a space dependent gravitational potential induces transverse energy currents proportional to the third derivative of the gravitational potential, the response to an analogous temperature profile is proportional to the first derivative of the temperature profile, and vanishes in limit of weak coupling to the thermal bath. Similarly, the Einstein relation, the analogy between the electrostatic potential and the internal chemical potential, is not valid in such a setup.

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[1] J. M Luttinger, Phys. Rev. 135, A1505 (1964).

# Exact analysis of the Liouvillian gap for the $SU(N)$ Fermi-Hubbard model with two-body loss

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The dynamics of the dissipative  $SU(N)$  Fermi-Hubbard model with two-particle loss has been studied experimentally and theoretically. The dynamics of Markovian dissipative systems is generated by the Liouvillian superoperator, which is usually more difficult to diagonalize than the Hamiltonian of a closed system. When the system is subject to two-body loss, the eigenvalue problem of the Liouvillian superoperator reduces to that of the Hubbard model with imaginary interaction strength. However, the exact analysis has been limited to the one-dimensional  $SU(2)$  Fermi-Hubbard model, where the Bethe ansatz is applicable.

Here we consider the  $SU(N)$  Fermi-Hubbard model with two-body loss at  $1/N$ -filling as a starting point and evaluate the Liouvillian gap, which characterizes the relaxation time towards the ferromagnetic steady state. On a  $d$ -dimensional hypercubic lattice with linear size  $L$ , the Liouvillian gap is upper bounded by a constant proportional to  $1/L^2$ , which is independent of the dimension  $d$ .

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# Floquet topological superconductivity induced by chiral many-body interactions

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Floquet theory enables us to design quantum phases of matter with exotic properties, via nontrivial modulation to the effective static Hamiltonian due to the time-periodic driving. In particular, we can control the band topology to realize various topological phases including Chern insulators without magnetic fields, in a dynamical way [1,2].

While extending this idea to topological superconductivity is an important application, the same mechanism does not apply to typical superconductors in a straightforward manner: The gap function does not directly couple to electromagnetic fields, so that it is difficult to modulate the pairing symmetry to induce topological phase transition.

In this study, we find that we can overcome this difficulty by taking account of correlation effects. Namely, we show that the d-wave superconductivity in the doped Hubbard model can be dynamically changed to the topological d+id one under the illumination of circularly-polarized light [3].

To this end, we first derive the Floquet t–J model by combining the Floquet theory and the Schrieffer-Wolff transformation. The obtained Hamiltonian has chiral many-body interactions with broken time-reversal symmetry, the scalar spin chirality term and so-called three-site terms with complex amplitudes. Then we show that these emergent interactions indeed modulate the pairing symmetry within the framework of Gutzwiller approximation, and demonstrate it by numerically calculating the phase diagram and transient dynamics.

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[1] T. Oka and H. Aoki, *Phys. Rev. B* **79**, 081406 (2009).

[2] T. Kitagawa, *et al.*, *Phys. Rev. B* **84**, 235108 (2011).

[3] S. Kitamura and H. Aoki, arXiv:2108.13626.

## Pump-Probe AC Susceptibility of $\text{LiHo}_x\text{Y}_{1-x}\text{F}_4$ ( $x = 4.5\%$ )

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$\text{LiHoF}_4$  under a transverse magnetic field exhibits one of the best understood examples of a quantum critical point. Substitutional doping of Ho with non-magnetic Yttrium may be used to study the effects of disorder [1]. In the highly diluted system  $\text{LiHo}_x\text{Y}_{1-x}\text{F}_4$  ( $x = 4.5\%$ ), investigated in our study, the nature of the ground state is still subject to intense experimental and theoretical studies [2]. To explore the ground state properties of this system, multiple studies employed so-called pump-probe susceptibility measurements [3-5]. We revisit this question and report a study of the pump-probe susceptibility as a function temperature and field orientation, covering a wide parameter range.

- [1] J. P. Gingras and P. Henelius, *J. Phys.: Conf. Ser.* **320**, 012001 (2011).
- [2] J. A. Quilliam *et al.*, *Phys. Rev. Lett.* **101**, 187204 (2008).
- [3] S. Ghosh *et al.*, *Science* **296**, 2195 (2002)
- [4] M. A. Schmidt *et al.*, *Proc Natl Acad Sci USA* **111**, 3689 (2014)
- [5] D. M. Silevitch *et al.*, *Nature Com.* **10**, 4001 (2019)

# Quantum thermodynamics of strongly correlated systems

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We study tunneling quenches when a hot-many body quantum system is brought into instantaneous contact with a cold many-body quantum system. The dynamics of such systems can be understood as a combination of early time von Neumann entropy gain and late time energy relaxation. We show that at the shortest timescales there is an energy increase in each system linked to the entropy gain and supported by the collective binding energy between the systems. Counterintuitively to the classical expectation, this implies that also the hotter of the two subsystems generically experiences an initial energy increase when brought into contact with a colder system. We explain this early time energy gain with a quantum thermodynamical relation that holds even for systems out of equilibrium and, in the limit where the energy relaxation overwhelms the quantum correlation build-up, reduces to a classical behavior. We use both, strongly correlated SYK systems and mixed field Ising chains with a tunneling quench to exhibit these characteristics, and study the contribution of quantum correlations to the von Neumann entropy.

# Exchange bias effect and inhomogeneous magnetism in 6H Ba<sub>3</sub>CoFeRuO<sub>9</sub>

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Structural, magnetic and electrical investigations on 6 layered hexagonal (6H) Ba<sub>3</sub>CoFeRuO<sub>9</sub> (BCFRO) reveals the role of two different octahedral *B*-site (2a and 4f sites) in creating competing antiferromagnetic and ferromagnetic interactions.

BCFRO forms in the  $P6_3/mmc$  space group. Temperature dependence of magnetism evidences spin glass transition at  $T_g \sim 50$  K. Glassy dynamics of magnetism in the system is further affirmed by the absence of long range ordering from Neutron diffraction as well as specific heat capacity measurement. Large exchange bias (EB) of 3.5 kOe is obtained at 3 K under a cooling field of 50 kOe. The EB in our system is a result of inhomogeneous magnetism owing to spatially varying chemical composition [1]. BCFRO 6H structure forms with site mixing with Co, Fe and Ru sharing 35 %, 49% and 16% each of the 2a site and similarly, 32%, 26% and 42% each of 4f site respectively. This site disorder along with mixed valency of magnetic ions leads to competing ferromagnetic and antiferromagnetic phases giving rise to spin glass behaviour. The exchange bias training effect in our system follows spin relaxation model of rotatable and frozen spins which are exchange coupled at the interface [2].

Strong electron localisation occurs by virtue of the specific 6H structure with corner shared octahedral 2a site and face shared octahedral 4f site. The electrical and thermal transport in BCFRO follows Efros-Shklovskii variable range hopping (ES VRH) model below 150 K [3].

[1] S. Middey *et al.*, Physical Review B **83**, 144419 (2011).

[2] S. K. Mishra *et al.*, Physical Review Letters **102**, 177208 (2009).

[3] A. L. Efros and B. I. Shklovskii, Journal of Physics C: Solid State Physics **8**, L49 (1975).

# **A hydrodynamic description for transport in the strange metal phase of cuprates**

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High temperature superconductors are strongly coupled systems which present a complicated phase diagram with many coexisting phases. This makes it difficult to isolate a particular mechanism which generates their singular transport properties. In strongly coupled systems one generically expects short equilibration times meaning that only long lived degrees of freedom are important. Hydrodynamics is the framework for describing such degrees of freedom. Because hydrodynamics mostly relies on the symmetries of the system, without referring to any specific microscopic mechanism, it constitutes a promising approach for analysing these materials.

In this talk I will argue that in the strange metal phase of the cuprates, a whole set of transport coefficients are described by a universal hydrodynamic framework. Integral to this description is the inclusion of the pseudo-spontaneous breaking of translation invariance, one manifestation of which is charge density waves.

We corroborate our theoretical prediction against the DC transport properties of Bi-2201 close to optimal doping. We measure all the DC transport properties of a given sample for several crystals. We use the subsequent data to demonstrate the consistency of our approach.

Finally, I will conclude by discussing some of the shortcomings of our model and how they may be overcome in the future.

# **Metal-insulator transition in the Hubbard model under external field**

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We investigate the metal-insulator transition of the dissipative Hubbard model driven by a constant electric field using the nonequilibrium dynamical mean field theory (NE-DMFT) with the steady state non-crossing approximation (SS-NCA) impurity solver. We discuss the effect of the coupling strength between the lattice fermions and the heat reservoir fermions on the phase diagram and compare them to the equilibrium solution obtained by NCA. We describe the various responses of the system across the metal-insulator transition lines of the phase diagram. The set of SS-NCA equations for a general impurity model on Keldysh formalism is presented in detail with a few numerical techniques for convergence. It can be used in a wide variety of systems out-of equilibrium including those requiring the cluster extension of NE-DMFT.



# Analysis of pump-probe spectroscopy in the extended Hubbard model in the infinite matrix-product-states representation

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Pump-probe spectroscopy measurements, such as time-resolved optical conductivity and time-resolved angle-resolved photoemission spectroscopy (trARPES), have been widely used to study the dynamical properties of strongly correlated electron systems. Especially, the ultrafast phenomena of one-dimensional (1D) Mott insulators, e.g., organic salt ET-F 2 TCNQ [1,2] and halogen-bridged transition-metal compounds [3], have been intensively explored in experiments, since it was expected that the optical response is significantly affected by the formation of doublon-holon bound states induced by photoexcitation. Namely, the emergence of a light-induced in-gap state and metallization was reported by analyzing the time-resolved optical conductivity in the 1D half-filled extended Hubbard model (EHM) with nearest-neighbor Coulomb repulsion, using time-dependent exact diagonalization (ED) [4] and density-matrix renormalization group [5] techniques. These previous calculations have been carried out, however, with finite systems and therefore depend strongly on the system size.

We calculate the nonequilibrium dynamics of the 1D EHM directly in the thermodynamic limit by imposing infinite boundary conditions (IBC) in the infinite matrix-product-states (iMPS) representation. Employing the (infinite) time-evolved block decimation technique [7], we perform time-evolution simulations to extract dynamical correlation functions. The time-resolved optical conductivity in the thermodynamic limit provides us with more precise information on the in-gap state. The other advantage of our numerical technique with IBC is that the momentum-dependent quantities, such as time-dependent photoemission spectra (PES), can also be computed with much higher resolution [8] than those by ED [9]. We will also demonstrate the numerical results of time-dependent PES in the 1D EHM after pulse irradiation, which are related to the trARPES experiments exhibiting gap collapse and reconstruction after photoexcitation.

[1] H. Okamoto *et al.*, Phys. Rev. Lett. **98**, 037401 (2007).

[2] S. Wall *et al.*, Nat. Phys. **7**, 114 (2011).

[3] H. Matsuzaki *et al.*, Phys. Rev. Lett. **113**, 096403 (2014).

[4] H. Lu, C. Shao, J. Bonča, D. Manske, and T. Tohyama, Phys. Rev. B **91**, 245117 (2015).

[5] J. Rincón and A. E. Feiguin, Phys. Rev. B **104**, 085122 (2021).

[6] V. Zauner *et al.*, J. Phys.: Condens. Matter **27**, 425602 (2015).

[7] G. Vidal, Phys. Rev. Lett. **98**, 070201 (2007).

[8] S. Ejima, F. Lange, and H. Fehske, Phys. Rev. Res. **4**, L012012 (2022).

[9] C. Shao, T. Tohyama, H. G. Luo, and H. Lu, Phys. Rev. B **101**, 45128 (2020).

# Local shot noise of the putative vortex Majorana modes in $\text{FeTe}_{0.55}\text{Se}_{0.45}$

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Vortices in a superconductor are local regions where quantized magnetic flux penetrates; their subgap states reflect both the pairing symmetry and the normal state properties [1]. In iron-based superconductors, vortices are reported to host elusive Majorana modes [2, 3], but the evidence remains controversial. Shot noise has been suggested [4] to act as a tell-tale probe into vortex physics, but despite much theoretical work, no experimental technique that can locally measure the shot noise of a vortex core has been successful. Here, we use local shot-noise spectroscopy to study the tunneling process into vortex subgap states for the first time in a conventional superconductor  $\text{NbSe}_2$  and the putative Majorana platform  $\text{FeTe}_{0.55}\text{Se}_{0.45}$ . We find that tunneling into vortex subgap states in both materials exhibit charge transfer of a single electron charge. Our data excludes the possibility of a Yu-Shiba-Rusinov state and is consistent with Majorana zero modes. However, we argue that our data is likely consistent with trivial vortex subgap states as well – further theoretical investigations taking into account dynamics and superconducting tips are necessary.

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[1] N. E. Hussey, *Adv. Phys.* 51, 1685 (2002).

[2] P. Zhang, et al., *Science* 360, 182 (2018).

[3] S. Y. Zhu, et al., *Science* 367, 189 (2020).

[4] C. J. Bolech and E. Demler, *Phys. Rev. Lett.* 98, 237002 (2007).

# Disentangling charge order and superconductivity in correlated kagome superconductor CsV<sub>3</sub>Sb<sub>5</sub>

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The kagome compounds possessing unique crystal structure, which leads to a non-trivial topological band structure, offer a unique platform to unfold the long-standing question of interdependence between strongly correlated quantum phenomena with close enough energy scales. Recently discovered series AV<sub>3</sub>Sb<sub>5</sub> (A = Rb, K, Cs) featuring such structural motif harbors a variety of intriguing phenomena namely competing chiral charge order (CO) and superconductivity (SC) [1-3]. CsV<sub>3</sub>Sb<sub>5</sub> is of particular interest because of the distinct M-dome like two peak behavior in superconducting transition temperature ( $T_c$ )-pressure phase diagram [4] signaling a close interplay between CO and SC. However, any microscopic experimental and theoretical understanding of such interplay remains elusive. We have carried out detailed muon spin relaxation experiments at ambient as well as under hydrostatic pressures up to 1.9 GPa aimed to comprehend the relationship between CO and SC in this compound. We observed nearly threefold enhancement of  $T_c$  and superfluid density at 1.74 GPa compared to their respective ambient pressure values [5,6]. Remarkably, similar to the pressure evolution of  $T_c$ , the superfluid density also manifest two-peak behavior with increasing pressure [6]. These results in conjunction with DFT calculations suggests a possible evolution of the CO of superimposed tri-hexagonal Star of David phase at low pressure (within the first dome), to a staggered tri-hexagonal phase at intermediate pressure (between first and second dome). Our findings suggest an unusual competition between CO and multiband SC in strongly correlated kagome superconductor CsV<sub>3</sub>Sb<sub>5</sub>.

# contributed equally

[1] T. Neupert, et al., Nature Physics **18**, 137 (2022).

[2] H. Zhao, et. al., Nature **599**, 216–221 (2021).

[3] C. Mielke III, et al., Nature **602**, 245 (2022).

[4] K. Chen, et al., Physical Review Letters **126**, 247001 (2021).

[5] R. Gupta et al., (arxiv: <https://doi.org/10.48550/arXiv.2108.01574>), accepted for publication in npj Quantum Materials.

[6] R. Gupta et al., (arxiv: <https://doi.org/10.48550/arXiv.2203.05055>)

# Structural and magnetic anisotropy in $\text{YBa}_2\text{Cu}_3\text{O}_7/\text{La}_{0.67}\text{Sr}_{0.33}\text{MnO}_3$ bilayer film on $\text{SrTiO}_3$ substrate

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The interplay between magnetism and superconductivity has been an intense field of research since the discovery of unconventional superconductivity in varied materials. The properties at interfaces of heterostructures have been found to be even more exotic and different from the behavior of the constituent layers. In order to probe the interplay between magnetism and superconductivity, and the influence of interface states, we fabricated the heterostructure thin film of superconducting layer  $\text{YBa}_2\text{Cu}_3\text{O}_7$  (YBCO) and ferromagnetic layer  $\text{La}_{0.67}\text{Sr}_{0.33}\text{MnO}_3$  (LSMO) on  $\text{SrTiO}_3$  (STO) (001) substrate using Pulsed Laser Deposition. X-ray diffraction shows the presence of (00 $l$ ) reflection from the YBCO as well as LSMO layer[1]. Reciprocal Space Mapping (RSM) shows the strained growth of the thin film with the Pole figure measurement confirming the single crystallinity of the bilayer film [2]. The temperature dependence of magnetic susceptibility measurements obtained for two different magnetic fields (100 Oe & 5000 Oe) along two directions, i.e.,  $H_{ext} \parallel c$  (out-of-plane) and  $H_{ext} \perp c$  (in-plane) direction exhibit a link between magnetic anisotropy and uniaxial growth of the thin film. The onset of superconducting transition temperature,  $T_c = 86$  K (in-plane) & 84 K (out-of-plane) under 100 Oe applied field and  $T_c = 82$  K (in-plane) & 76 K (out-of-plane) under 5000 Oe applied field indicating the dependence of onset temperature on the magnitude as well direction of externally applied magnetic field. In-plane magnetic measurements show suppression of diamagnetic behaviour which is indicative of the Meissner effect (typical in superconductors) as compared to out-of-plane measurements. The susceptibility signals are stronger for out-of-plane direction indicating the presence of higher ordering for  $\text{CuO}_2$  superconducting planes[3]. The Curie temperature is observed to be around 220 K for both the directions of the applied field. The dependence of magnetization on applied field shows superconducting behaviour in the temperature range 2-80 K and ferromagnetic behaviour with saturated magnetization in the temperature range 90-200 K. These results suggest that these LSMO/YBCO heterostructures are ideal playground for the study of interplay between magnetism and superconductivity that might help to unravel the underlying physics of unconventional superconductivity.

## References

- [1] A. K. Jha *et. al.* *J. Supercond. Nov. Magn.*, 27, 4, (2014).
- [2] J. J. Wisser *et. al.* *AIP Adv.*, 11,1, (2021).
- [3] H. S. Cornejo *et. al.* *J. Mater. Sci. Mater. Electron.*, 31, 23, (2020).

# Nonlinear optical responses in two-dimensional superconductors

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A wide variety of optical measurements have been used to obtain insight into the complex ordered states of quantum materials. Especially, nonlinear responses yield rich information about ordered states such as symmetry and geometric properties. There are many superconductors that show complex ordered states. Thus, the nonlinear optical response of superconductors is expected to be a useful tool for probing the symmetry of superconductors [1].

Second-order optical responses, in particular, appear in noncentrosymmetric materials. The representative examples are the photogalvanic effect and second-harmonic generation. The photogalvanic effect is the photo-induced direct current, and the second-harmonic generation is the process of converting the irradiated light into that with double frequency. Theories of the second-order nonlinear response in superconductors were recently formulated based on the Bogoliubov-de Gennes theory [2,3]. On the other hand, it is still unclear how the superconductivity influences the nonlinear optical properties. Thus, it is desirable to perform a comprehensive analysis of the superconducting nonlinear optical responses based on a canonical model.

To this end, we investigate the second-order nonlinear responses in superconductors with single-band model Hamiltonians. In the light of antisymmetric spin-orbit coupling, we present a systematic study of the superconducting nonlinear optical responses and elucidate the condition for characteristic behaviors such as the low-frequency divergence. Our study identifies a basic ingredient in superconducting nonlinear optics and may cover a broad range of noncentrosymmetric superconductors such as heavy-fermion and two-dimensional superconductors [4].

[1] J. Orenstein *et al.*, *Annu. Rev. Condens. Matter Phys.* **12**, 247 (2021).

[2] T. Xu *et al.*, *Phys. Rev. B* **100**, 220501 (2019).

[3] H. Watanabe *et al.*, *Phys. Rev. B* **105**, 024308 (2022).

[4] *Non-Centrosymmetric Superconductors: Introduction and Overview*, edited by E. Bauer and M. Sigrest, *Lecture Notes in Physics* Vol. **847** (Springer, Berlin, 2012); Y. Saito *et al.*, *Nat. Phys.* **12**, 144 (2016).

## ***Enhancement of pair correlations in the asymmetric Hubbard ladder***

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We investigated an extension of the asymmetric two-leg Hubbard ladder model [1,2] that consists of different on-site interaction  $U_y$  and intra-hopping  $t_y$  on each leg  $y$  using the density matrix renormalization group method. We calculated pair binding energy, charge, spin and single particle gaps as well as pairing correlation functions for several sets of model parameters. It is possible to adjust the asymmetry of model parameters to retain finite pair binding energy and enhanced pairing correlation functions similar to those appearing in symmetric two-leg Hubbard ladders. Such adjustment represents an interpolation between doped Mott insulator and doped charge transfer insulator.

[1] A. Abdelwahab, E. Jeckelmann, and M. Hohenadler, Phys. Rev. B **91**, 155119 (2015).

[2] A. Abdelwahab and E. Jeckelmann, Eur. Phys. J. B **91**, 207 (2018).

# Enhancement of the superconductivity due to quantum geometry in monolayer FeSe

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Monolayer FeSe is one of the high-temperature superconductors; surprisingly high mean-field transition temperature of more than 65 K [1,2] is in stark contrast to nearly 8 K of bulk FeSe[3]. Much research clarified the mechanism of the high mean-field transition temperature, which is attributed to the effect of the substrate. On the other hand, the high zero-resistance transition temperature, identified as the BKT transition temperature, has not been studied intensively. Considering the BKT transition temperature is determined by the superfluid weight, we study the mechanism enhancing the superfluid weight.

Recently, the superfluid weight of multi-band superconductors has been revealed to have a quantum geometric origin in addition to the Fermi-liquid contribution [4,5]. In monolayer FeSe, the small carrier density leads to a small Fermi-liquid contribution. In addition, since monolayer FeSe is the mother compound of the topological superconductor candidate FeSe<sub>1-x</sub>Te<sub>x</sub>, its band structure is expected to be geometrically nontrivial. Thus, the quantum geometric effect on the BKT transition temperature is a problem with considerable interest and attention.

In this work, we reveal that the quantum geometry significantly enhances the superconductivity through an increase of the superfluid weight [6]. First, we formulate the superfluid weight of unconventional superconductors based on the properties of the Bloch electrons. Then, we apply this theory to the monolayer FeSe. Surprisingly, the quantum geometric enhancement of the superconductivity does not depend on the superconducting symmetry. In addition, the enhancement of the BKT transition temperature is approximately 10 K in the typical parameter set.

[1] Wang, Q. Y, *et al.*, Chin. Phys. Lett. **29**, 037402 (2012).

[2] Y. Xu, *et al.*, Nat. Commun. **12** 2840 (2021).

[3] F.-C. Hsu, *et al.*, Proceedings of the National Academy of Science **105**, 14262 (2008).

[4] S. Peotta, *et al.*, Nat. Commun. **6**, 8944 (2015).

[5] L. Liagn, *et al.*, Phys. Rev. B **95**, 024515 (2017).

[6] T. Kitamura, *et al.* arXiv:2108:10002 (2021).

# Effect of hopping anisotropy on the critical temperature of unconventional, superconducting pairing states.

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Uniaxial strain affects pairing symmetry states in superconductors by changing the lattice symmetry, and by altering Fermi surface topology. We present a systematic study of these effects within a one-band negative-U Hubbard model for s, p and d-wave pairing states. We consider a general 2D model that can be applied to superconductors under uniaxial strain, modelled via hopping anisotropy, on a square lattice. The results presented here model an in plane compression along the x-axis, which reduces the lattice from a tetragonal to orthorhombic crystal space group exploring the affects of hopping anisotropy on the gap pairing. We show that changes in  $T_c$  are tune-able with hopping anisotropy and dependent on the orientation of the gap function in relation to the opening of the Fermi surface during the Lifshitz transition. In comparing the model results to experimental data for the case of Sr2RuO4 it is found that a d-wave pairing best describes the changes in  $T_c$  for the superconducting state in regards to its response to a small uniaxial strain.

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[1] A. Author *et al.*, Phys. Rev. B **1**, 1 (2020).

[2] A. Author and B. Author, Europhysics Letters **1**, 1 (2020).



# Microscopic evidence of the superconducting multiphase in the noncentrosymmetric heavy-fermion superconductor CeRh<sub>2</sub>As<sub>2</sub>

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The recently discovered heavy-fermion superconductor CeRh<sub>2</sub>As<sub>2</sub> exhibits a superconducting transition at  $T_{SC} \sim 0.3$  K, and in the  $c$ -axis magnetic field, superconducting (SC) multiphase have been reported [1]. As CeRh<sub>2</sub>As<sub>2</sub> has inversion symmetry in the crystal structure but no inversion symmetry at the Ce sites, CeRh<sub>2</sub>As<sub>2</sub> is called local inversion symmetry breaking system. In such system, the existence of two SC phases has been theoretically proposed: an even-parity SC state in low magnetic field and an odd-parity SC state in high magnetic field [2]. Actually, such phase diagram was experimentally shown [1].

To investigate the magnetic and superconducting properties of CeRh<sub>2</sub>As<sub>2</sub>, we performed <sup>75</sup>As-NQR (Nuclear Quadrupole Resonance)/NMR (Nuclear Magnetic Resonance) measurements. We observed site-dependent linewidth broadening below 0.25 K, indicating the antiferromagnetic transition below  $T_c$  [3]. In addition, we performed NMR measurements in  $H \parallel c$  and  $H \parallel ab$  to obtain information about the superconducting symmetry of the two phases. The response of antiferromagnetic order against magnetic fields was also investigated. We discuss the magnetic structure of the antiferromagnetic state and the relationship between superconductivity and magnetism on the basis of our NMR results.

[1] S. Khim *et al.*, Science 373, 1012 (2021).

[2] T. Yoshida *et al.*, Phys. Rev. B **86**, 134514 (2012).

[3] M. Kibune *et al.*, Phys. Rev. Lett. **128**, 057002 (2022).

# Heat capacity study of the type-I to type-II superconducting transition in the Dirac semimetal PdTe<sub>2</sub>

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PdTe<sub>2</sub> is a Dirac semimetal which becomes superconducting below 1.6 K [1]. Interestingly, it exhibits type-I superconductivity with an unusual surface state. This prompts the question whether the superconductivity at the surface is affected by the presence of topological surface states. Here we report heat capacity results around the superconducting transition when Pt is substituted for Pd to intentionally induce disorder in the type-I superconductor. Two single-crystalline batches Pd<sub>1-x</sub>Pt<sub>x</sub>Te<sub>2</sub> have been prepared with nominal doping concentrations  $x=0.05$  and  $x=0.10$ . Sample characterization by energy dispersive X-ray spectroscopy revealed Pt did not dissolve homogeneously in the crystals. By measuring the heat capacity near the superconducting transition we have successfully probed type-I superconductivity in the parent compound PdTe<sub>2</sub> and the  $x=0.05$  batch, as well as type-II superconductivity in the  $x=0.10$  batch [2,3]. This is accomplished by confirming the presence or absence of latent heat near the jump in heat capacity at the superconducting transition. Ac susceptibility results corroborate the evidence for the type-I to type-II superconducting transition. From transport measurements we determine that a residual resistivity  $\rho_0 = 1.4 \mu\Omega\text{cm}$  is sufficient to induce type-II superconductivity in PdTe<sub>2</sub>.

[1] H. Leng *et al*, Phys. Rev. B 96, 220506(R) (2017).

[2] M.V.Salis *et al*, Phys. Rev. B 103, 104502 (2021).

[3] M.V.Salis *et al*. Phys. Rev. B 105, 054508 (2022).

# Odd-frequency pairing in the system with Bogoliubov Fermi surface

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The conventional superconductors do not have Fermi surfaces in the superconducting state. On the other hand, it has been suggested theoretically that some of the superconductors have *Bogoliubov Fermi surfaces*: the Fermi surfaces appear even below the transition temperature in the inversion symmetric and time reversal symmetry broken multi-band system [1]. These exotic Fermi surfaces are composed of Bogoliubov quasi-particles (bogolons), which are quasi-particles characteristic for the superconducting state. The possibility of the existence of the Bogoliubov Fermi surface is implied experimentally in iron-based superconductor Fe(Se,S), which has a finite zero-energy density of state below  $T_c$  [2,3]. This finite density of state itself is the same as that in the normal Fermi liquid of the electrons. However, the Fermi surfaces in the superconducting state should be different from those in the normal state. In order to clarify this point, we need to study the behavior of bogolons near the Fermi level.

We investigate the impurity effect of the bogolons near the Bogoliubov Fermi surface. We have found that the *pure odd-frequency Cooper pairs* are induced by the effect of the self-energy, which is reflected in the density of states as a zero-energy peak [4]. We could have discussed the material-unspecific physics of Bogoliubov Fermi surfaces with this effective low-energy model. For more quantitative evaluation, we also analyze the more realistic situation using the tight-binding parameters FeSe. It has been confirmed that the physical properties remain qualitatively unchanged. We further study the bogolon's odd-frequency pair in terms of the original electron.

[1] D. F. Agterberg, P. M. R. Brydon, and C. Timm, Phys. Rev. Lett. **118**, 127001 (2017).

[2] Y. Sato *et al.*, Proc. Nat. Acad. Sci. **115**, 1227 (2018).

[3] T. Hanaguri *et al.*, Sci. Adv. **4**, eaar6419 (2018).

[4] T. Miki, S.-T. Tamura, S. Iimura, and S. Hoshino, Phys. Rev. B **104**, 094518 (2021).

# Quantum spin and charge excitations in high- $T_c$ cuprates: Variational theory and quantitative comparison with experiment

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The discovery of robust spin and charge collective excitations across the phase diagram of various classes of strongly-correlated electron materials, including copper-oxide superconductors, iron pnictides, and iridates, calls for a detailed investigation of their microscopic origin and relation to other thermodynamic properties (metal-insulator transitions, antiferromagnetism, and high- $T_c$  superconductivity). Recently, we have formulated and tested a new theoretical framework to address both equilibrium- and collective-dynamic properties of those materials on the same footing [1-5]. It combines Variational Wave Function (VWF) scheme and expansion in the inverse number of fermionic flavors ( $1/N$ ).

We overview theoretical paramagnon and plasmon spectra for the canonical models of high-temperature superconductors (Hubbard,  $t$ - $J$ , and  $t$ - $J$ - $U$ ), obtained using the VWF+ $1/N$  approach. The detailed evolution of the collective excitations from the Hubbard- to the  $t$ - $J$ -model limit is investigated. Our results are compared with available resonant inelastic x-ray scattering and inelastic neutron scattering data for La- and Bi-based cuprates from the underdoped to the overdoped regime, yielding a semi-quantitative agreement for a doping-independent set of microscopic model parameters. We also benchmark the VWF+ $1/N$  results against available determinant quantum Monte-Carlo data for both static- and dynamic spin and charge susceptibilities. Finally, we comment on possible microscopic mechanisms, resulting in apparent robustness of the paramagnons across the anti-nodal Brillouin-zone direction, as well as their rapid overdamping along the nodal line.

This work is supported by Grants OPUS No. UMO-2021/41/B/ST3/04070 and Miniatura No. DEC-2021/05/X/ST3/00666 from Narodowe Centrum Nauki.

- [1] M. Fidrysiak and J. Spaęek, Phys. Rev. B **102**, 014505 (2020).
- [2] M. Fidrysiak and J. Spaęek, Phys. Rev. B **103**, 165111 (2021).
- [3] M. Fidrysiak and J. Spaęek, Phys. Rev. B **104**, L020510 (2021).
- [4] M. Fidrysiak, D. Goc-Jaęło, and J. Spaęek J. Magn. Magn. Mater. **539**, 168395 (2021).
- [5] J. Spaęek, M. Fidrysiak, M. Zegodnik, and A. Biborski, Phys. Rep. **959**, 1–117 (2022).

# The edge currents and spin polarization of the chiral superconductor in the checkerboard triangular lattice

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The chiral superconducting state with non-zero Chern number topologically supports the chiral edge state carrying the spontaneous current. The influence of the spin-orbit coupling on the chiral edge state would be intriguing. Some of the authors analysed the chiral superconductors in the multi-orbital square lattice system and in the honeycomb one, both of which possessed the intrinsic spin-orbit coupling. They found the spontaneous spin current at the edge, and the coexistence of the charge and spin currents led to the spin polarization [1,2]. Their conclusion would be relevant for  $\text{Sr}_2\text{RuO}_4$  and  $\text{SrPtAs}$  [3].

In this paper, we investigate the chiral p-wave state in the checkerboard triangular lattice without inversion symmetry. We have the anti-symmetric spin-orbit coupling due to the inversion symmetry breaking and find the spin current and spin polarization. Unlike the results for the square and honeycomb lattices, the direction of the spin currents in both edges are parallel. Our result could be applied for the recently discovered superconductor  $\text{BaPtSb}$  [4,5,6]

[1] Y. Imai et al, Phys. Rev. B 85,174532(2012).

[2] J. Goryo et al, Phys. Rev. B 96,140502(2017).

[3] Y. Nishikubo et al, J. Phys. Soc. Jpn. 80, 055002(2011).

[4] K. Kudo et al, J. Phys. Soc. Jpn. 87, 063702(2018).

[5] T. Adachi et al., KEK-MSL REPORT 2017, 54(2018).

[6] M. Kudo et al, J. Phys.: Conf. Ser., 2164, 012015 (2022)

## Emergence of singlet states with superconductivity in $\text{CaFe}_2\text{As}_2$

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The many body Zhang-Rice singlet (ZRS) states in Cu-based superconductors which forms due to coupling of hole states at Cu  $3d$  and O  $2p$  and clearly detected as well screened state in the bulk sensitive Cu  $2p$  photoemission spectroscopy spectra, are believed to be important for the formation of Cooper pairs responsible for the high temperature superconductivity [1]. In order to explore such state in Fe-based compounds, we studied the electronic structure of a superconducting Fe-based system from 122-family,  $\text{CaFe}_{1.9}\text{Co}_{0.1}\text{As}_2$  ( $T_c = 15$  K), employing bulk-sensitive high-resolution hard  $x$ -ray photoemission spectroscopy (HAXPES) technique. The valence band HAXPES spectra shows significant spectral weight close to Fermi-level with doping with negligible change in the chemical potential. A new feature emerges close at Fermi-level with reduction of temperature. No change in As core level spectra is observed both with doping and temperature. The Ca  $2p$  HAXPES spectra show a gradually peak shift towards lower binding energies with cooling. The Fe  $2p$  spectra show emergence of a new feature towards the lower binding energy side from the screened Fe  $2p$  peak in the superconducting composition which was absent in the parent compound. Reduction of sample temperature shows increase in the spectral weight of the well-screened state [2]. Similar, low binding energy well-screened states have also been observed in the cuprates and are assigned as ZRS. Emergence of ZRS state in this superconducting compound and its temperature evolution indicates relevance of the state with the ground state properties of the Fe-based superconductors.

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[1] F. C. Zhang and T. M. Rice, Phys. Rev. B **37**, 3759(R) (1988).

[2] R. P. Pandeya et al., Phys. Rev. B **104**, 094508 (2021).

# Charge density waves and Fermi-surface reconstruction in the clean overdoped cuprate superconductor $\text{Tl}_2\text{Ba}_2\text{CuO}_{6+\delta}$

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Hall effect and quantum oscillation measurements on high temperature cuprate superconductors show that underdoped compositions have a small Fermi surface pocket [1] whereas when heavily overdoped, the pocket increases dramatically in size [2]. The origin of this change in electronic structure has been unclear, but may be related to the high temperature superconductivity. Here we use resonant inelastic x-ray scattering to show that the clean overdoped single-layer cuprate  $\text{Tl}_2\text{Ba}_2\text{CuO}_{6+\delta}$  (Tl2201) displays CDW order at  $\mathbf{Q} = (0.31, 0, 2.5)$  with a remarkably long correlation length  $\xi \approx 200 \text{ \AA}$  which disappears above a hole concentration  $p_{CDW} \approx 0.265$ . We show that the evolution of the electronic properties of Tl2201 as the doping is lowered may be explained by a Fermi surface reconstruction which accompanies the emergence of the CDW below  $p_{CDW}$  [3]. Our results demonstrate importance of CDW correlations in understanding the electronic properties of overdoped cuprates.

[1] D. LaBeouf *et al.*, Nature **430** 533 (2007).

[2] S. Badoux *et al.*, Nature **531** 210 (2016).

[3] C. C. Tam *et al.*, Nat. Commun. **13** 570 (2022).

# Investigation of the vortex lattice in NbS<sub>2</sub> – a potential FFLO candidate

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To date, several materials have been proposed as hosts for the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) spatially modulated superconducting state [1], but direct experimental proof has been challenging, with only the organic superconductors providing uncontested evidence for the state [2]. The FFLO state is expected to develop at high fields and low temperatures in materials with strong Pauli paramagnetic effects, an anisotropic Fermi surface, and clean superconductivity.

2H-NbS<sub>2</sub> has recently been proposed as a potential candidate material based on torque magnetometry, specific heat and thermal expansion measurements as a function of orientation in magnetic field. Transition metal dichalcogenides (TMDs) are strongly anisotropic layered superconductors in which the two-dimensional planes are weakly coupled by van der Waals forces. The upper critical field of superconducting TMDs in the basal plane is shown to be dramatically enhanced by a special form of Ising spin orbit coupling [3]. When the field is applied exactly in the plane, the upper critical field increases dramatically above 16 T, beyond the limit expected from the Pauli paramagnetic effect. This behaviour is reminiscent of the organic superconductors where the FFLO state is seen.

Using small angle neutron scattering, we have observed the vortex lattice in this material to test if this material is a good candidate to look for a direct FFLO diffraction signal. We have observed a strong intrinsic superconducting anisotropy between the c axis and the basal plane.

[1] J. Wosnitzer, *Annalen der Physik* 530, 1700282 (2017).

[2] C. Agosta, *Crystals* 8, 285 (2018).

[3] C.-W. Cho et al., *Nature Comm.* 12,3676 (2021).



## **1e shot noise below $T_c$ in superconducting tunnel junctions**

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Shot noise is a powerful tool for determining the effective charge in mesoscopic systems, including superconductors and fractional quantum Hall systems. In a superconductor-insulator-superconductor tunnel junction, Andreev reflection leads to an effective charge of multiple electron charges. This can be used to detect the possible phase-incoherent pre-formed electron pairs above the critical temperature of superconductors. I will present a newly developed, low temperature (1.5 K), wide bandwidth (100 kHz-5 MHz) noise-measurement amplifier with a resolution down to 0.002 nV<sup>2</sup>/Hz. I will show measured shot noise in Nb/Al-AlO<sub>x</sub>/Nb and NbN/oxide/Ag tunnel junctions, and describe possibilities to measure shot noise in superconducting tunnel junctions.

## Elastocaloric determination of the phase diagram of Sr<sub>2</sub>RuO<sub>4</sub>

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Many intriguing unconventional superconductors form a phase diagram containing strongly correlated states which can be tuned by doping, pressure, etc. In recent years, uniaxial pressure has shown capabilities of tuning the electronic structures of Sr<sub>2</sub>RuO<sub>4</sub> across a Van Hove singularity (VHS) [1-3]. Here, we perform high precision ac-elastocaloric effect measurements and map out the phase diagram of Sr<sub>2</sub>RuO<sub>4</sub>. Similar to many unconventional superconductors, Sr<sub>2</sub>RuO<sub>4</sub> has a superconducting dome in proximity to a magnetic phase. The superconducting dome is consistent with heat capacity measurements [4] and no second transition is observed below T<sub>c</sub>. Instead, we observe a strong entropy quench at the VHS upon entering the superconducting state. With a model calculation for pairing at VHS, our results strongly suggest a substantial gap opening at the VHS and put a strong constraint on the order parameter. Besides, we can calculate the entropy landscape and estimate the entropy change upon entering the magnetic phase in proximity to the superconducting dome. We believe this is the first thermodynamic study demonstrating the interplay between superconducting and magnetic phases in Sr<sub>2</sub>RuO<sub>4</sub>.

[1] A. Steppke et al. Science 355, eaaf9398 (2017).

[2] V. Sunko et al. npj Quant. Mat. 4, 2397–4648 (2019).

[3] V. Grinenko, et al., Nat. Phys. 17, 748—754 (2021).

[4] Y.-S. Li et al. Proc. Natl. Acad. Sci. USA 118, e2020492118 (2021).

## Correlating Structure with Superconductivity Variations in UTe<sub>2</sub>

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The spin-triplet candidate superconductor UTe<sub>2</sub> [1] crystallizes in the *Immm* space group (no. 71),  $a \sim 4.16 \text{ \AA}$ ,  $b \sim 6.14 \text{ \AA}$ , and  $c \sim 13.98 \text{ \AA}$ , and contains three crystallographic sites, one U site which occupies the  $4i$  position and two Te sites, where Te1 occupies the  $4j$  position and Te2 occupies the  $4h$  position [2]. An intrinsic multicomponent superconducting order parameter has been suggested to exist in UTe<sub>2</sub> [3] although contrasting reports indicate that the double superconducting transitions arise due to inhomogeneity within the crystal [4-6]. Recent work has optimized  $T_c$  by lowering growth temperatures, reaching the highest reported  $T_c$  of 2.0 K, with only one transition visible in heat capacity measurements. Lowering the growth temperature too far, however, completely removes any indication of superconductivity in heat capacity measurements. Although non superconducting samples have been shown to have U deficiencies and smaller  $b$  and  $c$  lattice parameters, [6-7] no structural parameter has been identified to correlate with the evolution of  $T_c$ .

This talk will focus on detailed single crystal X-ray diffraction studies to probe crystallographic differences in samples to elucidate the origin of the varying superconducting transitions. Additionally, the evolution of the superconducting transition(s) in UTe<sub>2</sub> will be explored as a function of annealing via thermodynamic measurements.

- [1] S. Ran et al. *Science* **365**, 684 (2019)
- [2] A. J. K. Haneveld et al. *J. Less-Common Met.* **21**, 45 (1970)
- [3] I. M. Hayes et al. *Science* **373**, 797 (2021)
- [4] L. P. Cairns et al. *J. Phys.: Condens. Matter* **32**, 415602 (2020)
- [5] S. M. Thomas et al. arXiv:2103.09194 (2021)
- [6] P.F.S. Rosa et al. arXiv:2110.06200 (2021)
- [7] Y. Haga et al. arXiv:2112.13468 (2021).

# Gate-tunable unconventional superconductivity in 2D oxide interfaces nanodevices

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In conventional Bardeen-Cooper-Schrieffer superconductors, inversion and time-reversal symmetries are preserved. The breaking of these symmetries is expected to lead to the formation of unconventional superconducting pairing. Two dimensional (2D) superconductors offer new opportunities to study and tailor unconventional superconducting order parameter, as they inherently lack inversion symmetry.

In this respect, the 2D electron systems in SrTiO<sub>3</sub> based heterostructures, such as LaAlO<sub>3</sub>/SrTiO<sub>3</sub>, is a paradigmatic non-centrosymmetric superconductor due to the coexistence of gate tunable large Rashba spin-orbit coupling and ability to modulate 2D superconductivity. Depending on the carrier density doping, single to multi-orbital electronic occupation takes place [1,2]. The system is expected to yield unconventional superconductivity. However, a convincing observation by phase-sensitive measurements has been elusive so far.

We present experimental evidence of unconventional superconductivity in the LaAlO<sub>3</sub>/SrTiO<sub>3</sub> interface nano-devices. The central observations are the giant anomalous enhancement of the critical current by small out-of-plane magnetic fields and the asymmetric response with respect to the magnetic field direction. These features have a unique trend in intensity and sign upon electrostatic gating that, together with their dependence on temperature and nanowire dimensions, cannot be accommodated within a scenario of spin-singlet superconductivity. We theoretically demonstrate that the hallmarks of the experimental observations unambiguously indicate the coexistence of Josephson channels with intrinsic phase shifts due to different sign of the order parameter [3].

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[1] Gyanendra Singh et al. Nature Materials 18, 948 (2019).

[2] Gyanendra Singh et al. Phys. Rev. B 18, 948 (2019).

[3] Gyanendra Singh et al. npj Quantum Mater. 7, 2 (2022).

## **Grain boundaries investigation in the heavy fermion superconductor CeCoIn<sub>5</sub>**

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The study of grain boundaries (GB) in superconductors has both fundamental and applied interests. In high-temperature cuprate superconductors studies of the critical currents ( $J_c$ ) across GBs have provided important information on the symmetry of the superconducting order parameter and are critical for the observation of spontaneously generated half-flux magnetic quanta [1,2]. Similar to cuprate superconductors, heavy fermion superconductors (HFS) host rich physics in the form of unconventional superconducting phases with nodal quasiparticles. However, there have been relatively few phase-sensitive measurements of the superconducting order parameter thereby emphasizing the need for investigations of  $J_c$  across GBs in HFS.

In this talk, I will present results on GBs in polycrystalline samples of the HFS CeCoIn<sub>5</sub>. Electron backscatter diffraction images of well-polished samples reveal that majority of grains are not randomly oriented as one would expect but grow at a misorientation angle of  $90^\circ$  with respect to their neighboring grain sharing a common axis. We performed  $J_c$  studies on various such GBs. Our investigations are crucial in understanding the superconducting order parameter symmetry of CeCoIn<sub>5</sub> and its potential use in devices for quantum information science.

\*This work was supported by USDOE Office of Science (SC).

[1] H. Hilgenkamp et al., Rev. Mod. Phys. 74, 485, 2002.

[2] C. C. Tsuei and J. R. Kirtley, Rev. Mod. Phys. 72, 969, 2000.

## Growth of FeSe on in-situ cleaved SnSe<sub>2</sub> (001) surfaces

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The interest in Fe-chalcogenides have significantly increased in the recent years, mainly due to particular superconducting properties of FeSe. FeSe has a critical temperature ( $T_c$ ) of 8 K in the bulk, but exhibits a 20-fold increase in  $T_c$  as a thin film on non-conductive oxide surfaces [1,2].

Previously, it was shown that FeSe monolayers can be grown on Bi<sub>2</sub>Se<sub>3</sub> topological insulator by Fe deposition and annealing process under ultra-high vacuum conditions [3]. Here, we show that a similar approach can be implemented for fabricating FeSe islands on in-situ cleaved SnSe<sub>2</sub> (001) van der Waals crystal surfaces via an on-surface reaction given as:  $\text{Fe} + \text{SnSe}_2 \rightarrow \text{FeSe} + \text{SnSe}$ . Previous reports on Sn doped bulk FeSe samples claim an improvement of superconductivity [4] in the presence of a SnSe phase, which makes thin FeSe layers on SnSe<sub>2</sub> a promising new material system to study unconventional superconductivity. The growth dynamics and the structure of the formed FeSe islands were examined at sub-monolayer and monolayer coverages with scanning tunneling microscopy (STM). The STM images reveal formation of FeSe islands on the surface with different orientations, which is supported by the low energy electron diffraction (LEED) patterns. The chemical and the electronic properties were further investigated by X-ray photoelectron spectroscopy (XPS) and angle resolved photoemission spectroscopy (ARPES) measurements. Si capped FeSe/SnSe<sub>2</sub> samples were used to investigate the transport properties at different temperatures.

[1] Qing-Yan W, *et al. Chinese Phys. Lett.* 29 037402 (2012).

[2] Liu D, *et al. Nat Commun* 3, 931 (2012).

[3] Cavallin A, *et al. Surf. Sci.* 646 72 (2016).

[4] Chen N, *et al. J. Alloys Compd.* 588 418-421 (2014).

# Spin susceptibility and multiband effects in the Emery model of the cuprate superconductors

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The dominant model in the study of superconductivity in the cuprate superconductors is the single-band Hubbard model, despite the fact that oxygen bands hybridize with the copper, leading to a charge-transfer situation. However, there are experimental probes that are in direct contradiction with the simplified single-band model. In this work we are focusing on the recent work Ref. [1] which studied the doping dependence of the NMR Knight shift and came to the conclusion that there is a nonnegligible contribution to the spin susceptibility from the oxygen spins.

We study the single-band Hubbard model and its three-band generalization, the Emery model using Dynamical Mean-Field Theory (DMFT) and cellular DMFT and measure a number of different physical observables. We study the antiferromagnetic phase diagram using physically relevant parameters [2] and account for the possibility of incommensurate order by solving the Bethe-Salpeter equation in certain parts of the phase diagram. Further we measure the impurity susceptibility and find that the experimental findings of Ref. [1] are qualitatively well reproduced in the three-band Emery model. At lower doping levels our preliminary results seem to support the idea of a single band description for single and two particle observables in small energy windows at low temperatures (at least qualitatively). At the same time, however, excitations beyond a couple of 100 meV as well as the high doping regime seem to be problematic for a static single band picture.

[1] M. Avramovska, D. Pavićević, and J. Haase, *Journal of Superconductivity and Novel Magnetism* **33**, 2621–2628 (2020).

[2] N. Kowalski, S. S. Dash, P. Sémon, D. Sénéchal, and A.-M. Tremblay, *PNAS* **118**, 40 e2106476118 (2021).

## Field-angle dependence reveals odd-parity superconductivity in CeRh<sub>2</sub>As<sub>2</sub>

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CeRh<sub>2</sub>As<sub>2</sub> is an unconventional superconductor with multiple superconducting phases and  $T_c = 0.26$  K. When  $H \parallel c$ , it shows a field-induced transition at  $\mu_0 H^* = 4$  T from a low-field superconducting state SC1 to a high-field state SC2 with a large critical field of  $\mu_0 H_{c2} = 14$  T. In contrast, for  $H \parallel ab$ , only the SC1 with  $\mu_0 H_{c2} = 2$  T is observed [1]. A simple model based on the crystal symmetry was able to reproduce the phase-diagrams and their anisotropy, identifying SC1 and SC2 with even and odd parity superconducting states, respectively. However, additional orders were observed in the normal state which might have an influence on the change of the superconducting state at  $H^*$  [2]. Here, we present a comprehensive study of the angle dependence of the upper critical fields using magnetic ac-susceptibility, specific heat and torque on single crystals of CeRh<sub>2</sub>As<sub>2</sub>. The experiments show that the state SC2 is strongly suppressed when rotating the magnetic field away from the  $c$ -axis and it disappears for an angle of 35°. This behavior agrees perfectly with our extended model of a pseudospin triplet state with  $\mathbf{d}$  vector in the plane and hence allows to nail down that SC2 is indeed the suggested odd-parity state.

[1] S. Khim and J. F. Landaeta *et al.* Science **373** (6558), 1012-1016 (2021)

[2] D. Hafner *et al.* Phys. Rev. X **12** (1), 011023 (2022)



# Impurity effect on superconducting diode effect

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The acquisition of new functionalities in superconductors is essential not only for engineering development, such as the creation of more energy-saving devices, but also for the development of the basic science of superconductivity. In recent years, nonreciprocal transport phenomena have attracted much attention as a new functionality of matter [1, 2]. In the field of superconductivity, the superconducting diode effect (SDE) has been observed in [Ni/V/Ta] artificial superlattice superconductors with inversion symmetry breaking [3]. The SDE refers to a current flow with zero electrical resistance in one direction and a finite resistance in the opposite direction (Fig.1). A theoretical explanation for the SDE was given in terms of the departing current [4-7], i.e., SDE by intrinsic mechanism. Moreover, the theory shows an interesting result suggesting that the sign change of SDE is closely related to the helical superconductivity [4], in which Cooper pairs are stabilized with a finite center-of-mass momentum. On the other hand, the time-reversal symmetry breaking by an applied magnetic field violates the assumption of Anderson's theorem [8], and indeed it is widely known that impurities have a significant effect on the physical properties of superconductivity [7, 9]. The evaluation of the effect of impurities on the SDE is interesting not only for the performance evaluation of superconducting diodes, but also for the development of the fundamental theory of noncentrosymmetric superconductors.

In this study, we investigate the impurity effect on the nonreciprocity in the departing current. Our results show that the superconducting diode effect is significantly diminished except in the sign-reversal region.

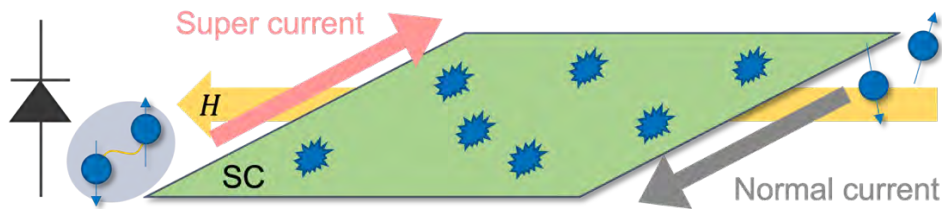


Fig. 1 Schematic figure for the SDE with impurities.

- [1] Y. Tokura and N. Nagaosa, *Nat. Commun.* **9**, 3740 (2018).
- [2] T. Ideue and Y. Iwasa, *Annu. Rev. Condens. Matter Phys.* **12**, 201 (2021).
- [3] F. Ando *et al.*, *Nature* **584**, 373 (2020).
- [4] A. Daido, Y. Ikeda, and Y. Yanase, *Phys. Rev. Lett.* **128**, 037001 (2022).
- [5] J. J. He *et al.*, *arXiv* :**2106**, 03575 (2021).
- [6] N. F. Q. Yuan and L. Fu, *PNAS* **119** (15) e2119548119 (2022).
- [7] S. Ilić and F. S. Bergeret, *arXiv* :**2108**, 00209 (2021).
- [8] P. W. Anderson, *J. Phys. Chem. Solids.* **11**, 26 (1959).
- [9] O. Dimitrova and M. V. Feigel'man, *Phys. Rev. B* **76**, 014522 (2007).

# Type-I Superconductivity in Non-centrosymmetric LaRhGe<sub>3</sub>

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Non-centrosymmetric (NCS) superconductors are theoretically proposed to have a mixture of singlet and triplet pairing in the superconducting state [1]. A novel spin-triplet state in a superconductor can host Majorana fermions, and can open up applications for quantum computing. A NCS with a strong triplet component will exhibit spontaneous time-reversal symmetry breaking (TRSB) as it enters the superconducting state in zero-field. A key ingredient to realizing triplet superconductivity is strong, asymmetric spin-orbit coupling (ASOC), which is generated by the lack of inversion and symmetry and scales with the atomic number. This ASOC the degeneracy of spin-up and spin-down bands, which can be directly probed via studies of the de Haas van Alphen (dHvA) effect. One family of materials where this has been demonstrated to occur is the intermetallic germanides LaTGe<sub>3</sub> (*T*: Fe, Co, Rh, Ir) [2], which crystalize in the non-centrosymmetric space group *I4mm* and are therefore a promising platform to search for spin-triplet superconductivity.

We have grown large single crystals of LaRhGe<sub>3</sub>, which have been obtained from a self-flux method for the first time. I present our discovery of Type-I superconductivity in LaRhGe<sub>3</sub> with evidence from heat capacity and  $\mu$ SR experiments, with a critical temperature  $T_c$  of 0.385 K and critical field  $H_c$  of 2.1 mT [3]. Despite the strong ASOC in LaRhGe<sub>3</sub>, we do not detect any evidence for TRSB across  $T_c$  in LaRhGe<sub>3</sub> in our zero-field  $\mu$ SR experiment. Our results are consistent with LaRhGe<sub>3</sub> being a weak-coupling *s*-wave superconductor with a dominant singlet pairing. We also characterize the normal state of LaRhGe<sub>3</sub> with temperature and field dependent electrical transport. We find a non-saturating magnetoresistance at 2 K of 800% at 9 T, which may be related to electron-hole compensation and topology in LaRhGe<sub>3</sub>. Finally, we find that above the onset of superconductivity, LaRhGe<sub>3</sub> exhibits an unusual temperature dependence in its resistivity,  $\rho \sim T^3$ , suggestive of possible non-Fermi liquid behavior.

[1] M. Smidman et al., Rep. Prog. Phys. **80**, 036501 (2017).

[2] T. Kawai et al., JPSJ **77**, 064717 (2008).

[3] M. Oudah, et al., in preparation.

# Chiral Superconductivity in $UPt_3$ observed by scanning SQUID Microscopy

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Symmetry and topology are tools to describe states of quantum matter: A long sought after indication for unconventional pairing of superconducting electrons is the breaking of additional symmetries other than gauge symmetry.

$UPt_3$  undergoes at low temperatures a strong electron mass renormalization (more than 100 times the free electron mass). These heavy fermions form superconducting Cooper pairs below 0.55 K. Superconductivity is expected to be mediated by spin fluctuations.

$UPt_3$  presents at ambient pressure three different superconducting phases A,B,C each with an order-parameter of different symmetry. Upon cooling in zero applied magnetic field the frontier between the A and the chiral B phase (breaking time reversal symmetry) is crossed at 0.5 K. In the B phase, energetically degenerate chiral domains are expected to appear: Theory predicts the existence of fractional vortices and an unusual flux distribution at the domain wall separating chiral domains.

With our scanning SQUID microscope we could observe in the B phase of  $UPt_3$  magnetic flux aligning with domain walls and detect half- $\Phi_0$  vortices. Half- $\Phi_0$  vortices are not observed in the A phase.

These direct observations are a strong indication for time reversal symmetry breaking and chiral superconductivity in  $UPt_3$ .

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## ***Investigation of the evolution of magnetic fluctuations in LSCO, measured in the quasi-elastic region***

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In cuprate superconductivity (SC), there is a subtle connection between SC and antiferromagnetism: [1,2] magnetic fluctuations are considered to play a decisive role as a “glue” that can bind together Cooper pairs, while on the other hand magnetic order suppresses SC [3]. Therefore, it is important to investigate the interplay between magnetism and SC to facilitate a common and detailed understanding of the elusive phenomena in unconventional SC.

The magnetism in  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  (LSCO), and similar cuprates, is found as static or dynamic stripes, i.e., small patches of antiferromagnetism, separated by ‘rivers’ of charge, giving rise to magnetic signals at incommensurate positions in q-space [4]. With neutrons we find that while dynamic stripes are present at all temperatures, static stripes appear only below the SC critical temperature. However,  $\mu\text{SR}$  measurements curiously find a much lower ordering temperature [5-8]. While this discrepancy has been attributed to the different time scales between the methods, no direct proof has been given to date.

In this work we present our preliminary results and first evidence on the transformation from static magnetism to magnetic fluctuations in  $\text{La}_{1.95}\text{Sr}_{0.05}\text{CuO}_4$  obtained on the IN16b backscattering instrument at Institute Laue Langevin (ILL), Grenoble [9].

We find evidence that the static magnetic signal is accompanied by a narrow (0.24  $\mu\text{eV}$ ) quasielastic signal at  $T = 2$  K. This discovery could lead to an explanation of the nature of the transition process between static and dynamic stripes, and thereby to the larger and crucial question of the relation between stripes and SC in the LSCO cuprates.

[1] B. Lake et al., *Nature* **400** 43 (1999)

[2] B. Keimer et al., *Nature* **518** 179 (2015)

[3] D. J. Scalapino, *Rev. Mod. Phys.*, **84** 1383 (2012)

[4] J. Tranquada et al., *Nature*, **375** 561 (1995)

[5] B. Keimer et al., *PRB* **45** 7430 (1992)

[6] T.P. Croft et al., *PRB* **89** 224513 (2014)

[7] N.E. Hussey et al., *Philos. Trans. A* **369** 1626 (2011)

[8] M. Kofu et al., *PRL* **102** 047001 (2009).

[9] ILL data set IN16-BATS (DOI 10.5291/ILL-DATA.TEST-3186)

# ***Thermodynamic evidence for two superconducting phases at ambient pressure in $UTe_2$***

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Three years ago, superconductivity was discovered in the paramagnetic compound  $UTe_2$  [1]. The possibility of triplet superconductivity, maybe driven by ferromagnetic fluctuations, and of topological superconductivity, triggered many studies. Nevertheless, the pairing symmetry and mechanism remain unknown.

A striking property of  $UTe_2$  at ambient pressure is the field reinforcement of superconductivity above 15 T along the hard magnetisation axis [2], up to a metamagnetic transition at 34.5 T.

We report new investigations under field along the three crystallographic axis of  $UTe_2$  by specific heat measurements up to 36 T [3]. We could establish the phase diagram of the superconducting phases. These measurements reveal the emergence of a second superconducting phase above 15 T when field is applied along the hard magnetisation axis. Thus, two superconducting phases are present, one at low fields with an extrapolated upper limit of 20 T, and the second at higher fields only limited by the metamagnetic transition at 34.5 T. These measurements emphasize that the two phases have different natures, requiring explanations beyond a simple change of symmetry of the superconducting order parameter as proposed in earlier theoretical studies [4,5]. Different scenarios for the explanation of the  $H_{c2}$  behaviour and the connection with the metamagnetic transition will be presented.

These measurements allow us to rediscuss the contradictory anisotropies observed between the upper critical field  $H_{c2}$  and the lower critical field  $H_{c1}$  [6]. They also confirm the presence of Lifshitz anomalies for fields along the easy magnetization axis [7].

[1] S. Ran et al. *Science*, 365, 684 (2019)

[2] G. Knebel et al. *JPSJ*, 88, 063707 (2019)

[3] A. Rosuel et al. *ArXiv* (2022)

[4] J. Ishizuka et al. *Phys. Rev. Lett.* **123**, 217001 (2019)

[5] T. Shishidou et al. *Phys. Rev. B* **103**, 104504 (2021)

[6] C. Paulsen et al. *Phys. Rev. B* **103**, L180501 (2021)

[7] Q. Niu et al. *Phys. Rev. Lett.* **124**, 086601 (2020)

## Puddle formation, persistent gaps, and non-mean-field breakdown of superconductivity in overdoped (Pb,Bi)<sub>2</sub>Sr<sub>2</sub>CuO<sub>6+δ</sub>

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The cuprate high-temperature superconductors exhibit many unexplained electronic phases, but it was often thought that the superconductivity at sufficiently high doping is governed by conventional mean-field Bardeen-Cooper-Schrieffer (BCS) theory<sup>[1]</sup>. However, recent measurements show that the number of paired electrons (the superfluid density) vanishes when the transition temperature  $T_c$  goes to zero<sup>[2]</sup>, in contradiction to expectation from BCS theory. The origin of this anomalous vanishing is unknown. Our scanning tunneling spectroscopy measurements in the overdoped regime of the (Pb,Bi)<sub>2</sub>Sr<sub>2</sub>CuO<sub>6+δ</sub> high-temperature superconductor show that it is due to the emergence of puddled superconductivity, featuring nanoscale superconducting islands in a metallic matrix<sup>[3,4]</sup>. Our measurements further reveal that this puddling is driven by gap filling, while the gap itself persists beyond the breakdown of superconductivity. The important implication is that it is not a diminishing pairing interaction that causes the breakdown of superconductivity. Unexpectedly, the measured gap-to-filling correlation also reveals that pair-breaking by disorder does not play a dominant role and that the mechanism of superconductivity in overdoped cuprate superconductors is qualitatively different from conventional mean-field theory

[1] B. Keimer *et al.*, *Nature* **518**, 179-186 (2015)

[2] I. Bozovic *et al.*, *Nature* **536**, 309-311 (2016)

[3] N.R. Lee-Hone *et al.*, *Phys. Rev. B* **96**, 024501 (2017)

[4] Z.-X. Li *et al.*, *NPJ Quantum Mater.* **6**, 36 (2021)

## Superconductivity in CaPd<sub>2</sub>Ge<sub>2</sub> and CaPd<sub>2</sub>As<sub>2</sub>: A $\mu$ SR study

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The quest of understanding the role of Fe in unconventional superconducting behavior in the family of FeAs-based superconductors have attracted considerable attention. In this context the investigations of iron-free 122-type superconductors are also considered important for a comparative study. CaPd<sub>2</sub>Ge<sub>2</sub> and CaPd<sub>2</sub>As<sub>2</sub> which exhibit type-II superconductivity with a  $T_c = 1.69$  K [2] and 1.27 K [3], respectively, are two such iron-free superconductors. Interestingly, despite a very sharp superconducting transition in both, the jump in their electronic specific heat at  $T_c$  yields much smaller values of  $\Delta C_e/\gamma_n T_c = 1.21$  for CaPd<sub>2</sub>Ge<sub>2</sub> single crystal [2] and 1.14 for CaPd<sub>2</sub>As<sub>2</sub> single crystal [3] compared to the BCS value of 1.43. Within the  $\alpha$ -model of BCS superconductivity, the reduced value of  $\Delta C_e/\gamma_n T_c$  corresponds to a reduced value of  $\alpha = \Delta(0)/k_B T_c = 1.62$  for CaPd<sub>2</sub>Ge<sub>2</sub> [2] and 1.58 for CaPd<sub>2</sub>As<sub>2</sub> [3] instead of the BCS value  $\alpha_{BCS} = 1.764$ .

The reduced value of  $\Delta C_e/\gamma_n T_c$  and hence  $\alpha$  is usually caused by an anisotropic superconducting order parameter, or due to the presence of multiple superconducting gaps [4]. Therefore in order to understand the nature of the superconducting order parameter in CaPd<sub>2</sub>Ge<sub>2</sub> and CaPd<sub>2</sub>As<sub>2</sub> we felt it necessary to probe the superconducting gap structure through the microscopic muon spin relaxation and rotation ( $\mu$ SR) measurements. Our  $\mu$ SR results of CaPd<sub>2</sub>Ge<sub>2</sub> and CaPd<sub>2</sub>As<sub>2</sub> are consistent with the weakly coupled phonon-mediated conventional BCS superconductivity in the dirty limit. From the analysis of the  $\mu$ SR spectra we infer single-gap isotropic s-wave superconductivity in both with preserved time-reversal symmetry.

[1] D. C. Johnston, Adv. Phys. **59**, 803 (2010).

[2] V. K. Anand *et al.*, J. Phys.: Condens. Matter **26**, 405702 (2014).

[3] V. K. Anand *et al.*, Phys. Rev. B **87**, 224510 (2013).

[4] Johnston D C 2013 Supercond. Sci. Technol. **26**, 115011 (2013).

# Tunneling spectroscopy at very high magnetic fields in the iron based superconductor $\text{KFe}_2\text{As}_2$

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We present scanning tunneling spectroscopy measurements in  $\text{KFe}_2\text{As}_2$ . This system is a superconductor with  $T_c=3.4$  K, which is at the end of the  $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$  series. It has been proposed to be a nodal superconductor [1]. The electronic effective mass is strongly enhanced due to the proximity to an orbital-selective Mott transition [1]. Here we make first STM measurements at very low temperatures and high magnetic fields [2]. At zero field, we identify a strong anisotropy of the superconducting gap. In the mixed state, we observe the vortex lattice at very large values of the magnetic field. We finally present measurements of the bandstructure in the superconducting and normal phases, obtained at zero magnetic field and at a magnetic field of 20 T from quasiparticle interference scattering.

[1] F. Hardy et al., Phys. Rev. Lett. 111, 027002 (2013)

[2] M. Fernández-Lomana et al, Rev. Sci. Instrum. 92, 093701 (2021)



# **Exploring the limits of unconventional superconductivity with a novel complex impedance scanning tunneling microscope**

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Superconductors exhibit fascinating properties, including zero resistivity, a diamagnetic Meissner effect, and macroscopic quantum phenomena, with promising applications in quantum computing and electrical engineering. Conventional superconductors can be described by a single macroscopic order parameter, from which we derive expressions for the hallmark properties. In unconventional superconductors, which are not understood, the situation is remarkably different. Importantly, the superfluid can be inhomogeneous in space down to the nanoscale, yielding different regions with different properties, not all showing on the same scale. To understand why such an inhomogeneous state exists and what determines the length scales over which it persists, we need a probe to extract the local behaviour of both superconducting and normal carriers. I will develop a complex impedance scanning tunneling microscope to probe the local normal- and superfluid carrier density, thereby visualizing local and macroscopic phase coherence and both periodic and non-periodic inhomogeneity. Can we relate these inhomogeneities to fluctuations taking place at the critical temperature? Are their patterns to be found within the inhomogeneity? By spatially resolving the frequency dependence of the complex conductivity over temperature, I will study the local resistivity and Meissner effect in a quest to answer these questions.

# High Pressure-Tuning of Electron-Doped Cuprate Superconductors

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In the cuprate superconductors  $Ln_{2-x}Ce_xCuO_4$ , electron-doping through Ce substitution leads to a seemingly prototypical phase diagram featuring a suppression of a Mott insulating antiferromagnetic (AFM) phase, a sudden emergence of unconventional superconductivity, and a Fermi surface reconstruction across optimal doping. Yet despite this apparent generic picture, the interplay between the aforementioned electronic phases remains poorly understood [1]. In particular for  $Ln = Pr$ , conflicting reports exist concerning the extent of the AFM phase and whether or not it may coexist with superconductivity (e.g. [2,3]). Similarly, the existence of a quantum critical point below the superconducting dome, and if and how it is related to the AFM phase and to the Fermi surface reconstruction remain open questions. One challenging aspect of cuprate superconductors is that sample growth and annealing procedures depend on the exact doping concentration  $x$ , which may explain the hitherto inconclusive results.

Here, we will present a new approach by employing hydrostatic pressures to tune underdoped single-crystals of  $Pr_{2-x}Ce_xCuO_4$  across the phase boundaries. Pressure is expected to tune  $Pr_{2-x}Ce_xCuO_4$  in a different way compared to Ce doping by controlling the bandwidth instead of the formation of in-gap states, whilst also reducing the sample dependence on growth and annealing conditions. We will discuss our initial high-pressure transport, Hall effect and penetration depth measurements which confirm the suppression of the insulating/AFM phase, but with reduced quasiparticle scattering and thus closer to the clean limit.

[1] N. Armitage *et al.*, Rev. Mod. Phys. **82**, 2421 (2010).

[2] E.M. Motoyama *et al.*, Nature **445**, 186 (2007).

[3] Y. Dagan *et al.*, Phys. Rev. Lett. **92**, 167001 (2004).

# Superconducting Instabilities in Strongly-Correlated Infinite-Layer Nickelates

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The discovery of superconductivity in infinite-layer nickelates [1] has added a new family of materials to the fascinating growing class of unconventional superconductors. By incorporating the strongly correlated multi-orbital nature of the low-energy electronic degrees of freedom [2], we compute the leading superconducting instability from magnetic fluctuations relevant for infinite-layer nickelates. Specifically, by properly including the doping dependence of the Ni  $d_{x^2-y^2}$  and  $d_{z^2}$  orbitals as well as the self-doping band, we uncover a transition from d-wave pairing symmetry to nodal  $s_{\pm}$  superconductivity, driven by strong fluctuations in the  $d_{z^2}$ -dominated orbital states [3]. We discuss the properties of the resulting superconducting condensates in light of recent tunneling [4] and penetration depth experiments [5,6] probing the detailed superconducting gap structure of these materials.

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- [1] D. Li, *et al.*, Superconductivity in an infinite-layer nickelate, *Nature* **572**, 624 (2019).
- [2] F. Lechermann, Multiorbital processes rule the  $\text{Nd}_{1-x}\text{Sr}_x\text{NiO}_2$  normal state, *Phys. Rev. X* **10**, 041002 (2020).
- [3] Andreas Kreisel, Brian M. Andersen, Astrid T. Rømer, Ilya M. Eremin, Frank Lechermann, arXiv:2202.11135 (2022).
- [4] Q. Gu, *et al.*, Single particle tunneling spectrum of superconducting  $\text{Nd}_{1-x}\text{Sr}_x\text{NiO}_2$  thin films, *Nature Communications* **11**, 6027 (2020).
- [5] L. E. Chow, *et al.*, Pairing symmetry in infinite-layer nickelate superconductor, arXiv:2201.10038 (2022).
- [6] S. P. Harvey, *et al.*, Evidence for nodal superconductivity in infinite-layer nickelates, arXiv:2201.12971 (2022).

## mK STM studies of FeSe

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FeSe is a superconductor with strong two-dimensional character and electron and hole bands crossing the Fermi level. There is a set of hole bands centered at the Brillouin zone which are highly elongated along one in-plane crystalline axis and another set of electron bands at the corners and sides of the Brillouin zone that are also highly in-plane anisotropic. Different measurements show that the Fermi energy in one or several of these bands might be very small, comparable to the superconducting gap size. This is at stark contrast to most superconductors, where the gap size is usually negligible with respect to the Fermi energy.

Here we study the superconducting density of states of FeSe using millikelvin Scanning Tunneling Microscopy. We trace the quasiparticle dispersion relation and find a strongly electron-hole anisotropic density of states. In particular, we show that the superconducting density of states close to the quasiparticle peaks is in-plane anisotropic for hole excitations but four-fold symmetric for electron excitations. This peculiar electron-hole anisotropy is due to a band whose Fermi level is even smaller than the superconducting gap. Furthermore, we analyze in detail the quasiparticle density of states very close to defects and find of in-gap features in the tunneling conductance connecting quasiparticle states among different impurities

# Majorana zero modes on parallel one-dimensional p-wave superconducting wires

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The one-dimensional topological superconductor is known to have two Majorana zero modes on the edge [1].

Consider the model of parallel p-wave superconductor wires. The phase difference between parallel wires is  $\varphi$ , which can be tweaked so that the Majoranas between the parallel wires will have different coupling modes. When there is no coupling between the parallel wires, there will definitely be four Majorana zero modes on the edge of both chains. However, if the perpendicular hopping amplitude is not 0, the Majoranas between the parallel wires will couple with each other in different ways. We analyze how many Majorana zero mode will emerge when the chemical potential and the perpendicular hopping amplitude satisfy different conditions.

What is more, we connect the parallel p-wave superconductor wires to the normal conductors and show that the differential conductance can also be quantized even without Majorana zero modes. The differential conductance will be calculated by the recursive green function method [2].

[1] A. Y. Kitaev, *Physics-Uspekhi* **44**, 131 (2001).

[2] D. Takagi, S. Tamura, and Y. Tanaka, *Phys. Rev. B* **101**, 024509 (2020).

# Pairing symmetries in Sr<sub>2</sub>RuO<sub>4</sub> from first-principles

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Using DFT+DMFT method, we investigate feasible symmetries of the superconducting gap function in Sr<sub>2</sub>RuO<sub>4</sub>. Spin and charge susceptibilities are evaluated and then used to construct an effective BCS gap equation within the linearized Eliashberg formalism. Most stable solutions include nodal s-wave (s') and  $d_{x^2-y^2}$  which are nearly degenerate, as well as odd-parity interorbital pairings which can lead to a chiral gap function, all in spin-singlet channel. We argue that adopting a fully frequency dependent two-particle vertex in susceptibility calculation is essential to obtain such gap symmetries.

# Effect of pressure on normal and superconducting states of YFe<sub>2</sub>Ge<sub>2</sub>

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The iron-germanide superconductor YFe<sub>2</sub>Ge<sub>2</sub> displays a large Sommerfeld coefficient  $C/T \sim 100$  mJ/mol K<sup>2</sup> and a  $T^{1.5}$  non-Fermi liquid form of the normal-state resistivity, indicating the presence of strong electronic correlations [1-3]. The coexistence of strong ferro- and antiferromagnetic fluctuations probed by inelastic neutron scattering [4], the clear detrimental effect of lattice disorder on superconductivity [2-3], and theoretical predictions from DFT calculations [5] all point towards an unconventional superconducting pairing mechanism, the origin of which demands further investigation.

YFe<sub>2</sub>Ge<sub>2</sub> is paramagnetic, but the isostructural and isoelectronic sister compound LuFe<sub>2</sub>Ge<sub>2</sub> exhibits spin-density-wave (SDW) order below  $T_N \sim 9$  K. Moderate substitution of Lu by Y suppresses  $T_N$ , whereas hydrostatic pressure boosts the SDW transition in LuFe<sub>2</sub>Ge<sub>2</sub> to higher temperatures [6, 7]. This suggests that LuFe<sub>2</sub>Ge<sub>2</sub> and YFe<sub>2</sub>Ge<sub>2</sub> sit on either side of an SDW quantum critical point, which could be connected to superconductivity and non-Fermi liquid properties and might be accessible through application of hydrostatic pressure in YFe<sub>2</sub>Ge<sub>2</sub>.

Here, we present results of electrical transport and magnetic susceptibility measurements in high-quality YFe<sub>2</sub>Ge<sub>2</sub> single crystals under applied hydrostatic pressure up to and beyond 70 kbar. Our data show a gradual full suppression of superconductivity and non-Fermi liquid transport signatures without evidence for a pressure-induced magnetic transition, suggesting different effects of pressure and composition tuning in YFe<sub>2</sub>Ge<sub>2</sub> and providing an expanded view of the interplay between superconducting and normal state properties for theoretical analysis.

[1] J. Chen *et al.*, Phys. Rev. Lett., **116**, 127001 (2016).

[2] J. Chen *et al.*, Phys. Rev. B, **99**, 020501(R) (2019).

[3] J. Chen *et al.*, Phys. Rev. Lett., **125**, 237002 (2020)

[4] H. Wo *et al.*, Phys. Rev. Lett. **122**, 217003 (2019)

[5] A. Subedi, Phys. Rev. B **89**, 024504 (2014); D. J. Singh, Phys. Rev. B **89**, 024505 (2014).

[6] S. Ran *et al.*, Philos. Mag. **91**(34), 4388–4400 (2011).

[7] T. Fujiwara *et al.*, J. Phys. Soc. Jpn. **76**, 60–61 (2007).

## **Cooper pairs sizes in two orbital superconductor with d-wave pairing**

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We study the temperature behavior of the sizes of Cooper pairs in particular orbitals with a d-wave symmetry at various band fillings in the framework of two-orbital superconductivity model with intra-site intra-orbital attractive Hubbard correlations together with inter-site inter-orbital pair transfer interactions. It is found that the sizes of Cooper pairs can decrease with the temperature substantially stronger compared to the behavior in a single-orbital system.



# Temperature-dependent angle resolved photoemission spectroscopy study of the possible topological Kondo insulator CeNiSn

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Kondo insulators (KI's) have attracted revived attention as they can be topological Kondo insulators (TKI's) due to their strong spin-orbit coupling and the odd parity of the f states [1]. In fact, robust conducting surface states were observed in transport measurements for SmB<sub>6</sub>, which is considered a representative KI [2]. Recently, it was reported theoretically that CeNiSn, a KI having the non-symmorphic symmetry, could have a topological state [3]. Hence, it is important to investigate the electronic structure of CeNiSn experimentally to confirm whether CeNiSn belongs to a TKI. In this work, we have performed a temperature-dependent angle resolved photoemission spectroscopy (ARPES) study of CeNiSn, which is a TKI candidate. We have measured the Fermi surfaces and band structures for three orthogonal crystallographic planes, and compared them with the density functional theory calculations. Then, in order to investigate the role of Ce 4f states in determining the TKI property of CeNiSn, we have performed temperature-dependent ARPES measurements near the Ce 4f resonance. In this presentation, we will discuss the correlation between the Kondo effect and the possible topological states in CeNiSn.

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[1] M. Dzero, J. Xia, V. Galitski, and P. Coleman, *Annu. Rev. Condens. Matter Phys.* **7**, 249 (2016).

[2] S. Wolgast *et al.*, *Phys. Rev. B* **88**, 180405 (2013).

[3] Po-Yao Chang *et al.*, *Nat. Phys.* **13**, 794 (2017).

# Numerical study of screening clouds around quantum impurities subject to disorder and anisotropy

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Dilute quantum impurities in metals induce complex correlations in real space that are difficult to calculate due to their multi-scale nature, so that studies of screening clouds are often reduced to the s-wave scattering in clean hosts. Although universal behavior of spatial correlations induced on electronic states have been extensively studied in asymptotic regimes, a full microscopic description including the interplay with disorder and spatial anisotropies is still an open problem. We present an efficient and robust algorithm based on the recursive generation of natural orbitals, that are eigenvectors of the truncated single-particle density matrix.

This method is tailored for impurity problems, where the full many-body problem reduces to few degrees of freedom [1], and provides well-converged many-body wave functions on lattices with up to tens of thousands of sites. Taking advantage of the efficiency of the algorithm, we compute the disorder induced distribution of Kondo temperatures over thousands of realizations, at the same time gaining access to the full screening cloud in each sample [2].

While the charge screening cloud is typically shortened due to the polarization of the impurity by the disorder potential, we surprisingly find that rare disorder configurations preserve the long range nature of Kondo correlations in the electronic bath.

Finally we study the screening cloud around an adatom impurity in a 2-dimensional clean host with a square lattice of  $9e4$  sites, that goes beyond any existing numerical method, and show that absence of rotational invariance leads to strong anisotropy of spatial correlations.

[1] M. Debertolis, S. Florens, and I. Snyman, *Phys. Rev. B* **103**, 235166 (2021).

[2] M. Debertolis, I. Snyman, and S. Florens, arXiv:2203.13041 (2022).

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Michael Lang

## From magnetic order to valence-change crossover in $\text{EuPd}_2(\text{Si}_{1-x}\text{Ge}_x)_2$ using He-gas pressure

We are interested in novel collective phenomena in correlated electron materials which originate from a particularly strong coupling between electronic-, magnetic- and lattice degrees of freedom.  $\text{EuPd}_2\text{Si}_2$  is a promising target material for this purpose as it is one of the rare examples where a strong valence-change crossover can be induced merely by variation of temperature. This  $\text{Eu}^{(2+\delta)+}$  to  $\text{Eu}^{(3-\delta'+)}$  valence change is accompanied by pronounced lattice effects along with significant changes of the material's magnetic properties [1]. According to magnetic and thermodynamic measurements, this material is located on the high-pressure side (crossover range) of the second-order critical endpoint. This endpoint terminates the first-order valence transition in the generalized  $p$ - $T$  phase diagram of Eu-based intermetallics [2]. The aim of this study is to identify a suitable chemical modification, corresponding to a negative chemical pressure, so that the critical endpoint can be accessed via fine pressure tuning by using He-gas techniques. On approaching the critical endpoint we expect to enter a strong-coupling regime characterized by anomalous lattice and electronic properties reflecting distinct cross correlations between the various degrees of freedom [3].

Here we present magnetic susceptibility measurements taken on high-quality single crystals of  $\text{EuPd}_2(\text{Si}_{1-x}\text{Ge}_x)_2$  for  $0 \leq x \leq 0.2$  and temperatures  $2 \text{ K} \leq T \leq 300 \text{ K}$ . Measurements have been performed at ambient pressure and finite He-gas pressure  $p \leq 500 \text{ MPa}$ . For  $x = 0$  and ambient pressure we observe a pronounced valence crossover centered around  $T_v \sim 160 \text{ K}$  with a non-magnetic ground state. This valence-change crossover is characterized by an extraordinarily strong pressure dependence of  $dT_v/dp \approx 80 \text{ K/GPa}$ . As expected,  $T_v$  shifts to lower temperatures with increasing Ge-concentration, reaching  $T_v \sim 90 \text{ K}$  for  $x = 0.05$ , while still showing a non-magnetic ground state. Remarkably, on further increasing  $x$  to 0.2 we find a magnetic ground state with long-range antiferromagnetic order setting in below  $T_N = 47.5 \text{ K}$ . This compound with  $x = 0.2$  is of particular interest in the context of this study as the ground state turns out to be highly sensitive to pressure: through the application of slight pressure as low as 100 MPa the long-range magnetic order can be suppressed giving way to a non-magnetic ground state with pronounced valence fluctuations. We therefore consider this compound a promising target material for studying pressure-induced strong-coupling effects.

[1] B. Batlogg, A. Jayaraman, V. Murgai, L. C. Gupta, R. D. Parks, M. Croft, in *Valence Instabilities*, ed. P. Wachter and H. Boppert, North-Holland Publishing Company, 229, (1982)

[2] Y. Onuki, A. Nakamura, F. Honda, D. Aoki, T. Tekeuchi, M. Nakahima, Y. Amako, H. Harima, K. Matsubayashi, Y. Uwatoko, S. Kayama, T. Kagayama, K. Shimizu, S. Esaki, Muthu, D. Braithwaite, B. Salce, H. Shiba, T. Yara, Y. Ashitomi, H. Akamine, K. Tomori, M. Hedo, T. Nakama, *Philosophical Magazine* **97**, 3399 (2017).

[3] E. Gati, M. Garst, R.S. Manna, U. Tutsch, B. Wolf, L. Bartosch, H. Schubert, T. Sasaki, J.A. Schlueter, M. Lang, *Science Advances* **2**, e1601646 (2016).

# Valence fluctuations and structural collapse in Eu-based phosphides $\text{EuT}_2\text{P}_2$

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Studies of enhanced coupling between electrons and phonons is focussed on materials exhibiting phase transitions involving both electronic and lattice degrees of freedom. Europium in intermetallic systems can exhibit different magnetic ground states: If the ground state is  $\text{Eu}^{2+}$ , the system shows long range magnetic order; if the ground state is  $\text{Eu}^{3+}$ , no magnetic order is observed. In between, different intermediate valence states are stabilized [1].

When looking at europium based phosphides  $\text{EuT}_2\text{P}_2$  ( $T = \text{Fe}, \text{Co}, \text{Ni}, \text{Ru}$ ) in the  $\text{ThCr}_2\text{Si}_2$  structure, the ground state of europium interrelates with the crystal structure. There are two states for the  $\text{ThCr}_2\text{Si}_2$  crystal structure, referred to as the non-collapsed and the collapsed state. In the latter, covalent bonds between phosphorus atoms of neighbouring interlayers are established [2]. While  $\text{EuFe}_2\text{P}_2$  [3],  $\text{EuRu}_2\text{P}_2$  [4] and  $\text{EuCo}_2\text{P}_2$  [5] exhibit different magnetic order and appear in the non-collapsed phase of the crystal structure,  $\text{EuNi}_2\text{P}_2$  exhibits a valence fluctuation crossover and appears in the collapsed phase [6]. The structural collapse in  $\text{EuT}_2\text{P}_2$  ( $T = \text{Fe}, \text{Co}, \text{Ru}$ ) can be introduced by pressure, which has previously been studied on powder samples, showing a sharp first order transition for  $\text{EuCo}_2\text{P}_2$  and broad transitions for  $\text{EuFe}_2\text{P}_2$  and  $\text{EuRu}_2\text{P}_2$  at room temperature [7].

In this work, we revisit the structural collapse in  $\text{EuT}_2\text{P}_2$  ( $T = \text{Fe}, \text{Co}, \text{Ru}$ ), reporting on single crystal diffractometry at high pressures at 15K and 300K. Additionally, we show characterizations of the electronic and structural contributions to the valence fluctuations in  $\text{EuNi}_2\text{P}_2$ .

[1] Y. Onuki *et al.*, *Philos. Mag.* **97**, 3399 (2017).

[2] R. Hoffmann, C. Zheng, *J. Phys. Chem.* **89**, 4175-4181 (1985).

[3] C. Feng *et al.*, *Phys. Rev. B* **82**, 094426 (2010).

[4] P. Proschek *et al.*, *J. Alloys and Compounds* **864**, 158753 (2021).

[5] N.S. Sangeetha *et al.*, *Phys. Rev. B* **94**, 014422 (2016).

[6] Y. Hiranaka *et al.*, *J. Phys. Soc. Jpn.* **82**, 083708 (2013).

[7] C. Huhnt *et al.*, *Physica B* **252**, 44-54 (1998).

# Magnetic hard-direction ordering in anisotropic Kondo systems

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We present a generic mechanism that explains why many Kondo materials show magnetic ordering along directions that are not favoured by the crystal-field anisotropy. Using a renormalization-group (RG) analysis of single impurity Kondo models with single-ion anisotropy, we demonstrate that strong fluctuations above the Kondo temperature drive a moment re-orientation over a wide range of parameters, e.g. for different spin values  $S$  and number of Kondo channels  $N$ . In tetragonal systems this can happen for both easy-plane or easy axis anisotropy. The characteristic crossing of magnetic susceptibilities is not an artefact of the weak-coupling RG treatment but can be reproduced in brute-force perturbation theory. Employing numerical renormalization group (NRG), we show that for an under-screened moment ( $S = 1$ ,  $N = 1$ ) with easy-plane anisotropy, a crossing of magnetic susceptibilities can also occur in the strong-coupling regime (below the Kondo temperature). This suggests that collective magnetic ordering of such under-screened moments would develop along the magnetic hard axis.

# Magnetic hard-direction ordering in anisotropic Kondo systems

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## ***Kondo systems with periodically driven dipole transitions***

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In this work, we study the effects of light irradiation on a magnetic impurity. The impurity is modelled by the single impurity Anderson model where the local impurity is coupled to the conduction electrons via dipole coupling. Therefore, the application of a strong laser field induces a time-periodic hybridization. This can be treated within Floquet Green's function method combined with the slave boson non-crossing approximation [1].

What we see is that the Kondo peak is robust against small driving strengths, and then it gets strongly suppressed when the driving strength increases. However, we find that the destruction of the Kondo effect occurs much faster in terms of driving strength compared to a situation where the energy level of the impurity is itself driven independently.

[1] B. H. Wu and J. C. Cao, Physical Review B 81, 085327 (2010).

## *Microscopic essence of magnetism in Ce<sub>2</sub>Pd<sub>2</sub>In at ambient and elevated pressures*

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Among the  $R_2T_2X$  intermetallics adopting the Shastry-Sutherland-like tetragonal structure ( $P4/mbm$ ), Ce<sub>2</sub>Pd<sub>2</sub>In represents the rare example of Ce-based ferromagnet ( $T_C = 4.16$  K), however the ground state is reached via the antiferromagnetic ( $T_N = 4.65$  K) interphase [1].

Anisotropic properties of Ce<sub>2</sub>Pd<sub>2</sub>In observed both at ambient and elevated pressure are strongly related to the details of crystal structure. Investigation of lattice temperature evolution has shown the basal plane varying with temperature more than the  $c$ -direction, probably related to the additional degree of freedom in  $R-4h$  and  $T-4g$  crystallographic positions. Pressure effect on the lattice is a subject of recent high pressure X-ray diffraction experiment. However, similar trend can be expected, based on the comparison with La<sub>2</sub>Pd<sub>2</sub>In analogue showing  $a$ -direction more sensitive to both temperature and pressure variations [2,3].

Ambient-pressure neutron powder diffraction confirmed the character of magnetic orderings and the antiferromagnetic state was described as incommensurate one with propagation vector  $k \approx (0.21, 0, 0)$ . Development of magnetism upon pressure was found to depend on the way of pressure acting. Hydrostatic pressure, supposed to act towards increase of  $c/a$  ratio, leads to the suppression of ferromagnetic state at  $p_c \approx 4.0(3)$  GPa accompanied with the significant Kondo-like anomaly formation. Contrarily, uniaxial pressure applied along the  $c$ -direction has rather opposite effect resulting in only slight increase of  $T_C$ . Comparison of the lattice evolution of the magnetic Ce- and the nonmagnetic La-based system leads to conviction of the  $4f$  electronic states being the base of both – structural and magnetic behavior of Ce<sub>2</sub>Pd<sub>2</sub>In at elevated pressure.

[1] M. Klicpera *et al.*, J. Magn. Magn. Mater. **404**, 250 (2016).

[2] P. Král *et al.*, J. Alloys Compd. **878**, 160304 (2021).

[3] P. Král *et al.*, J. Phys. Condens. Matter **34**, 145403 (2022).



# Thermoelectric signatures of Majorana-Kondo interplay in double quantum dots

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Majorana bound states (MBSs) and strong correlations are two directions at the forefront of modern condensed matter physics. The search for MBSs is stimulated by their potential ability to serve as qubits in quantum computing devices. Transport measurement on the quantum dot attached to the end of topological superconducting nanowire has been used for verification of their presence there and for exploration of their properties with partial success [1]. On the other hand, in various systems at low temperatures strong electronic correlations give rise to rich phase diagrams comprising unconventional phases [2].

In this contribution we bridge these two fields with theoretical investigations of the signatures of MBSs in the electric and thermoelectric transport properties of a T-shaped double quantum dot coupled to a Majorana wire [3]. Addressing the two-stage Kondo regime by means of the density-matrix numerical renormalization group method, we demonstrate new aspects of the interplay of the Kondo and Majorana physics. We show that a modified Wiedemann-Franz law holds for the considered system. We further demonstrate that the Seebeck coefficient and spin thermopower both exhibit an additional sign change in the presence of MBSs. Finally, we also discuss finite current spin polarization in the system induced by the coupling to Majorana wire. These findings complement conventional zero-bias peak in the spectral density observed in MBS candidates.

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[1] M. T. Deng *et al.*, *Science* **354**, 1557 (2016).

[2] S. Paschen and Q. Si, *Nat. Rev. Phys.* **3**, 9 (2021).

[3] P. Majek, K. P. Wójcik, and I. Weymann, *Phys. Rev. B* **105**, 075418 (2022).

# Magnetic phase diagram and novel electronic phase in $U_2Rh_3Si_5$

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The intermetallic  $5f$  material  $U_2Rh_3Si_5$  exhibits a unique first order antiferromagnetic transition at  $T_N = 25.6$  K [1]. This was attributed to the so-called bootstrapping effect [2,3], in which the crystal field splitting in combination with the magnetoelastic interactions occurring close to a magnetic transition leads to changes in the crystal field scheme. This in turn influences magnetic order and triggers a first-order magnetic transition.

Recently, we presented a detailed study of the magnetic properties of  $U_2Rh_3Si_5$  in pulsed magnetic fields up to 65 T, revealing a complex magnetic phase diagram and strong anisotropy among the three crystallographic axes [4]. Moreover, our resistivity measurements indicated the presence of a novel phase of electronic nature slightly above the Néel temperature [4].

To shed light on the physics of this novel phase, we have conducted extensive studies on the electronic properties of  $U_2Rh_3Si_5$  by means of electrical resistivity in high magnetic fields and Hall effect measurements. Here, for the first time, we present the temperature dependence of the Hall coefficient. Surprisingly, we observe a non-linear in-field Hall response in particular close to  $T_N$ , which we discuss in relation to a possible electronic phase transition.

[1] B. Becker et al., Phys. Rev. Lett. **78**, 1347 (1997).

[2] Y.-L. Wang and B. R. Cooper, Phys. Rev. **172**, 539 (1968).

[3] R. G. Leisure et al., Phys. Rev. Lett. **95**, 075506 (2005).

[4] J. Willwater et al., Phys. Rev. B **103**, 054408 (2021).

# Orbital anisotropy probed by hyperfine couplings in Kondo lattice materials

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Heavy-fermion metals are described by strong electron-electron interactions that can be tuned across a quantum phase transition between localized  $f$ -electron magnetism and itinerant heavy-mass Fermi liquid behavior. Therefore, the overlap between neighboring atomic wave functions is a central feature and gives rise to a range of emergent phenomena, including antiferromagnetism, unconventional superconductivity, and the ability to tune from one ground state to the other in this class of materials. Nevertheless, measuring the degree of this hybridization by conventional methods is challenging and indirect.

Here we provide an approach using NMR to determine the magnetic couplings between the  $f$  electrons and neighboring nuclear spins in a series of Kondo lattice materials and find that the hybridization is strongly direction dependent in this significant class of superconducting heavy-fermion materials.[1] The experimental data are discussed in terms of a change in Ce's  $4f$  orbitals that arises from evolution of crystal-electric field (CEF) energy levels upon doping/pressure. We demonstrate that the hyperfine coupling probed by NMR provides a quantitative measure of orbital anisotropy.

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[1] P. Menegasso *et al.*, Phys. Rev. B **104**, 035154 (2021).

# Quadrupole phase transition in a cubic $4f^2$ compound PrCdNi<sub>4</sub> with a non-Kramers doublet ground state

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Cubic praseodymium-based intermetallic compounds with  $4f^2$  electrons have received much interests because the quadrupolar degrees of freedom of the nonmagnetic  $\Gamma_3$  doublet ground state under the crystalline electric field (CEF) shows a variety of phenomena [1]. Recently, we reported that PrMgNi<sub>4</sub> crystallizing in the cubic MgSnCu<sub>4</sub>-type structure [2] with an fcc sublattice of the Pr ions has the  $\Gamma_3$  doublet ground state [3,4]. At around 0.7 K, both magnetic specific heat  $C_m(T)$  and electrical resistivity  $\rho(T)$  exhibit broad anomalies, which could be ascribed to development of short-range correlation of quadrupolar degrees of freedom.

In the present work, we have synthesized an isostructural compound PrCdNi<sub>4</sub> and measured  $\rho(T)$ , magnetic susceptibility  $\chi$ , isothermal magnetization, and  $C(T)$  of polycrystalline samples. The  $\rho(T)$  shows a shoulder at around 15 K and  $C(T)$  exhibits a broad maximum at around 4 K. The maximum of  $C(T)$  is reproduced by a doublet-triplet two-level model with an energy gap of 12 K. Thereby, the CEF ground state is the  $\Gamma_3$  doublet. Upon further cooling, a clear peak manifests itself in  $C(T)$  at  $T_0 = 1.0$  K, indicating a phase transition. Because the transition at  $T_0$  is robust against magnetic fields up to 5 T, the transition is not magnetic but quadrupolar in origin. Thus, PrCdNi<sub>4</sub> is found to be the first fcc Pr-based compound exhibiting a long-range quadrupole order. (220/250 words)

[1] T. Onimaru and H. Kusunose, J. Phys. Soc. Jpn. **85**, 082002 (2016).

[2] Y. Kusanose *et al.*, J. Phys. Soc. Jpn. **88**, 083703 (2019).

[3] K. Kadir *et al.*, J. Alloys Compd. **345**, 140 (2002).

[4] Y. Kusanose *et al.*, JPS Conf. Proc. **30**, 011160 (2020).

## Magnetic properties of TbCuBi<sub>2</sub> Intermetallic compound

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In this work, we have investigated the physical properties of recently synthesized single crystals of the TbCuBi<sub>2</sub> compound. The single crystals are grown by the Bi-metallic flux method. X-ray diffraction analyzed by the Rietveld method reveals a tetragonal structure with space group P4/nmm. Measurements of magnetic susceptibility reveal an easy c-axis magnetic anisotropic with an increase of T<sub>N</sub> = 18 K for Tb compound. When compared to the GdCuBi<sub>2</sub> T<sub>N</sub> = 13.6 K in single crystals [1], our result shows a breakdown of the De Gennes scaling factor for the Tb-based compound. This breakdown was also observed in the lights rare-earth in the RCuBi<sub>2</sub> family of compounds [1,2], indicating a strong influence of the CEF effects and competition between distinct magnetic exchange interaction. Additionally, the field dependent magnetization reveals steps and hysteresis, indicating complex magnetic ordering below T<sub>N</sub> for TbCuBi<sub>2</sub>. The observed magnetic properties were described and reproduced using a mean-field model that includes an anisotropic exchange interaction between nearest neighbors and the tetragonal CEF Hamiltonian. Our results suggest that the CEF effects seem to rule the magnetic properties of these family of compounds RCuBi<sub>2</sub> (R = Ce, Pr, Nd, Sm, Gd) [1,2], as well as in others relates structures of Tb-based compounds [3].

[1] C.B.R. Jesus *et al.* Journal of Applied Physics **115**, 17E115 (2014).

[2] C. Adriano *et al.* Phys. Rev. B, **90(23)**, 235120 (2014).

[3] R. Lora-Serrano *et al.* Phys. Rev. B, **74**, p. 214404, Dec 2006.

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## Detailed magnetic phase diagram in CeCoSi for single crystal

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CeCoSi crystallizes in the tetragonal CeFeSi-type structure with the space group  $P4/nmm$  (No. 129,  $D_{4h}^7$ ) [1]. This compound exhibits two successive phase transitions: an antiferromagnetic (AFM) ordering at  $T_N = 9.4$  K and a hidden ordering at  $T_0 \sim 12$  K [2]. Co-NQR measurements have suggested that the hidden ordering phase is an electric multipole ordering, such as an antiferroquadrupole ordering [3]. However, the details of the hidden ordering state are unclear. In addition, it has been reported that the magnetic moment is directed in the [100] direction in the antiferromagnetic phase [4]. However, this requires multifaceted verification. To deepen our understanding of these ordered states, it is necessary to construct the detailed magnetic phase diagrams including their anisotropy with respect to the magnetic field  $B$  direction. Recently, our research group has reported the magnetic field-temperature phase diagrams of single crystal CeCoSi for the magnetic field applied parallel to the tetragonal [100] and [001] axes, where the presence of high- $B$  regions was revealed [5]. In the present study, we performed the magnetization and electrical resistivity measurements for a single crystalline CeCoSi under  $B$  up to 14 T in order to construct the magnetic phase diagram for  $B \parallel [110]$ . We will compare the characteristics of the magnetic phase diagrams obtained for all the  $B$  directions and discuss the novel ordering states in CeCoSi.

\*This work was supported by JSPS KAKENHI Grants Nos. JP20K03825 and 18H03683.

[1] O. I. Bodak *et al.*, J. Stuct. Chem. **11**, 283 (1970).

[4] H. Tanida *et al.*, J. Phys. Soc. Jpn. **88**, 054716 (2019).

[3] M. Manago *et al.*, J. Phys. Soc. Jpn. **90**, 023702 (2021).

[4] S.E. Nikitin *et al.*, Phys. Rev. B **101**, 214426 (2020).

[5] H. Hidaka *et al.*, arXiv:2203.09754

## ***Crystal-Electric-Field excitations of CeCoSi unveiled by Raman spectroscopy***

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CeCoSi is an unusual system due to several unidentified states that coexist with a strong Kondo effect [1-3]; yet these states are also distinct from the antiferromagnetic state below 9.5K [1] and other conventional magnetic orderings, which is reminiscent of other ‘hidden-order’ systems. It has been argued that all of the unidentified states are intimately related to excitations between a trio of Kramers doublets that form from the splitting of the  $\text{Ce}^{3+}$   $J=5/2$  multiplet under the action of a tetragonal crystal-electric-field (CEF). Recent neutron scattering measurements have determined the positions of the two excited states at 10.5meV and 14.1meV in agreement with specific heat measurements [3].

In this work, we use polarised Raman spectroscopy to identify the energies and symmetries of the CEF transitions. At low temperatures and amongst the phonons that are expected for the CeFeSi-type structure, we observe multiple excitations that are within the energy range of neutron scattering measurements [3]. We clearly identify the CEF scheme of the Ce site to be  $\Gamma_7 - \Gamma_7 - \Gamma_6$ . Surprisingly, more than the two expected CEF modes are observed below 42K, which corresponds to one of the unidentified phases at ambient pressure.

[1] E. Lengyel *et al.*, *Physical Review B*, **88**(15), 155137, (2013).

[2] H. Tanida *et al.*, *Journal of the Physical Society of Japan*, **88**(5), 1–10. (2019).

[3] S. Nikitin *et al.*, *Physical Review B*, **101**(21), 214426. (2020)

# Crystalline electric field effect and anisotropic magnetic interactions in RTBi<sub>2</sub> (R = Ce, Pr, Nd; T = Cu, Au)

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In this work we have performed a comprehensive study of the crystalline electric field (CEF) effects on the macroscopic magnetic properties of the RTBi<sub>2</sub> (R = Ce, Pr, Nd; T = Cu, Au) intermetallic compounds. Single crystalline samples were grown by the self-flux method. Macroscopic measurements of magnetic susceptibility, heat capacity, and electrical resistivity were previously carried out, with supplementary energy-dispersive X-ray spectroscopy and X-ray diffraction [1-4]. A mean-field model that includes anisotropic exchange interactions between nearest neighbors and tetragonal CEF effects was employed to simultaneously fit the magnetic susceptibility and magnetization data. These fits yielded the CEF scheme, parameters, and the values of the exchange interactions for each compound in the RTBi<sub>2</sub> series.

Using our analysis, we suggest that the chemical substitution of Cu for a larger ion (Au) enhances the axial CEF effect contribution, which leads to an increase of magnetic anisotropy for all studied rare-earth members. Moreover, the consequent decrease in distance between antiferromagnetically coupled axial first neighbors and the larger separation between second axial neighbors, which are ferromagnetically coupled, reduces the magnetic frustration and increases the ordering temperature. The in-plane exchange interactions also play a role in reducing magnetic frustration. Our results reveal how the CEF effects and the competition between magnetic interactions govern the magnetic properties of these compounds, leading to the observed breaking of the de Gennes scaling factor [1-4]. The propose scenario can be verified by measurements of the CEF schemes by Inelastic Neutron Scattering and/or X-ray Absorption measurements.

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[1] C. Adriano, et al, Phys. Rev. B **90**, 235120 (2014).

[2] M. M. Piva, et al, Phys. Rev. B **101**, 214431 (2020).

[3] C. B. R. Jesus, et al, J. of App. Phys. **115**, 17E115 (2014).

[4] C. B. R. Jesus, et al, Physics Procedia **75**, 618-624 (2015).



# Probing field-induced CEF mixing in CeRhIn<sub>5</sub> with field-angle dependence measurements

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Interesting states of matter can be stabilized by magnetic fields in *f*-electron materials, such as reentrant superconductivity in UTe<sub>2</sub> and the *Q*-phase of CeCoIn<sub>5</sub>. Another interesting example occurs in the heavy fermion material CeRhIn<sub>5</sub>. For fields applied near the *c*-axis, a so-called electronic nematic phase is stabilized above ~30T, within the antiferromagnetic order [1]. It was suggested that this exotic phase emerges from a change of the Fermi surface caused by field-enhanced Kondo hybridization [2]. The hybridization enhancement would be caused by a change of the 4*f* orbital character, a direct consequence of excited CEF levels mixing within the ground state due to the magnetic field. On the other hand, neutron spectroscopy has revealed a field-induced moment anisotropy in CeRhIn<sub>5</sub>, an effect that would also arise from CEF mixing [3].

In order to clarify the role of CEF levels in the field-induced properties of CeRhIn<sub>5</sub>, we performed field-angle dependent measurements of the specific heat, resistivity and ultrasound velocity. Considering that CEF mixing is different for different field directions, these measurements are sensitive to different field-induced multipoles. Our results reveal only a weak anisotropy for fields up to 16T applied in the tetragonal plane. Mean-field models that can describe the CeRhIn<sub>5</sub> phase diagram are constrained by these results and will be discussed.

[1] F. Ronning, *et al.*, Nature **548**, 313 (2017).

[2] P.F.S. Rosa, *et al.*, Phys. Rev. Lett. **122**, 016402 (2019).

[3] D.M. Fobes, *et al.*, Nature Physics **14**, 456 (2018).

## Magnetoelastic coupling in PrNi<sub>5</sub>

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The well-known concept of the Born-Oppenheimer approximation treats the motion of nuclei and electrons independently in order to simplify theoretical calculations. Nevertheless, multiple strongly correlated materials cannot be always treated this way and deserve a more complex approach due to their strong magnetoelastic coupling.

Pr-based compounds usually do not order down to the low temperatures due to the crystalline electric field (CEF) singlet ground state. One of the intermetallic compounds from this family is PrNi<sub>5</sub> being Van Vleck paramagnet. Its low-lying CEF modes are crossing acoustic phonons, which could resolve in the formation of hybridized modes. Such crosstalk was predicted by Aksenov et al. [1] and was studied by our recent inelastic neutron scattering study [2].

In this work, we present results of thermal conductivity measurements by two different methods performed on high-quality single crystals of PrNi<sub>5</sub> and its non-magnetic analog LaNi<sub>5</sub> down to 1.8 K under a magnetic field up to 14 T. Proper analysis of the thermal transport data of 4*f*-electron systems is a useful tool to study the scattering of phonons on magnetic ions due to the magnetoelastic coupling. Our analysis shows a contribution from the magnetic excitations to the heat transport in PrNi<sub>5</sub>. These results are compared with the former data on polycrystalline samples of PrNi<sub>5</sub> published by Reiffers et al. [3].

[1] V. Aksenov et al., *Physica B-condensed Matter* **120**, 310-313 (1983).

[2] Š. Venclík, et al., *to be published*

[3] M. Reiffers et al., *Czechoslovak Journal of Physics B* **38**, pages 197–200 (1988)

## Crystal fields and Magnetic frustration in SrTm<sub>2</sub>O<sub>4</sub>

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The SrTm<sub>2</sub>O<sub>4</sub> belongs to the family of orthorhombic rare-earth oxides where two inequivalent rare-earth sites form zig-zag chains along the *c*-axis and distorted honeycomb in the *ab*-projection. The previous report on this system has shown that the system does not order down to 65mK [1]. Our crystal field model predicts the singlet ground state for both Tm sites. The model reveals that the lowest dispersing excited state originates from one of the sites and the next excited state from the other [2]. The dispersing excitations were modeled using RPA. Modeling of dispersing excitation has revealed that one of the chains is dimerized while the other chain is frustrated, and this system cannot be driven to the thermal phase transition. However, the dimer chain starts ordering into the *XY*-AFM phase above 4 T.

Additionally, unique zero-field mSR results show signs of long-range order contradicting Ref. [1,2]. However, we show that the muon implantation distorts the crystal fields and leads to nuclear hyperfine enhancement and thus concurring with other results.

[1] H. Li et al. *J. Mater. Chem. C*, 3, 7658-7668 (2015).

[2] A. B Kademane et al. *JMMM*, 551, 169020 (2022).

## Cobalt substitution induced ferromagnetism in PdCrO<sub>2</sub>

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Pd based ABO<sub>2</sub> delafossites with B=Co and Cr are known to be the best examples of the coexistence of insulating and a nearly free electron like metal behaviour in a single material based on the lattice planes [1]. In contrast to PdCoO<sub>2</sub>, a non-magnetic band insulator, PdCrO<sub>2</sub> is a Mott insulator ordered in a long-range 120<sup>0</sup> antiferromagnetic (AFM) state at ~38 K [1, 2]. There is experimental evidence of the release of interlayer frustration by applied external uniaxial stress on single crystalline samples [2].

Here, we have studied the effect of Co substitution on Cr site in PdCrO<sub>2</sub> which acts like internal stress. A robust ferromagnetic state has been clearly observed in magnetization measurements just by substitution of a minimal amount of 10% Co. Isothermal magnetization measurements revealed that ferromagnetic state exist up to 100 K with a coercive field of ~4500 Oe. First principal calculations on Pd (Cr<sub>1-x</sub>Co<sub>x</sub>)O<sub>2</sub> also support that the observed ferromagnetism is due to uncompensated AFM in its nearest neighbourhood.

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[1] V Sunko et al. *Sci. Adv.* **6** : eaaz0611 7 (2020).

[2] Dan Sun *et al.*, *Phys. Rev. B* **100**, 094414 (2019).

# High field magnetism of the triangular lattice antiferromagnet CsFeCl<sub>3</sub> under high pressure

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The triangular lattice antiferromagnet CsFeCl<sub>3</sub> (Fe<sup>2+</sup>, effective spin  $S = 1$  at low energies) possesses a spin singlet ground state with a spin gap to the excited doublet state due to a single-ion anisotropy  $D$  with a positive sign (easy-plane type). By increasing applied pressure at zero field, the gap diminishes and then vanishes above  $P_c \sim 0.90$  GPa to exhibit magnetically ordered state with 120° spin structure in the  $ab$ -plane at low temperatures [1,2]. Under ambient pressure, the magnetization at 1.3 K for  $H \parallel c$  increases gradually up to 4 T, and then increases rapidly between 4 and 12 T. Above 12 T, the magnetization becomes nearly saturated and then exhibits a metamagnetic transition around 33 T [3]. This metamagnetic transition was suggested to be caused by an unconventional level crossing between the lowest triplet and the excited quintet states [4]. In this study, we performed magnetization (induction method and  $LC$ -circuit technique using a proximity detector oscillator) measurements of CsFeCl<sub>3</sub> in high magnetic fields of up to 51 T under high pressure of up to 2 GPa. The metamagnetic transition field shifted linearly to a lower field with increasing pressure and decreased to approximately 23 T at 2 GPa. In this presentation, we report these experimental results and discuss the origin of the metamagnetic transition observed in the present compound.

- [1] N. Kurita and H. Tanaka, Phys. Rev. B **94**, 104409 (2016).
- [2] S. Hayashida *et al.*, Phys. Rev. B **97**, 140405 (2018).
- [3] M. Chiba *et al.*, Solid State Commun. **63**, 427-430 (1987).
- [4] H. Hori *et al.*, Physica B **155**, 299 (1989).

# Gauge-flux-driven Kondo screening in $\alpha$ -Ru<sub>1-x</sub>Cr<sub>x</sub>Cl<sub>3</sub>

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The Kondo effect, describing the many-body screening of magnetic impurities in electron baths, is one of the most intriguing phenomena in condensed-matter physics. Beyond normal metals, the scope of Kondo physics has continued to expand into quantum dots, graphene, topological insulators, Weyl semimetals, and even quantum spin liquids. Singularly, a  $S=1/2$  Kitaev model on the honeycomb lattice offers a prominent testing ground for Kondo effects as the incorporation of magnetic impurities in a Kitaev spin-liquid host is proposed to enable Kondo screening by binding Kondo impurities to gauge fluxes. By combining magnetic susceptibility, specific heat, and muon spin relaxation/rotation measurements, we give experimental evidence of gauge-flux-driven Kondo screening in the Kitaev antiferromagnet  $\alpha$ -RuCl<sub>3</sub> with dilute Cr ( $S=3/2$ ) impurities. Logarithmic singularities in the static magnetic response and the muon spin relaxation rate are consistent with the predicted Kondo screening by impurity fluxes. Linear temperature dependence of the magnetic specific heat lends further credence to metallic transport of Majorana fermions in the background of thermally fluctuating fluxes. Our discovery opens up new avenues for multi-channel Kondo physics in quantum spin liquids.

## Metastable antiphase boundary ordering in $\text{CaFe}_2\text{O}_4$

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$\text{CaFe}_2\text{O}_4$  is an  $S = 5/2$  antiferromagnet exhibiting two seemingly distinct magnetic orders that shows regions of coexistence at some temperatures. Using a Green's function formalism, we model neutron scattering data of the spin wave excitations in this material, elucidating the microscopic spin Hamiltonian. In doing so, we suggest that the low temperature A phase order ( $\uparrow\uparrow\downarrow\downarrow$ ) finds its origins in the freezing of antiphase boundaries created by thermal fluctuations in a parent B phase order ( $\uparrow\downarrow\uparrow\downarrow$ ). The low-temperature magnetic order observed in  $\text{CaFe}_2\text{O}_4$  is thus the result of a competition between the exchange coupling along the c-axis, which favors the B phase, and the single-ion anisotropy, which stabilizes thermally generated antiphase boundaries, leading to static metastable A phase order at low temperatures [1]

[1] H. Lane *et al*, Phys. Rev. B **104**, 104404 (2021)

# Probing Flat Band Physics in Spin Ice Systems via Polarized Neutron Scattering

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In this Poster, following [1], we illustrate how polarized neutron scattering can be used to isolate the spin-spin correlations of modes forming flat bands in a frustrated magnetic system hosting a classical spin liquid phase. In particular, we explain why the nearest-neighbor spin ice model, whose interaction matrix has two flat bands, produces a dispersionless (i.e., “flat”) response in the non-spin-flip (NSF) polarized neutron scattering channel and demonstrate that NSF scattering is a highly sensitive probe of correlations induced by weak perturbations that lift the flat band degeneracy. We use this to explain the experimentally measured dispersive (i.e., non-flat) NSF channel of the dipolar spin ice compound  $\text{Ho}_2\text{Ti}_2\text{O}_7$ .

[1] Chung *et al.* Phys. Rev. Lett. **128**.107201 (2022)



## Kasteleyn transition in a Coulomb phase.

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We apply a magnetic field along the [111] direction for spin ice in the monopole crystal phase - a strongly fragmented phase in which a longitudinal fragment of the magnetic moments show antiferromagnetic long range order characteristic of a monopole crystal while the remainder, the transverse part forms a Coulomb phase with dipolar correlations [1,2,3]. The magnetic field couples to the transverse component, driving it towards saturated ferromagnetic state via a Kasteleyn transition [4].

We present numerical results generated from a worm Monte Carlo algorithm confirming the Kasteleyn transition. Tilting the field away from the [111] direction, the system orders in one of four topological sectors over a sphere of solid angle  $4\pi$ .

We show that the specific heat and susceptibility diverge logarithmically at the transition, consistently with the system being at the lower critical dimension. The reduced symmetry for the Coulomb phase correlations due to the applied field shows up in the evolution of simulated neutron scattering plots as the transition is approached. These show pinch point patterns that are continuously deformed as the field strength grows.

[1] M. E. Brooks-Bartlett, S. T. Banks, L. D. C. Jaubert, A. Harman-Clarke, P. C. W. Holdsworth. Magnetic-Moment Fragmentation and Monopole Crystallization. *Physical Review X*, American Physical Society, 2014, 4, pp.011007.

[2] A. A. Turrini et al. Tunable critical correlations in kagome ice. 2021. arXiv:2102.06546 [cond-mat.stat-mech].

[3] V. Cathelin et al. “Fragmented monopole crystal, dimer entropy, and Coulomb interactions in Dy<sub>2</sub>Ir<sub>2</sub>O<sub>7</sub>”. In: *Phys. Rev. Research* 2 (3 Sept. 2020), p. 032073. doi:10.1103/PhysRevResearch.2.032073.

[4] R. Moessner and S. L. Sondhi. “Theory of the [111] magnetization plateau in spin ice”. In: *Phys. Rev. B* 68 (6 Aug. 2003), p. 064411. doi:10.1103/PhysRevB.68.064411.

# Single Crystal Growth and Physical Properties of Distorted Triangular Lattice quantum magnet $\text{La}_2\text{CuGe}_2\text{O}_8$

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Geometrically frustrated quantum magnets are attracting widespread research interest among condensed-matter physicists because of their possible realization of unconventional magnetism manifest as exotic ground states and excitations [1]. Large crystals are essential for further detailed investigation of frustrated quantum magnetism using advanced measuring techniques including inelastic neutron scattering (INS). Therefore, a large single crystal (4 mm×4 mm×10 mm) of the potential highly geometrically frustrated candidate compound  $\text{La}_2\text{CuGe}_2\text{O}_8$  have been grown for the first time using the traveling-solvent floating zone (TSFZ) method, and this crystal has been characterized with regard to phase purity and crystallinity using powder X-ray diffraction, energy dispersive X-ray analysis, and Laue diffraction. Low temperature heat capacity measurement reveals a Long-range magnetic order occurs below 0.93 K (see fig 1). The ordering temperature is clearly suppressed compared to the Curie-Weiss temperatures which is -5.7K, which implies the presence of frustrated antiferromagnetic interactions [2]. INS and neutron powder diffraction analysis are in progress.

## Acknowledgment

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[1] Balents, Leon. *Nature* 464.7286 (2010): 199-208.

[2] H. Cho, et al *Phys. Rev. B.* 95, 144404 (2017)

# Thirty-Year Anniversary of $\kappa$ -(BEDT-TTF)<sub>2</sub>Cu<sub>2</sub>(CN)<sub>3</sub>: Reconciling the Spin Gap in a Spin-Liquid Candidate

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In 1991, the Argonne group led by Jack Williams [1] reported the first synthesis of  $\kappa$ -(BEDT-TTF)<sub>2</sub>Cu<sub>2</sub>(CN)<sub>3</sub>. Although, originally, the focus was on the superconducting properties under pressure, this frustrated Mott insulator with a triangular lattice (Fig. 1c) has been the most promising quantum-spin-liquid candidate for almost two decades [2], widely believed to host gapless spin excitations down to  $T = 0$  [3]. The recent observation of a spin gap by the Stuttgart group [4] rules out a gapless spin liquid with itinerant spinons and puts severe constraints on the magnetic ground state. Here I evaluate magnetic, thermal transport, and structural anomalies around  $T^* = 6$  K [5]. The opening of a spin gap yields a rapid drop of spin susceptibility [4], NMR Knight shift [6], spin-lattice relaxation rate, and  $\mu$ -SR spin fluctuation rate, but is often concealed by impurity spins [5]. The concomitant structural transition at  $T^*$  manifests in thermal expansion [7], THz phonons and <sup>63</sup>Cu NQR relaxation. Based on the field dependence of  $T^*$ , a critical field of order 60 T is estimated for the underlying spin-singlet state [5]. Overall, the physical properties are remarkably similar to those of spin-Peierls and valence-bond-solid phases. Thus, a strong case is made that the ‘6K anomaly’ in  $\kappa$ -(BEDT-TTF)<sub>2</sub>Cu<sub>2</sub>(CN)<sub>3</sub> is the transition to a valence-bond-solid state and it is suggested that such a scenario is rather the rule than the exception in materials with strong magnetic frustration [5].

- [1] U. Geiser *et al.*, *Inorg. Chem.* **30**, 2586–2588 (1991).
- [2] Y. Shimizu *et al.*, *Phys. Rev. Lett.* **91**, 107001 (2003).
- [3] S. Yamashita *et al.*, *Nat. Phys.* **4**, 459–462 (2008).
- [4] B. Miksch *et al.*, *Science* **372**, 276–279 (2021).
- [5] A. Pustogow, *Solids* **3**, 93–110 (2022).
- [6] Y. Saito *et al.*, *Phys. Rev. B* **98**, 205141 (2018).
- [7] R. S. Manna *et al.*, *Phys. Rev. Lett.* **104**, 016403 (2010).

## Nonlinear stress-strain relation of PdCrO<sub>2</sub>

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PdCrO<sub>2</sub> is a delafossite with an antiferromagnetic triangular lattice and a Neel temperature of 38 K [1]. It has a double-q magnetic structure, in which the direction of spin rotation alternates from layer to layer [2]. Under uniaxial stress, PdCrO<sub>2</sub> undergoes a transition from this double- to a single-q structure [3]. Here, we will show stress-strain data on PdCrO<sub>2</sub>, collected using a piezoelectric-driven strain cell that allows simultaneous measurement of uniaxial stress and strain. We will show that the change in lattice constant across this magnetic transition is quite large and that the transition evolves in a nontrivial way as temperature is raised.

[1] H. Takatsu et al., Phys. Rev. B **79**, 104424 (2009)

[2] H. Takatsu et al., Phys. Rev. B **89**, 104408 (2014)

[3] D. Sun et al., New J. Phys. **23**, 123050 (2021)

## **Magnon contributions to thermal conductivity in non-collinear magnets**

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Magnetic memory and logic devices, including prospective ones based on skyrmions, inevitably produce heat. Thus, controlling heat flow is essential for the performance. Here we study thermal conductivity in the most basic noncollinear magnet with a spin spiral ground state. We focus on the magnon scattering in a quasi-one dimensional spiral magnet. We start from a model Hamiltonian with competing nearest and next-nearest neighbor interactions and expand the spin-spin interaction up to the third order in bosonic operators using the Holstein-Primakoff transformation. This results in the magnon scattering matrix that is used in the description of the dynamics of the excitations via a kinetic equation. We adopt the relaxon formalism [1] and compute the magnetic contribution to the thermal conductivity.

[1] A. Cepellotti, N. Marzari, Phys. Rev. X 6, 041013 (2016)

## A $\mu$ SR study of novel magnetic ordering in LiYbO<sub>2</sub>

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The stretched diamond lattice material LiYbO<sub>2</sub> has recently been reported to exhibit two magnetic transitions ( $T_{N1} = 1.1$  K,  $T_{N2} = 0.45$  K) via specific heat, magnetization, and neutron scattering measurements [1]. Here we report complementary magnetic measurements down to  $T = 0.28$  K via the local probe technique of muon spin relaxation. While we observe a rapid increase in the zero-field muon depolarization rate at  $T_{N1}$ , we do not observe any spontaneous muon precession for  $T < T_{N1}$ , which is typically associated with long-range magnetic ordering. The depolarization rate in the ordered state shows a surprising sensitivity to magnetic fields applied along the initial spin polarization direction. Using a simple one-dimensional model, we show that these results are consistent with the unusual random-phase bipartite incommensurate magnetic structure proposed [1] for the intermediate temperature range  $T_{N2} < T < T_{N1}$ . We also find evidence for temperature-independent magnetic fluctuations persisting to our lowest temperatures, but no obvious signature of the transition or spontaneous muon precession at and below  $T_{N2}$ , respectively. This result is suggestive of quantum dynamics within a highly degenerate ground state.

\* This work is based on experiments performed at the Swiss Muon Source S $\mu$ S, Paul Scherrer Institute, Villigen, Switzerland. MMB and SDW were supported by the US Department of Energy Office of Basic Energy Sciences, Division of Materials Science and Engineering under award DE-SC0017752.

[1] Bordelon et al., Phys. Rev. B **103**, 014420 (2021).

# ***Engineering antiferromagnetic skyrmions and antiskyrmions at metallic interfaces***

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We identify a mechanism to convert skyrmions and antiskyrmions into their antiferromagnetic (AFM) counterparts via interface engineering. The key idea is to combine properties of an antiferromagnet and a spin-orbit (SO) coupled metal. Utilizing hybrid Monte Carlo (HMC) simulations for a generic microscopic electronic Hamiltonian for the interfacial layers, we explicitly show the emergence of AFM skyrmions and AFM antiskyrmions. We further show that an effective spin Hamiltonian provides a simpler understanding of the results. We discuss the role of electronic itinerancy in determining the nature of magnetic textures, and demonstrate that the mechanism also allows for a tuning of antiskyrmion size without changing the SO coupling.

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# Dynamical Spin Structure Factor of the spin- $\frac{1}{2}$ $J_1 - J_2$ Heisenberg Model on the Triangular Lattice

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The spin- $\frac{1}{2}$  Heisenberg model with antiferromagnetic nearest and next-to-nearest neighbour interactions on a triangular lattice exhibits—driven by the highly frustrated spins—a rich phase diagram including a spin liquid phase and is relevant for various two-dimensional quantum materials. Using large-scale density matrix renormalization group and time evolution algorithms for matrix product states, we obtain the dynamical spin structure factor of the triangular  $J_1 - J_2$  Heisenberg model depicting the low-energy excitations both in the  $120^\circ$ -ordered phase at  $J_2 = 0$  and the spin liquid phase at  $J_2/J_1 = 0.125$ . This method allows us to compare the low-energy properties of the isotropic Heisenberg model with previous analytical and numerical approaches.

In the ordered phase, we observe the same avoided decay of the magnon-branch as first reported by Verresen et al. [1] for a modified Heisenberg model with an easy-axis anisotropy, thus demonstrating the generic nature of this phenomenon. Our findings in the spin-liquid phase support the field-theoretical predictions by Song et al [2,3], in particular the emergence of low-lying monopole excitations at the corners of the Brillouin zone.

[1] R. Verresen, R. Moessner and F. Pollmann, Nat. Phys. **15**, 750 (2019).

[2] X.-Y. Song *et al.*, Nat. Comm. **10**, 4254 (2019).

[3] X.-Y. Song *et al.*, Phys. Rev. X **10**, 011033 (2020).



## Possible chiral spin liquid state in the $S = 1/2$ kagome Heisenberg model

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The ground state for the kagome antiferromagnetic Heisenberg model is a long-standing problem that has been attracting increasing interests from the condensed matter community. This is not only because the kagome lattice is a representative geometrically frustrated lattice that can host a quantum spin liquid ground state, but also attributed to emerging material realizations with a variety of compounds. While it is commonly accepted that this model has a quantum spin liquid ground state, the nature of this spin liquid state remains a puzzle.

We revisit this challenging problem and provide strong numerical evidence that its ground state is a chiral spin liquid [1]. Exploiting newly developed Gutzwiller-boosted-DMRG and analytical analyses, we demonstrate that the previously observed chiral spin liquid phase in the model with longer-range couplings is stable in a broader region, including the point with only nearest neighboring couplings. A phase diagram consisting of a chiral spin liquid phase, two valence-bond-crystal phases, and a magnetically ordered phase has been established.

The chiral spin liquid state has been identified by (i) computing energy derivatives and wavefunction fidelities, (ii) revealing ground-state degeneracy arising from spontaneous breaking of time-reversal symmetry, and (iii) targeting the topological semion sector in addition to the identity sector. The latter two were thought to be “Mission Impossible” in the framework of traditional DMRG.

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[1] R.-Y. Sun *et al.*, arXiv: 2203.07321

## Pressure effects on the magnetism of the $S = 1/2$ spin ladder $\text{Cu}(\text{DEP})\text{Br}_2$

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$\text{Cu}(\text{DEP})\text{Br}_2$  (DEP = 2,3-diethylpyrazine) is an antiferromagnetically coupled  $S = 1/2$  ( $\text{Cu}^{2+}$  ion) two-leg spin-ladder system [1]. The exchange constant along the rung is  $J_{\text{rung}}/k_{\text{B}} = 16.5$  K, and its ratio to the leg constant is  $J_{\text{rung}}/J_{\text{leg}} \sim 2$  [1, 2]. The spin gap ( $\Delta_{\text{s}}/k_{\text{B}}$ ) between the non-magnetic singlet ground state and the first-excited triplet state is evaluated to be approximately 13.3 K in the specific heat measurements [1]. The  $\Delta_{\text{s}}$  is expected to vanish by the application of magnetic field and/or external pressure. Above the critical field or pressure, a magnetic state would be induced. In the present study, we investigated the pressure effects on magnetism of  $\text{Cu}(\text{DEP})\text{Br}_2$ .

Magnetic susceptibility of  $\text{Cu}(\text{DEP})\text{Br}_2$  under high pressure of up to 1.5 GPa was measured by an  $LC$  resonance method utilizing a proximity detector oscillator (PDO). A non-destructive pulse magnet was used for applying the external magnetic fields of up to 50 T.

At ambient pressure and 1.4 K, the transition field to the gapless state is  $H_{\text{c1}} \sim 8$  T, and the saturation field is  $H_{\text{c2}} \sim 24$  T.  $H_{\text{c1}}$  decreased monotonically with increasing pressure and seemed to disappear at about 1.7 GPa, resulting in the gapless state.  $H_{\text{c2}}$  decreased with increasing pressure up to 0.98 GPa, and then turned to increase. The  $J_{\text{rung}}/J_{\text{leg}}$  gets closer to one by applying more pressure than 0.98 GPa. In this presentation, we discuss the pressure-induced quantum criticality near 1.7 GPa and the change in magnetism of  $\text{Cu}(\text{DEP})\text{Br}_2$ .

[1] Z. Honda *et al.*, J. Phys. Soc. Jpn. **81**, 113710 (2012).

[2] M. Ikeda *et al.*, J. Low Temp. Phys. **170**, 296 (2013).

# The Skyrmion Phase of the Chiral Antiferromagnet EuPtSi Studied by Transport Measurements

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A magnetic skyrmion is a local vortex-like whirl of the spin configuration in a magnetic material. The rare-earth compound EuPtSi, crystallizing in a non-centrosymmetric chiral structure with the  $P2_13$  space group, similar to that of MnSi, orders antiferromagnetically below  $T_N=4\text{K}$ . Recently it has been shown that inside the antiferromagnetic phase, a unique magnetic skyrmion phase, called the A-phase, is formed [1].

Here, we studied the magnetic phase diagram of EuPtSi for magnetic fields applied along [001] and [111] by Seebeck, Nernst effect, thermal conductivity and resistivity measurements. In addition to the so-called A-phase, we also confirm the newly discovered B-phase which appears for a field applied along [100] above the A-phase. The measurements of the Seebeck effect in a wide field and temperature range give evidence for additional energy scales linked to different magnetic phases at low temperatures.

Furthermore, we report the presence of quantum oscillations in the Seebeck and Nernst signals. The observed frequencies have been analysed using the Pantsulaya-Varlamov fit of the temperature dependence of the amplitude of the oscillations, revealing the corresponding cyclotron masses which are in very good agreement with previous dHvA experiments [2].

[1] M. Kakihana et al., J. Phys. Soc. Jpn. 87, 023701 (2018).

[2] M. Kakihana et al., J. Phys. Soc. Jpn. 88, 094705 (2019).

## Evidences for a Skyrmion phase formation in $\text{Eu}_2\text{Pd}_2\text{Sn}$

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The magnetic phase diagram of  $\text{Eu}_2\text{Pd}_2\text{Sn}$  is revisited with detailed measurements of susceptibility  $\chi(T, B)$  in order to investigate the possibility of a Skyrmion phase formation. According to theory, this compound fulfills the conditions for the appearance of such a phase [1] because: a) the Intra-layer ferromagnetic nearest neighbor exchange  $\mathcal{J}_{\text{NN}}(\text{FM})$  between divalent  $\text{Eu}^{2+}$  atoms, b) the antiferromagnetic exchange  $\mathcal{J}_{\text{NNN}}(\text{AFM})$  between next NN and c) the frustrated Inter-layer  $\mathcal{J}_{\text{LL}}$  exchange.

The Eu-Eu interatomic spacing within the Eu puckered chains: 3.734 Å [2], is nearly 7% smaller than twice the  $\text{Eu}^{2+}$  radius (2.0Å) favoring the formation of Eu-Eu dimers which is driven by the strong  $\mathcal{J}_{\text{NN}}(\text{FM})$  interaction. This process is detected by  $\chi(T)$  and magnetization measurements in the range  $70\text{K} > T > T_{\text{N}}$  and confirmed by the entropy gain at  $T = T_{\text{N}} = 13.5\text{K}$ . At that ordering temperature a modulated collinear arrangement is expected according the temperature dependence of specific heat [3].

This revisited phase diagram coincides with some of the theoretic propositions [1] that correspond to zero next Inter-layer interaction  $\mathcal{J}_{\text{NLL}} = 0$ . The frustrated  $\mathcal{J}_{\text{LL}}$  interaction rises between sequential layers formed by a series of stacked ABA'B'... bilayers, each one presenting Eu chains forming a 114° dihedral angle among them [2], close to 120° proposed by theory [1]. Taking into account that Eu-Eu dimers possess a total angular momentum  $\mathbf{J}_{\text{D}} = 7$  instead of the individual  $\mathbf{J}_{\text{Eu}^{2+}} = 7/2$ , this is a unique case with the largest magnetic moment at low temperature

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[1] Lin et al., Phys. Rev. Lett. 120 (2018) 077202.

[2] Giovannini et al., Inorg. Chem. 60 (2021) 8085.

[3] Blanco et al., Phys. Rev. B 43 (1991) 13145

# EPR and SQUID Interrogations of Chromium Trimer Complexes in the MIL-101(Cr) and Bimetallic MIL-100(Al/Cr) MOFs

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Metal-organic frameworks (MOFs) are a novel and the most prominent class of microporous materials for the applications such as gas storage and separation, catalysis, heat storage and liquid purification, owing to their unique structural diversity and tunability. [1]

Herein, electron paramagnetic resonance (EPR) spectroscopy at X- (9.4 GHz), Q- (34 GHz) and W-band (94 GHz), and superconducting quantum interference device (SQUID) measurements on MIL-101(Cr) and bimetallic MIL-100(Al/Cr):10%Cr MOFs were investigated. The intra trimer interaction of Cr<sup>3+</sup> in the metal-oxo trimers of the supertetrahedra units and their Al/Cr composition in case of MIL-100 are elucidated. The temperature-dependent magnetization of the studied MOF materials at 0.01 T and 0.5 T fields indicates antiferromagnetic interactions for both MIL-101(Cr) as well as for the magnetically diluted MIL-100(Al/Cr). Also, the magnetic susceptibility data from the SQUID are in accordance with the temperature-dependent intensity of the Cr<sup>3+</sup> EPR signals of the MOF materials extracted from X-band EPR measurements. The g-value of the Cr<sup>3+</sup> trimers is found to be  $g \approx 1.78$  at 7 K in MIL-101(Cr) from the X-band EPR measurement is smaller than the usual Cr<sup>3+</sup> g value of 1.96~2.00. It could be attributed to the Dzyaloshinsky-Moriya (D-M) interaction, and the Cr<sup>3+</sup> trimers behave like a spin 1/2 paramagnetic species at the low temperatures.[2,3]

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## References

1. M. Bracci, P. C. Bruzzese, A. Famulari, D. Fioco, A. Guidetti, Y.-K. Liao, L. Podvorica, S. F. Rezayi, I. Serra, K. Thangavel, and D. M. Murphy, *Electron Paramag. Reson.* **27**, 1-46 (2021).
2. M. Honda, M. Morita, and M. Date, *J. Phys. Soc. Jpn.* **61**, 3773 (1992).
3. A. Vlachos, V. Psycharis, C. P. Raptopoulou, N. Lalioti, Y. Sanakis, G. Diamantopoulos, M. Fardis, M. Karayanni, G. Papavassiliou, and A. Terzis, *Inorganica Chimica Acta* **357**, 3162 (2004).

# **Y<sub>2</sub>CuTiO<sub>6</sub>: A novel low temperature dynamic correlated 3D-paramagnet on a randomly diluted planar triangular lattice**

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Interacting spins on a lattice usually leads to magnetically ordered states at temperatures comparable to the exchange interaction strengths. However, magnetic frustration, such as in a triangular lattice with antiferromagnetic interactions, arising from competing exchange interactions can lead to such orderings being strongly suppressed, leading to, in extreme cases, quantum spin liquid-like states [1,2]. An alternate approach to realizing magnetically disordered states is to introduce sufficient magnetic disorder in the lattice; this usually leads to a magnetically glassy state. Combining the two approaches, namely frustration and disorder, we explore Y<sub>2</sub>CuTiO<sub>6</sub> where magnetic spin- $\frac{1}{2}$  Cu<sup>2+</sup> ions are arranged on a triangular lattice with 50% of the sites randomly occupied by nonmagnetic Ti<sup>4+</sup> atoms, giving rise to a realization of a simultaneous presence of frustration and disorder. We establish [3] that this system does not achieve a magnetic ordering or a glassy state down to 50 mK, though the magnetic interaction strength is nearly 3000 times larger than this temperature. Various experiments and specific scaling behaviors of thermodynamic properties with temperature and magnetic fields suggest that the system remains in a disorder-driven dynamic cooperative paramagnetic state, opening new possibilities to explore the field of frustrated magnetism aided by the disorder.

[1] P.W. Anderson, *Mater. Res. Bull.* **8**, 153 (1973)

[2] L. Balents, *Nature (London)* **464**, 199 (2010)

[3] S. Kundu, A. Hossain *et al.*, *Phys. Rev. Lett.* **125**, 117206 (2020)

## Single-crystal growth and low temperature properties of ErB<sub>2</sub>

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Single crystals of the hexagonal rare-earth diboride ErB<sub>2</sub> were synthesized by means of the self-adjusted flux travelling solvent optical floating zone technique and metallurgically characterized. [1] The magnetic phase diagram of single-crystalline ErB<sub>2</sub> was inferred from measurements of the specific heat, the magnetisation, the ac susceptibility, and the electrical transport for fields applied along major crystallographic axes. We find behavior characteristic of an easy-plane antiferromagnet below  $T_N = 14$  K. Linear Curie-Weiss fits of the ac susceptibility data in zero field indicate ferromagnetic coupling along the easy in-plane directions  $\langle 100 \rangle$  and  $\langle 210 \rangle$ , and antiferromagnetic coupling along the hard out-of-plane direction  $\langle 001 \rangle$ . For magnetic fields applied along the hard axis  $\langle 001 \rangle$  we observe a spin-flip transition at  $B_N = 12$  T.

Most notably, the Hall resistivity below  $T_N$  for fields applied along the hard axis exhibits a large anomalous contribution that does not scale with the uniform magnetization. Possible origins include spin-chirality mechanisms [2] and large Berry curvatures associated with a canted spin structure, or more exotic types of magnetic order [3].

[1] A. Bauer *et al.*, *physica status solidi (b)* p. 2100159 (2021).

[2] Y. Machida *et al.*, *Physical Review Letters*, vol. 98, p. 057203, (2007).

[3] S. Nakatsuji *et al.*, *Nature*, vol. 527, pp. 212–215, (2015).

# Frustration model and spin excitations in the helimagnet FeP

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The metallic compound FeP belongs to the class of materials that feature a complex noncollinear spin order driven by magnetic frustration. While its double-helix magnetic structure with a period  $\lambda_s \approx 5c$ , where  $c$  is the lattice constant, was previously well determined, the relevant spin-spin interactions that lead to that ground state remain unknown. By performing extensive inelastic neutron scattering measurements, we obtained the spin-excitation spectra in a large part of the momentum-energy space. The spectra show that the magnons are gapped with a gap energy of  $\sim 5$  meV. Despite the 3D crystal structure, the magnon modes display strongly anisotropic dispersions, revealing a quasi-one-dimensional character of the magnetic interactions in FeP. The physics of the material, however, is not determined by the dominating exchange, which is ferromagnetic. Instead, the weaker two-dimensional antiferromagnetic interactions between the rigid ferromagnetic spin chains drive the magnetic frustration. Using linear spin-wave theory, we were able to construct an effective Heisenberg Hamiltonian with an anisotropy term capable of reproducing the observed spectra. This enabled us to quantify the exchange interactions in FeP and determine the mechanism of its magnetic frustration.



# Low temperature thermodynamic characterization of the spin-1/2 triangular antiferromagnet $\text{Na}_2\text{BaCo}(\text{PO}_4)_2$

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$\text{Na}_2\text{BaCo}(\text{PO}_4)_2$  is a geometrically frustrated triangular antiferromagnet and a quantum spin liquid candidate. Its crystal structure features  $\text{Co}^{2+}$  ions arranged on the undistorted triangular lattice. The combination of crystal-field splitting and spin-orbit coupling results in the effective spin  $\frac{1}{2}$  behavior at low temperatures.

Despite several previous publications, the low-temperature properties of this compound are controversial. Earlier thermodynamic measurements revealed a clear transition in the heat capacity data at 140mK in zero magnetic field [1]. On the other hand, the AC magnetic susceptibility data and muon spin rotation experiments (ZF- $\mu$ SR) indicate a dynamically fluctuating ground state down to at least 80mK [2]. Furthermore, recent theoretical calculations [3] confirm that  $\text{Na}_2\text{BaCo}(\text{PO}_4)_2$  is an almost ideal realization of the spin  $\frac{1}{2}$  triangular-lattice antiferromagnet that would allow an experimental observation of high-field phases predicted for this model.

In order to uncover the field-temperature phase diagram of  $\text{Na}_2\text{BaCo}(\text{PO}_4)_2$ , we performed measurements of the heat capacity and magnetic Grüneisen parameter, as well as thermal expansion and magnetostriction down to 40mK and for two field directions, namely, along the  $c$  axis and in the  $ab$ -plane.

From these measurements we derived the complete field-temperature phase diagram of  $\text{Na}_2\text{BaCo}(\text{PO}_4)_2$  and compare it with the literature results and recent theoretical predictions [1, 3].

[1] N. Li *et al.*, Nat. Commun. 11, 1-9 (2020)

[2] S. Lee *et al.*, Phys. Rev B 103, 024413 (2021)

[3] Y. Gao *et al.*, *arXiv preprint arXiv:2202.05242* (2022)

# NMR studies of the spin liquid candidate material, $\kappa$ -(BEDT-TTF)<sub>2</sub>Cu<sub>2</sub>(CN)<sub>3</sub>, with varying magnetic field and pressure

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An organic triangular-lattice Mott insulator,  $\kappa$ -(BEDT-TTF)<sub>2</sub>Cu<sub>2</sub>(CN)<sub>3</sub>, is the first candidate for a quantum spin liquid material [1]. Even 20 years after the first report of this phenomenon, the nature of spin liquid state has still been debated. One of key phenomena to this issue is the so-called *6K-anomaly*, which refers to the anomalies that appear in magnetic, thermodynamic, dielectric and lattice properties around 6K [2]. We performed the in-depth study of the 6K-anomaly, combining <sup>1</sup>H and <sup>13</sup>C NMR measurements in two ways; one is to examine the magnetic-field dependence of the anomaly and the other is to trace the fate of the anomaly upon the Mott transition to a metallic phase by pressure [3].

At ambient pressure, <sup>13</sup>C NMR spectra show a significant decrease in the spin shift and a simultaneous line broadening suggestive of an inhomogeneous state below 6K. Moreover, we found that the 6K-anomaly is robust against the magnetic field up to 15Tesla. The  $1/T_1$  at <sup>1</sup>H sites, where the hyperfine coupling with conduction electrons is smaller than that at <sup>13</sup>C sites, obeys similar temperature dependence to that at <sup>13</sup>C sites down to 6K; however, below that,  $1/T_1$  shows quite different temperature variations at the <sup>1</sup>H and <sup>13</sup>C sites, indicative of different relaxation mechanisms at the <sup>13</sup>C and <sup>1</sup>H sites at low temperatures. This can be a key to understanding the anomalous state below 6K.

With <sup>1</sup>H NMR measurements under pressure variation, we found that the 6K-anomaly suddenly and completely disappear when the system enters into the metallic.

[1] Y. Shimizu *et al.*, Phys. Rev. Lett. **91**, 107001 (2003).

[2] Yi Zhou, Kazushi Kanoda, and Tai-Kai Ng, Rev. Mod. Phys. **89**, 025003 (2017).

[3] T. Komatsu *et al.*, J. Phys. Soc. Jpn. **65**, 1340 (1996). T. Furukawa *et al.*, Nature commun. **9**, 307 (2018).

# Quantum spin nematic liquid in the low-dimensional anisotropic magnets

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The spin nematic phase is one of interesting topics in the field of the strongly correlated electron systems. The previous theoretical and numerical studies predicted that the spin nematic order would be induced by the frustration of the ferromagnetic and antiferromagnetic exchange interactions, or the biquadratic interaction[1-3]. The spin nematic order is characterized by the long-range four spin correlation and the two-magnon bound state. The previous numerical diagonalization study had indicated that a similar two-magnon bound state can occur in the  $S=1$  antiferromagnetic chain with the single-ion anisotropy under magnetic field[4]. The recent calculation of the critical exponents of the spin correlation functions suggested that this two-magnon bound state includes the spin nematic liquid phase, as well as the SDW liquid one. Some phase diagrams with respect to the anisotropy and the magnetization were obtained by the numerical diagonalization of finite size clusters[5]. The same numerical analysis indicated that the spin nematic liquid phase appears in the magnetization process of the  $1/2$  spin ladder system with the anisotropic ferromagnetic rung interaction[6,7].

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[1] A. F. Andreev and A. Grishchuk, *Sov. Phys. JETP* **60**, 267 (1984).

[2] H. H. Chen and P. M. Levy, *Phys. Rev. Lett.* **27**, 1383 (1971).

[3] T. Hikihara, L. Kecke, T. Momoi and A. Furusaki, *Phys. Rev. B* **78**, 144404 (2008).

[4] T. Sakai, *Phys. Rev. B* **58**, 6268 (1998).

[5] T. Sakai, H. Nakan, K. Okamoto and R. Furuchi, *J. Phys.: Conf. Ser.* **2164**, 012030 (2022).

[6] T. Sakai, K. Okamoto and T. Tonegawa, *phys. Status solidi B* **247**, 583 (2010).

[7] T. Sakai, R. Nakanishi, T. Yamada, R. Furuchi, H. Nakano, H. Kaneyasu, K. Okamoto, T. Tonegawa, in preparation.

# Feasibility study of Kitaev quantum spin liquid for ultracold polar molecules and higher spin materials

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The Kitaev model is an  $S = 1/2$  quantum spin model with bond-dependent anisotropic interactions [1]. Despite its strong frustration, this model is exactly solvable, and the ground state is a quantum spin liquid, often called the Kitaev quantum spin liquid (KQSL). Here we investigate the feasibility of the KQSL for two extensions of the model, by using the pseudofermion functional renormalization group method.

The first one is for ultracold polar molecules. While the implementation of the Kitaev-type interaction was proposed [2], the stability of the KQSL has not been clarified so far. Studying a model with long-range angle-dependent interactions, we find that the ground state is a magnetically ordered state in both ferromagnetic and antiferromagnetic cases. Moreover, we also unravel how the KQSL becomes fragile while changing the range of the interaction.

The other is the extension to higher-spin systems. While candidate materials with  $S > 1/2$  were proposed [3], the stability of the KQSL has not been systematically elucidated for general spin  $S$  in the presence of non-Kitaev interactions. Studying the ground state phase diagram of the spin- $S$  Kitaev-Heisenberg model, we find that the KQSL remains stable for  $S < 2$ , while the regions in the phase diagram are quickly shrunk while increasing  $S$ .

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[1] A. Kitaev, *Ann. Phys.* **321**, 2 (2006).

[2] S. R. Manmana *et al.*, *Phys. Rev. B* **87**, 081106 (2013); A. V. Gorshkov, K. R. A. Hazzard, and A. M. Rey, *Mol. Phys.* **111**, 1908 (2013).

[3] P. P. Stavropoulos, D. Pereira, and H.-Y. Kee, *Phys. Rev. Lett.* **123**, 037203 (2019); C. Xu *et al.*, *npj Comput. Mater.* **4**, 57 (2018).

# Theory of absorption in Shastry-Sutherland material $\text{SrCu}_2(\text{BO}_3)_2$

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Quasi two-dimensional magnet  $\text{SrCu}_2(\text{BO}_3)_2$  is well known as a realization of the Shastry-Sutherland model, of which the ground state is rigorously described as a direct product of dimer singlet states. The magnetic behaviors of  $\text{SrCu}_2(\text{BO}_3)_2$ , *e.g.* spin gap excitations and magnetization plateaus, have been studied from experimental and theoretical point of view [1]. Spin excitation spectra have been investigated by ESR and far-infrared spectroscopy and one-triplet and bound state of two triplet excitations have been observed. However, the comprehensive understanding of the mechanism and the selection rule has not yet been established.

In magnetoelectric multiferroics, there is a strong coupling between magnetization and electric polarization. Such a coupling induces an electromagnon, *i.e.*, an electro active magnon [2]. We show that such electromagnetic couplings can exist even in  $\text{SrCu}_2(\text{BO}_3)_2$  and spin gap excitations can be active by the electric components of light through the couplings. In the Shastry-Sutherland model with Dzyaloshinskii-Moriya interactions, we clarify the mechanism and the selection rule in  $\text{SrCu}_2(\text{BO}_3)_2$ .

[1] S. Miyahara and K. Ueda, *J. Phys.:Condens. Matter* **15**, R327 (2003).

[2] H. Katsura, A.V. Balatsky, and N. Nagaosa, *Phys. Rev. Lett.* **98**, 027203 (2007).

# Vibrating-coil and membrane-based-Faraday magnetometry of the magnetic phase diagram of $\text{Gd}_3\text{Ga}_5\text{O}_{12}$ at low temperatures

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The magnetic properties of  $\text{Gd}_3\text{Ga}_5\text{O}_{12}$  (GGG) originate in large, classical spins ( $J = S = 7/2$ ) that interact antiferromagnetically on two interpenetrating hyperkagome lattices. It has long been recognized that this implies a high degree of frustration with some kind of classical spin liquid at low temperatures [1]. Yet, dipolar interactions are large and may normally be expected to relieve the effects of geometric frustration. Therefore, it has been considered surprising that GGG at zero magnetic field exhibits spin-freezing without evidence for long-range order, where the recent observation of antiferromagnetic correlations on ten-spin rings [2], suggests a nematic order parameter, or director [3]. We report vibrating coil magnetometry (VCM) and membrane-based Faraday magnetometry of the orientation dependence of the magnetic phase diagram of GGG down to mK temperatures, where the applied magnetic field stabilizes a complex sequence of cross-overs and phase transitions that reflect the underlying antiferromagnetic interactions. While the VCM is ideally suited for studies under very carefully controlled temperature versus field histories, the membrane-based Faraday magnetometer as combined with a set of superconducting gradient coils permits delineation of force and torque components.

- [1] P. Schiffer *et al.*, Phys. Rev. Lett. **73**, 18 (1994).
- [2] S.Ghosh *et al.*, Phys. Rev. Lett. **101**, 157205 (2008).
- [3] Joseph A. M. Paddison *et al.*, Science **350**, 179 (2015).

# Advanced magnetocaloric materials for adiabatic demagnetization Spin dynamics of the quantum dipolar magnet $\text{Yb}_3\text{Ga}_5\text{O}_{12}$

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Aside from fundamental interest, delayed magnetic ordering in conjunction with a large unfrozen entropy makes frustrated materials interesting for low temperature magnetic cooling [1]. Developing space applications and increasing costs of helium motivate a continuing search for new refrigerant materials for adiabatic demagnetization refrigeration in the 0.1 - 4 K temperature range [2]. In this context,  $\text{Yb}_3\text{Ga}_5\text{O}_{12}$ , a frustrated spin system consisting of magnetic ytterbium ions on the hyperkagome lattice, is of specific interest since it exhibits an enhanced magnetocaloric effect [3] together with unconventional magnetic properties.

Magnetisation, specific heat and neutron scattering measurements are used to further understand the magnetocaloric effect in  $\text{Yb}_3\text{Ga}_5\text{O}_{12}$ . Polarised neutron scattering measurements show the building of Q-dependent magnetic correlations below 500 mK [4,5] and inelastic neutron scattering measurements have found field induced excitations which are consistent with spin-wave calculations [4] assuming dominant dipole-dipole interactions. These results highlight the presence of a microscopic contribution to the magnetocaloric effect in  $\text{Yb}_3\text{Ga}_5\text{O}_{12}$  determined by collective excitation modes. In addition, recent high energy resolution time-of-flight measurements could better resolve the different modes, opening the way to the determination of the system Hamiltonian.

We have also measured two materials with non-magnetic Y substituted on the Yb site. Finding greater than expected magnetic moments and a high magnetocaloric power. This provides further evidence that the spin correlations in  $\text{Yb}_3\text{Ga}_5\text{O}_{12}$  are predominantly dipolar in nature and opens a new possibility for improving the capabilities of these materials in the context of adiabatic demagnetisation refrigeration.

[1] M. Zhitomirsky, Phys. Rev. B 67, 104421 (2003).

[2] P. Wikus et al., Cryogenics 62, 150 (2014).

[3] D.A. Paixao Brasiliano et al., Cryogenics 105, 103002 (2020).

[4] E. Lhotel et al., Phys. Rev. B 104, 024427 (2021).

[5] L. Ø. Sandberg et al., Phys. Rev. B 104, 064425 (2021).

# A cluster extension of the spin wave theory for spin excitation spectra

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Spin wave theory (SWT) has often been used to analyze the spin excitation spectra of magnetic materials. Recent experimental research showed that the standard SWT failed to sufficiently explain the inelastic neutron scattering spectrum of the  $S = 1/2$  triangular antiferromagnet  $\text{Ba}_3\text{CoSb}_2\text{O}_9$  in the  $120^\circ$  Néel phase [1,2]. This provided a clear example of the fact that the semiclassical approach was not appropriate to describe the spin excitation of highly-quantum spin systems, especially in the presence of strong frustration. Moreover, the SWT does not work at all when the ground-state phase is strongly affected by quantum effects since it treats the spin fluctuations only around the classical ground state.

In this work, we develop a method for providing a better description of spin excitation spectra by combining the SWT with the cluster mean-field theory (CMFT). In the CMFT, we divide the lattice sites into clusters consisting of  $N$  sites, and exactly treat the spin interactions inside each cluster while those between the clusters are approximated by means of the mean-field decoupling. Based on the CMFT ground state and excited states, we calculate the spin excitation spectra via a generalized Bogoliubov transformation followed by a multi-boson Holstein-Primakoff transformation. It should be emphasized that the result can be improved in a systematic way by increasing the cluster size  $N$ . We demonstrate the effectiveness of our method by taking the case of the spin-1/2 Heisenberg model on square lattice as an example.

[1] J. Ma, Y. Kamiya *et al.*, Phys. Rev. Lett. **116**, 087201 (2016).

[2] S. Ito, N. Kurita *et al.*, Nat. Commun. **8**, 235 (2017).



# Bose-Einstein Condensations in quasi-2D Diluted $S = 3/2$ Quantum Magnets

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Bose-Einstein Condensation (BEC) in quantum magnets is an intensively studied subject and regarded as a test field for theoretical works of quantum critical phenomena as well as a promising arena for the emergence of exotic phases of matter near the BEC quantum critical point (QCP) [1]. Previous experimental studies have been mainly focused on  $S = 1/2$  and  $S = 1$  magnets because strong quantum effects are expected. On the other hand, higher spin ( $S > 1$ ) systems potentially possess richer physics due to the multiple spin excitation levels on a single site level. However, such a structure is easily masked by the inter-site exchange interaction, which makes the experimental exploration challenging.

Here, we study the evolution of the magnetic phase diagram of an  $S = 3/2$  quantum magnet  $\text{Ba}_2\text{CoGe}_2\text{O}_7$  with partial substitution of non-magnetic Zn for magnetic Co, which effectively reduces the magnetic interaction. Pulsed high-field measurements up to 50 T and low-temperature measurements down to 0.4 K reveal that the single dome of the antiferromagnetic phase for the pristine compound transforms into two BEC domes intervened by a disordered state with 25 % Zn substitution. Furthermore, we find that the evolution of the phase diagram deviates from the mean-field behavior probably due to the randomness effect induced by the site dilution. As a result, the emergence of the spin Bose/Mott glass is suggested in the vicinity of BEC-QCP.

[1] V. Zapf *et al.*, Rev. Mod. Phys. **86**, 563 (2014).

# Hole Spectral Function of a Chiral Spin Liquid in the Triangular Lattice Hubbard Model

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Quantum spin liquids are fascinating phases of matter, hosting fractionalized spin excitations and unconventional long-range quantum entanglement. These exotic properties, however, also render their experimental characterization challenging and finding ways to diagnose quantum spin liquids is therefore a pertinent challenge. Here, we numerically compute the spectral function of a single hole doped into the half-filled Hubbard model on the triangular lattice using techniques based on matrix product states. At half filling the system has been proposed to realize a chiral spin liquid at intermediate interaction strength, surrounded by a magnetically ordered phase at strong interactions and a superconducting/metallic phase at weak interactions. We find that the spectra of these phases exhibit distinct signatures. By developing appropriate parton mean-field descriptions, we gain insight into the relevant low energy features. While the magnetic phase is characterized by a dressed hole moving through the ordered spin background, we find indications of spinon dynamics in the chiral spin liquid. Our results suggest that the hole spectral function, as measured by Angle-Resolved Photoemission Spectroscopy (ARPES), provides a useful tool to characterize quantum spin liquids.

# Spin-orbit mixed states in an electromagnetic field

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Spin-orbit mixing is an important problem in condensed matter. For instance, spin-orbit entanglement in the  $t_{2g}$  manifold may play an important role in exotic phenomena, like quantum spin liquids in 4d and 5d systems. An interesting question is how these states interact with electromagnetic fields, which may hold potential to tune their properties and reveal interesting physics. Motivated by our recent discovery of large gyrotropic signals in some Jahn-Teller manganites [1], here we explore the interaction of light with spin-mixed  $t_{2g} - e_g$  states in 3d metals. We show that spin-orbit mixing enables electronic transitions that are sensitive to circularly polarized light, giving rise to a gyrotropic response. Such interactions offer the opportunity to use electromagnetic waves at optical wavelengths to entangle orbital and spin degrees of freedom. Interestingly, we find that, in addition to spin-orbit coupling, orthorhombic Jahn-Teller interactions are relevant to enhance the observed optical gyrotropy in solid-state 3d systems with octahedral symmetry. Our approach, which includes a group-theoretical treatment of spin-orbit coupling, has wide applicability and provides a versatile tool to explore the interaction of electromagnetic fields with electronic states in transition metals with arbitrary spin-orbit coupling strength and point-group symmetries..

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[1] B. Casals et al., Phys. Rev. Lett. **117**, 026401 (2016).

# Three-Dimensional Skyrmions in chiral non-collinear antiferromagnets

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The dimensionality and topology of the order parameter space determines the shape of defects in uniformly ordered states. Thus collinear (anti)ferromagnets with an order parameter taking values on the two-dimensional (2D) sphere can host 2D baby Skyrmions (Skyrmion tubes) or 3D Hopfions. If spins inside the magnetic unit cell form a non-collinear ordering, such as the  $120^\circ$ -ordering in triangular antiferromagnets, the rotational symmetry is completely broken. The order parameter space is then  $SO(3)$  or  $O(3)$  [1-3]. Such systems host different topological solitons:  $Z_2$  vortices and 3D Skyrmions closely related to solitons in the non-linear sigma model originally studied by T.H.R. Skyrme.

We discuss stability of 3D Skyrmions in a chiral cubic magnet with three mutually orthogonal magnetic sublattices. These particle-like defects are stable in the conical spiral state induced by Dzyaloshinskii-Moriya (DM) interactions. We present results of numerical studies of a microscopic spin model with Heisenberg and DM interactions, in which this physics is realized.

[1] Dombre, T., Read, N., Phys. Rev. B **39**, 6797-6801 (1989).

[2] Batista, D. *et al.*, Phys. Rev. Lett. **121**, 227201 (2018).

[3] Barts, E., Mostovoy, M., Npj Quantum Mater. **6**, 104 (2021).

# Fractonic behaviors of skyrmions in chiral magnets

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Skyrmions are robust, spatially localized, topological spin textures, which carry a topological charge and have been found in many magnetic systems. In two-dimensional incommensurate chiral magnets, their dynamics obeys at least two conservation laws: the conservation of the topological charge and the conservation of energy-momentum tensor associated with the translational invariance of the system. These lead to a constrained dynamics which preserves both the topological charge and its higher moments [1]—a characteristic feature of fractons, which are excitations in fractonic phases of matter [2, 3]. As a result, a single skyrmion, like a fracton, is immobile and can move only by creating dipoles of the topological charge. A gas of skyrmions features interesting dynamics due to the interplay between the conservation laws and inter-skyrmion interactions. For instance, two like-charge skyrmions, if experiencing a mutual attraction while obeying the conservation laws, can exhibit a planetary motion akin to that of a binary star system. Motivated by all these, we theoretically study the fractonic behaviors of skyrmions in the field polarized phase of a two-dimensional chiral magnet model. We demonstrate how skyrmions can couple to a higher-rank  $U(1)$  gauge field. We also explore how the presence of thermally-excited magnons can influence the dynamics of a skyrmion gas by mediating an inter-skyrmion force or by screening the force mediated by the gauge field.

\*This work is supported by the DPG grant SPP 1237.

[1] N. Papanicolaou, T.N. Tomaras, Nucl. Phys. B **360**, 425 (1991).

[2] R. M. Nandkishore and M. Hermele, Annu. Rev. Condens. Matter Phys **10**, 295 (2018).

[2] M. Pretko, X. Chen and Y. You, Int. J. Mod. Phys. A **35**, 2030003 (2020).

## Thermal Hall transport calculations in Kitaev-Heisenberg model.

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The honeycomb lattice Mott insulating systems such as  $\alpha$ -RuCl<sub>3</sub>, have emerged as candidates for realizing the Kitaev spinons. Motivated by the experimental observation of quantized (likely half-integer) thermal Hall conductivity in  $\alpha$ -RuCl<sub>3</sub>, we study the thermal Hall conductivity of a non-integrable Kitaev-Heisenberg model numerically, using tensor network techniques. Our tensor network analysis uses the purification method to represent mixed quantum states at finite temperature as pure states on an enlarged Hilbert space carrying both physical and ancilla sites. We compare our findings with reported quantized thermal Hall conductivity results. We also study the topological entanglement entropy - a measure of topological order - as a function of the model parameters. Our study confirms continued persistence of topological order deep in the spin density wave order phase.

## ***ClassiC, a package for simulating classical spin dynamics at finite temperatures***

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At low temperatures, the dynamics of semi-classical spin systems is well understood from the linear spin wave theory [1], valid for both ferromagnets and antiferromagnets as implemented in the package SpinW [1]. However, the spin wave theory considers spin dynamics as a perturbation of an ordered state, so at elevated temperatures, comparable to the Néel temperature  $T_N$ , the theory breaks down. Even more problematic is the situation for frustrated spin systems, where the ordering temperature is considerably suppressed [3]. Here, spins are typically strongly correlated even at temperatures far above  $T_N$ . In these cases other methods, e.g. computer simulations, must be taken in use to explain the physics of the spin systems.

We here present the Copenhagen Langevin Spin Simulation Code (ClassiC) that is developed and optimized for modeling spin dynamics of highly frustrated spin systems. This code can define a generally anisotropic spin Hamiltonian on a (potentially periodic) finite lattice. The program solves the semi-classical equations of motion using the method of Langevin dynamics to take into account temperature effects on an absolute scale [4]. From the simulated spin data, observables are calculated, such as magnetic energy, magnetisation/susceptibility, static spin correlations, and the dynamical correlation function  $S^{\alpha\alpha}(\mathbf{q},\omega)$ , describing the outcome of neutron scattering experiments. Our code is in this respect rather similar to the more general UPPASD code where lattice dynamics and spin-lattice couplings are also taken into account [5].

We exemplify the ClassiC code by spin chains in magnetic field and finite temperatures, as well as frustrated clusters of spins on the triangular and kagome lattice, with and without periodic boundary conditions. We will compare our results and code performance with analytical expressions, UPPASD, and recent experimental findings on frustrated systems (e.g. the triangular lattice of h-YMnO<sub>3</sub> as found in [6]).

[1] F. Bloch, Z. Phys. **61**, 206 (1930); J. C. Slater, Phys. Rev. **35**, 509 (1930); T. Holstein and H. Primakov, Phys. Rev. **58**, 1098 (1940)

[2] S. Toth and B. Lake, J. Phys. Cond. Matt. **27**, 166002 (2015)

[3] C. Lacroix, P. Mendels, and F. Mila, *Introduction to frustrated magnetism*, Springer Series in Solid State Sciences, vol. 164 (2011)

[4] P. Langevin, C. R. Acad. Sci. Paris **146**, 530 (1908)

[5] J. Hellsvik et al, Phys. Rev. B **99**, 104302 (2019)

[6] S. Janas et al, Phys. Rev. Lett. **126**, 107203 (2021)

## Tuning exchanges in frustrated diamond-lattice antiferromagnet: $\text{MnSc}_2\text{Se}_4$

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$\text{MnSc}_2\text{S}_4$ , a magnetically frustrated thiospinel with  $\text{Mn}^{2+}$  forming a diamond lattice, shows multistep long-range ordering as a function of applied field,  $H$  and temperature,  $T$  [1]. Recently, neutron scattering studies established  $H$ - $T$  phase boundaries of the triple- $k$  state and thorough Monte Carlo simulations revealed the additional anisotropy terms in the spin Hamiltonian that stabilize the fractional antiferromagnetic skyrmion triple- $k$  state [2]. Motivated by these results, we investigate now the sister compound  $\text{MnSc}_2\text{Se}_4$ . We find a reduction of Curie-Weiss  $\Theta_{CW}$  and ordering  $T_N$  temperatures, and diminished energy range of spin excitations on replacing S by Se. The main features of  $H$ - $T$  phase diagram remain similar compared to  $\text{MnSc}_2\text{S}_4$  but the exchange constants are significantly smaller. I will discuss our magnetization and neutron scattering results which demonstrate that through frustrated interactions,  $\text{MnSc}_2\text{Se}_4$  is a host for realizing exotic states akin to magnetic skyrmions and vortices.

[1] S. Gao, O. Zaharko, et al. Nature Physics, 13, 157–161 (2016).

[2] S. Gao, H.D. Rosales, et al. Nature, 586, 37 (2020).



# Engineering magnetic frustration with impurities

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Sometimes, a little bit of frustration makes life interesting. Although controversial, this statement is certainly correct in physics, where frustration has opened an entire field of research with materials of exotic properties. Frustration refers to the presence of competing forces that cannot be simultaneously satisfied. Frustrated magnets often order in unconventional ways, or do not order at all, even at the lowest temperatures. In this context it is usually believed that pristine crystals are necessary, and impurities are unwanted perturbations.

Our motivation is to take the opposing view, and use impurities as a tool to engineer the properties of frustrated magnets. Motivated by recent experiments on the rare-earth pyrochlore oxide  $\text{Er}_2\text{Ti}_{2-x}\text{Sn}_x\text{O}_7$  [1], the idea is to tune the Hamiltonian of our system via non-magnetic dilution  $x$ . In other words, to use impurities as a knob to explore unknown parts of the phase diagram. Interestingly, this approach brings us at the frontier between (geometric) frustration and spin glasses. We report the phase diagram of  $\text{Er}_2\text{Ti}_{2-x}\text{Sn}_x\text{O}_7$  for  $0 \leq x \leq 2$ , using classical Monte Carlo simulations. Our calculations reproduce the shape of the experimental phase diagram [1], with a competition between two different types of antiferromagnetic orders and a pronounced asymmetry. We explain the origin of this asymmetry and find that this competition induces an intermediate spin glass phase where magnetic order disappears. To build a detailed theory, we extract from simulations the specific heat, susceptibility, neutron-scattering structure factor, microscopic fluctuations and spin dynamics.

**Keywords**— condensed matter, statistical physics, magnetic frustration, spin glass

[1] M. Shirai, R. S. Freitas, J. Lago, S. T. Bramwell, C. Ritter, and I. Zivkovic, “Doping-induced quantum crossover in  $\text{Er}_2\text{Ti}_{2-x}\text{Sn}_x\text{O}_7$ ” *Physical Review B*, **96**, 180411 (2017).

# Quantum oscillations in heat capacity and charge transport of the unconventional insulator SmB<sub>6</sub>

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We present results of low temperature heat capacity and charge transport experiments on floating zone-grown single crystals of SmB<sub>6</sub> in high magnetic field and compare the observed quantum oscillations with those detected in this unconventional insulator by other authors[1,2]. Details of sample properties can be found in [3]. A robust numerical method for detecting small quantum oscillations in physical quantities was developed. The analysis of our results shows that the quantum oscillations, both in heat capacity and electrical resistivity, appear mainly at oscillation frequencies ranging from 244 T to 568 T and that their frequency spectrum is similar. Based on this parallel observation of quantum oscillations (in heat capacity and electrical resistivity) we suppose that their origin is intrinsic and comes from the insulating bulk, which in high field becomes gradually metallized. However, the frequency spectrum of our quantum oscillations is shifted towards lower frequencies when compared with those observed by other authors. The reason for this discrepancy is not yet clear, but it may be related with the different quality of samples used for heat capacity and resistance measurements, and with the different crystallographic orientation of investigated single crystalline samples towards magnetic field.

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[1] P. G. LaBarre *et al.* arXiv:2111.03758v3 (2021).

[2] M. Hartstein *et al.* iScience **23**, 101632 (2020).

[3] M. Orendac *et al.* Physical Review B **96**, 115101 (2017).

# Exploring $\text{Eu}_5\text{In}_2\text{Sb}_6$ , a non-symmorphic antiferromagnet: from macroscopic to atomic length scales

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We combine bulk measurements with scanning tunneling microscopy/spectroscopy (STM/S) to investigate the Zintl phase  $\text{Eu}_5\text{In}_2\text{Sb}_6$ , which is a non-symmorphic antiferromagnetic (AFM) insulator.  $\text{Eu}_5\text{In}_2\text{Sb}_6$  crystallizes in an orthorhombic structure (space group 55, Pbam), characterized by infinite  $[\text{In}_2\text{Sb}_6]^{10-}$  double chains along the crystallographic  $c$  axis [1]. At low temperatures, two magnetic transitions ( $T_{M1} \approx 14\text{K}$  and  $T_{N2} \approx 7\text{K}$ ) revealed in our magnetization, heat capacity, and magneto-transport measurements, point to a complex, presently not fully elucidated magnetic structure. Interestingly, the reported emergence of colossal magnetoresistance (CMR), an anomalous Hall effect (AHE), and a deviation of the susceptibility from a Curie-Weiss-type behavior suggested the formation of magnetic polarons [2]. Here, we also report concomitant features in the frequency and field-dependent ac-susceptibility.

By performing STM/S measurements, we obtained local insights into the electronic structure and surface morphology.  $\text{Eu}_5\text{In}_2\text{Sb}_6$  was successfully cleaved *in situ* at  $T \approx 20\text{K}$ . The STM topography revealed atomically flat and non-reconstructed areas. For the (010) and (081) planes, our STS data indicated gap-like spectra with a very low, but finite conductance at the Fermi level. To further elucidate the electronic structure, we also conducted DFT calculations. In order to calculate the density of states (DOS), different magnetic configurations and calculation schemes were considered. Qualitatively, the STS data agree with the calculated DOS for the a-AFM ground state in the energy range from  $-1$  to  $+1$  eV. From our investigations, direct experimental evidence of the predicted topological surface states remains elusive, although future experimental efforts will focus on optimizing cleaved (001) surfaces [3].

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[1] S.-M. Park et al., J. Mater. Chem. 12, 1839 (2002).

[2] P. Rosa et al., npj Quantum Materials (2020) 5:52.

[3] B. J. Wieder et al., Science 361, 246 (2018). N. Varnava et al., [arXiv:2203.06212](https://arxiv.org/abs/2203.06212) (2022).

## Orbital Differentiation in Sr<sub>2</sub>RuO<sub>4</sub> under Uniaxial Stress

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The Hall coefficient of unstressed Sr<sub>2</sub>RuO<sub>4</sub> changes sign twice with temperature, at  $\approx 120$  K and  $\approx 30$  K [1]. It has been proposed that this behavior is due to strong differentiation of the inelastic scattering between the Ru  $d_{xy}$  and  $d_{xz/yz}$  orbitals, which is a predicted consequence of Hund's coupling [2,3]. Here, we report the Hall resistance of Sr<sub>2</sub>RuO<sub>4</sub> under tunable uniaxial stress, which induces a Lifshitz transition, *i.e.* a topological transition in the Fermi surface structure [4,5]. We find that in the elastic regime below  $\sim 1.5$  K, both the Hall and longitudinal resistivities are unchanged across this Lifshitz transition. At temperatures where the resistivity is dominated by electron-electron scattering, the Hall coefficient becomes strongly electron-like beyond the Lifshitz transition, which is opposite to expectations from the change in topology, and indicates a crucial change in the orbital-dependent scattering. We present a model for this behavior, and more generally show how Hall effect data under uniaxial stress can be used to obtain information on  $k$ -dependent scattering in multiband metals.

[1] A. P. Mackenzie *et al.*, Phys. Rev. B **54**, 7425 (1996).

[2] M. Zingl *et al.*, Npj Quantum Mater. **4**, 1 (2019).

[3] J. Mravlje *et al.*, PRL **106**, 096401 (2011).

[4] A. Steppke *et al.*, Science **355**, eaaf9398 (2017).

[5] M. E. Barber *et al.*, Phys. Rev. Lett. **120**, 076602 (2018).

## Angle-resolved photoelectron spectroscopy of $\text{Yb}(\text{Ni}_{1-x}\text{Co}_x)_3\text{Ga}_9$

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A chiral compound  $\text{YbNi}_3\text{Ga}_9$  is a typical valence fluctuation system with Kondo temperature ( $T_K$ )  $\sim 570$  K [1]. The magnetic susceptibility shows a broad maximum around 190 K without Curie-Weiss behavior and decreases to constant in low temperature region. A specific heat measurement reported a Sommerfeld coefficient of  $\gamma \sim 30$  mJ/(mol·K<sup>2</sup>) that implies a moderate mass-enhancement [1]. Recently, pressure induced quantum critical behavior and a transition to antiferromagnetic phase above  $P_c \sim 9$  GPa have been reported in  $\text{YbNi}_3\text{Ga}_9$  [3]. The Co-substitution to  $\text{YbNi}_3\text{Ga}_9$  works as a hole doping and reduces  $T_K$ . In  $\text{Yb}(\text{Ni}_{0.9}\text{Co}_{0.1})_3\text{Ga}_9$ ,  $T_K$  decreases to 270 K and a Sommerfeld coefficient increases to  $\gamma \sim 65$  mJ/(mol·K<sup>2</sup>) [4].

We performed angle-resolved photoelectron spectroscopy (ARPES) to study the band structure of  $\text{Yb}(\text{Ni}_{1-x}\text{Co}_x)_3\text{Ga}_9$  ( $x = 0, 0.1$ ). We have revealed complex band structures and Fermi surfaces of both  $\text{YbNi}_3\text{Ga}_9$  and Co-substituted compound. In the vicinity of Fermi energy, a nondispersive  $\text{Yb}^{2+} 4f^{7/2}$  band was clearly observed in both compounds. Moreover, we observed an evidence of hybridization between  $4f$  and valence bands [5]. Due to the hole doping, the  $\text{Yb}^{2+} 4f^{7/2}$  band shifts toward the Fermi energy in Co-substituted compound. The detail of the ARPES results will be discussed in the poster presentation.

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[1] Y. Yamashita *et al.*, J. Phys. Soc. Jpn. **81**, 034705 (2012).

[2] Y. Utsumi *et al.*, Phys. Rev. B **86**, 115114 (2012); JPS Conf. Proc. **1**, 012117 (2014).

[3] K. Umeo *et al.*, Phys. Rev. B **98**, 024420 (2018); K. Matsubayashi *et al.*, Phys. Rev. Lett. **114**, 086401 (2015).

[4] T. Fukuta *et al.*, JPS Conf. Proc. **3**, 011048 (2014).

[5] Y. Utsumi *et al.*, J. Phys. Soc. Jpn. **89**, 044711 (2020).

## Compass-like manipulation of nematicity in $\text{Sr}_3\text{Ru}_2\text{O}_7$

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Strong electron interactions in correlated materials give rise to a variety of emergent phases, including electronic nematic phases. Electronic nematicity has been found in a range of different materials, exhibiting strong symmetry-breaking reconstruction of electronic states without a significant lattice distortion. An enigmatic example of an electronic nematic state is found in  $\text{Sr}_3\text{Ru}_2\text{O}_7$ , where nematicity was shown to be stabilized by external magnetic field and manifests in anisotropic in-plane resistivity [1].

Recently, STM measurements have revealed a symmetry breaking electronic structure at the surface of  $\text{Sr}_3\text{Ru}_2\text{O}_7$  which occurs even in zero magnetic field, providing new insights into the mechanism stabilizing the nematicity [2]. At the same time, it presents a valuable opportunity for spectroscopic study of nematic order in an external field.

Here, we use low-temperature scanning tunnelling microscopy to study the nematicity in  $\text{Sr}_3\text{Ru}_2\text{O}_7$  in vector magnetic fields. We find the low-energy electronic structure is strongly affected by the in-plane direction of external field, and demonstrate control over the nematic axis even with modest magnetic fields. Quasiparticle interference measurements allow us to relate the observed angle dependence with the previously reported electronic structure of this material.

This result establishes compass-like control over the electronic structure in the surface layer of  $\text{Sr}_3\text{Ru}_2\text{O}_7$  and emphasizes the importance of spin-orbit coupling in the formation of the field-controlled nematic state [3]. We also discuss possible implications for the field-induced nematicity found in the bulk.

[1] R. A. Borzi *et al.*, *Science* **315**, 214 (2007).

[2] C. A. Marques *et al.*, *arXiv:2202.12351* (2022).

[3] S. Raghu *et al.*, *Phys. Rev. B* **79**, 214402 (2009)

## Fermi surface and nested magnetic breakdown in WTe<sub>2</sub>

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The transition metal dicalcogenide WTe<sub>2</sub> has been studied extensively since the observation of a large non-saturating magnetoresistance in 2014 due to charge carrier compensation in this type-II Weyl semimetal [1]. The exact morphology of two small electron and hole pockets in the Fermi surface of WTe<sub>2</sub> has been under debate ever since. We present a detailed Shubnikov-de Haas (SdH) study up to 29 T where in addition to the fundamental orbits, magnetic breakdown (MB) is observed [2]. Using the SdH results to guide our density functional theory calculations, we are able to accurately determine its Fermi surface by employing a moderate Hubbard U term. The tunneling mechanism causing MB is different from other materials since the onset of MB is solely determined by impurity damping due to a small breakdown gap. Secondly, the pockets are located in a Matruschka doll nesting that causes the breakdown gap to remain small upon rotating the magnetic field orientation resulting in the observation of MB over a wide range of angles.

[1] Ali, M., Xiong, J., Flynn, S. et al. Large, non-saturating magnetoresistance in WTe<sub>2</sub>. *Nature* **514**, 205–208 (2014)

[2] Linnartz, J.F., Müller, C. S. A., Hsu, Y. et al. Fermi surface and nested magnetic breakdown in WTe<sub>2</sub>. *Phys. Rev. Research* **4**, L012005 (2022)

# Investigation of temperature dependent thermal transport in $\text{Sr}_2\text{RuO}_4$ and $\text{Sr}_3\text{Ru}_2\text{O}_7$ over a wide temperature range

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Using optical methods to investigate a material is a powerful non-contact way to explore fundamental physics. In our work, we use optics to study thermal transport by modifying a typical laser pump-probe technique. However, a direct measurement of thermal conductivity is not only inconvenient, but also very challenging at high temperatures. In contrast, our method allows us to directly obtain the absolute value of temperature dependent diffusivity over a wide range of temperature, from 10K up to 330K. As thermal diffusivity is the ratio of the thermal conductivity to the heat capacity of a material, we can access the higher temperature thermal conductivity by an optical measurement of diffusivity and standard heat capacity measurement.

We have used this technique to measure thermal diffusivity of two strongly correlated metals, the ruthenates  $\text{Sr}_2\text{RuO}_4$  and  $\text{Sr}_3\text{Ru}_2\text{O}_7$ . This temperature dependent thermal transport combined with the resistivity measurements help us derive a temperature dependent Lorenz ratio  $L(T)$ . This offers an insight into the electronic and phononic contributions to the quasiparticle scattering. On comparing the experimentally obtained  $L(T)$  in the above ruthenates with the metals like Nb that are known for their strong electron phonon coupling, we can identify the dominant scattering mechanisms.



# Emergent Phase Diagram of Ruthenates : SrRuO<sub>3</sub>-SrTiO<sub>3</sub> Heterostructure

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Ruthenates are unique class of system that manifest a variety of quantum phenomena such as an unconventional superconductivity, Hund metallicity, and Mott-insulating phases. At the core of the fascinating properties, there are intricate balance among the electron correlation, spin and orbital physics. Here, we demonstrate that the SrRuO<sub>3</sub>-SrTiO<sub>3</sub> heterostructure, in conjunction with epitaxial strain, is a unique platform to manipulate the emergent electronic and magnetic properties. Employing the density functional theory plus dynamical mean field theory, we show that the strain can tune the orbital selective electronic correlation from Hund metal with simultaneous control of different magnetic orders at competition, which covers various known and even unknown phase of bulk ruthenates.

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## Localized-to-itinerant crossover in CeIn<sub>3</sub>

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dHvA study has revealed drastic change of the Fermi surface around the antiferromagnetic quantum critical pressure  $P_c$  in CeRhIn<sub>5</sub>, CeRh<sub>2</sub>Si<sub>2</sub> and CeIn<sub>3</sub> [1]. These results apparently imply the transition from the small Fermi surface with localized 4f-electron to the large Fermi surface with itinerant 4f-electron. However, recent Hall effect, resistivity and thermal expansion measurements in CeRh<sub>2</sub>Si<sub>2</sub> revealed the existence of two critical pressures, the localized-to-itinerant transition pressure  $P^*$ , and the antiferromagnetic quantum critical pressure  $P_c$  with  $P^* < P_c$ . Thus, the Hall effect is a powerful probe to seek the existence of localized-to-itinerant transition or crossover.

We measured the resistivity and the Hall coefficient in CeIn<sub>3</sub> under pressure down to about 200 mK. The discontinuous variation of the Hall coefficient at 200 mK was observed around  $P^* \sim 1.1 \text{ GPa} < P_c = 2.4 \text{ GPa}$ , which strongly implies the change of the Fermi surface related to the localized-to-itinerant crossover of 4f electron in antiferromagnetic (AFM) phase. The anomaly smeared out at higher temperatures than about 1 K. On the other hand, the resistivity at 200 mK shows strong enhancement around  $P^*$ . This anomaly can be traced within AFM phase and is smoothly connected to the localized-to-itinerant crossover line observed in the paramagnetic phase [2]. The Hall coefficient around  $P^*$  shows the characteristic temperature dependence, which may be explained by the existence of the valence fluctuations.

[1] Y. Ōnuki and R. Settai, *Low Temp. Phys.* **38**, 89 (2012).

[2] S. Kawasaki et al., *Phys. Rev. B* **77**, 064508 (2008).

## Electronic structure across the antiferromagnetic transition of NiO

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Most of the 3d transition metal oxides (TMOs), despite their partially filled 3d orbitals, have insulating ground states in contrast to expectations based on elementary band theoretical considerations. Nickel Oxide, NiO is one such material which arguably has been the most discussed compound as the archetype of an insulating state with a partially filled 3d shell with diverse explanations over the decades. While it is now generally believed that the presence of strong electron-electron interactions is the primary reason for the insulating state, often referred to as the Mott-Hubbard insulators [1,2], the role of the antiferromagnetic order, established at a high temperature of ~525 K for NiO and originally proposed by Slater [3] as a mechanism to derive the insulating state, has often been addressed experimentally and theoretically by probing the valence band (VB) and Ni 2p core level photoemission spectra of NiO across the antiferromagnetic transition temperature ( $T_N$ ) [4-6] with little agreement between different reports. We address this issue by performing Hard X-ray Photoelectron Spectroscopy (HAXPES) on NiO single crystals with 6000 eV photon energy to study the influence of magnetic ordering on the electronic structure. We have collected the VB and the Ni 2p core level spectra at different temperatures across the  $T_N$ . Interestingly, we observe no change in VB as well as in the core level spectra as a function of temperature across the  $T_N$ . Our experimental results establish that the long range magnetic ordering does not appreciably influence the electronic structure of NiO; this result is in contrast with the available theoretical results that predict substantial changes in core and valence photoemission spectra across  $T_N$  with the assumption of a completely disordered magnetic state above the transition temperature. Therefore, our results suggest the existence of short-range spin correlations on the Ni sites in NiO in the high temperature paramagnetic state with the electronic structure being dominantly influenced by short-range interactions.

[1] N. F. Mott, *Proc. Phys. Soc. London, Sect. A* **62**, 416 (1949).

[2] J. Hubbard, *Proc. R. Soc. London, Ser. A* **276**, 238 (1963).

[3] J. C. Slater, *Phys. Rev.* **81**, 385 (1951).

[4] O. Tjernberg *et al.*, *Phys. Rev. B* **54**, 10245 (1996).

[5] A. Hariki *et al.*, *J. Phys. Soc. Japan* **82**, 1 (2013).

[6] C. Y. Kuo *et al.*, *Eur. Phys. J. Spec. Top.* **226**, 2445 (2017).

# Investigation of de Haas-van Alphen oscillations under temperature modulation in Bi

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Starting with the discovery of quantum oscillatory phenomena in the 1930s [1], the properties of Bi have become the drosophila of studies of the electronic structure and the Fermi surface of metals, providing access to both the most basic phenomena [2,3] as well as the extreme quantum limit [4,5]. However, an inherent constraint of present-day detection techniques of quantum oscillations encountered especially in strongly correlated topological materials, concerns the separation of signal components of vastly different amplitude as associated with large differences of the effective charge carrier masses. We report the development of a detection technique for measurements of the de Haas-van Alphen effect by means of an inductive signal pick-up that is driven by temperature oscillations of the sample [2]. Resulting in an effective convolution of the oscillatory signal components with the derivative of the effective charge carrier mass with respect to temperature, our setup permits to discriminate elegantly light from heavy masses, and allows the direct (in-situ) determination of the charge carrier effective masses. Using this setup, we have revisited de Haas-van Alphen effect in Bi, focusing on the nature and character of the electron pockets as well as the effects of partial valley polarization when approaching the quantum limit under large magnetic fields.

- [1] W. J. de Haas and P. M. van Alphen, *Commun. Phys. Lab. Leiden* **212a**, 3 (1930).
- [2] D. Shoenberg, *Magnetic oscillations in metals*, Cambridge Monographs in Physics.
- [3] V.S. Edel'man, *Adv. Phys.* **25**, 555 (1976).
- [4] K. Behnia, *et al.*, *Science* **317**, 1729 (2007).
- [5] Z. Zhu *et al.*, *J. Phys.: Condens. Matter* **309**, 313001 (2018).

# Mutually stabilised electronic and structural transition in high-pressure sulphur

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Charge density waves (CDW's) affect various electronic and structural phenomena in condensed matter systems, including metal-insulator transitions and superconductivity, e.g. in cuprates. Sulfur is one of the few elements that exhibits a CDW between 83 and 153 GPa as well as superconductivity. The CDW S-IV phase is an incommensurate modulation of a body-centered monoclinic crystal structure with the monoclinic structure being a distortion of the rhombohedral lattice present at higher pressures [1,2].

Here, we present Raman spectroscopy results as an alternative probe of the CDW state [3] – the displacement mode of the atomic positions is always Raman-active. Our Raman measurements of sulfur up to 155 GPa track the CDW mode across the entire S-IV range. Surprisingly, we find that the CDW mode in S-IV retains a finite frequency up to the transition to S-V, suggesting a weakly first order transition when the CDW breaks down. We use first-principles electronic structure and phonon calculations to show that only by combining both the CDW displacement mode and the monoclinic lattice distortion the two phases are stabilised. The coupling between the two distortions causes the weak first-order transition including the quantum phase transition in the zero temperature limit.

Our work suggests that the formation of CDW states can be more complex than hitherto assumed, e.g. *via* interactions with lattice degrees of freedom, but also demonstrates the potential of spectroscopic measurements in combination with electronic structure calculations to unravel those interactions.

[1] O. Degtyareva, *et al.*, Phys. Rev. B **71**, 214104 (2005).

[2] C. Hejny, *et al.*, Phys. Rev. B **71**, 020101(R) (2005).

[3] T. Kume, *et al.*, Phys. Rev. Lett. **94**, 065506 (2005).

# Nodes of different speeds: anisotropy of the nodal electronic structure in single-layered Pb-Bi2201 high- $T_c$ superconductors

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The single-layered cuprates  $(\text{Pb,Bi})_2\text{Sr}_{2-x}\text{La}_x\text{CuO}_{6+\delta}$  (Pb-Bi2201) are low-dimensional materials hosting strong electronic correlations that lead to a highly anomalous normal state and high-temperature superconductivity. Historically, Pb-Bi2201 was believed to be tetragonal [1], though more recent refinement studies have shown that the system stabilizes in an orthorhombic structure [2] with inequivalent in-plane lattice parameters. It is not known, however, how this orthorhombicity influences electronic properties such the Fermi velocity  $v_F$  and the Fermi wave vector  $k_F$ . Here, we employ angle-resolved photoemission spectroscopy (ARPES) and low-temperature thermal conductivity measurements to study the effect of orthorhombicity on the in-plane properties of Pb-Bi2201, in particular the in-plane anisotropy of  $k_F$  and  $v_F$ .

Strikingly, in synchrotron ARPES data we find a sizeable ( $\sim 10\%$ ) anisotropy in the nodal  $k_F$  determined between the orthogonal in-plane  $\Gamma X$  and  $\Gamma Y$  directions of Pb-Bi2201 [3]. Using high-resolution laser-ARPES we have also examined the corresponding  $v_F$  values along the  $\Gamma X$  and  $\Gamma Y$  nodes. The observed anisotropies are compared with the anisotropy observed in low- $T$  thermal conductivity measured on the same crystals along the two orthogonal nodal directions. In the proposed presentation, I will discuss these results and build the argument for the role of crystal structure in shaping the electronic properties of Pb-Bi2201.

[1] J.B. Torrance et al., Solid State Communications, 66(7):703-706, 1988.

[2] Ito et al. Physical Review B, 58(5):2851-2858, 1998.

[3] S. Smit et al., (in preparation)

# Cubic Rashba effect and 2D-ferromagnetism at the iridium-silicide surfaces of antiferromagnetic $\text{GdIr}_2\text{Si}_2$ and mixed-valent $\text{EuIr}_2\text{Si}_2$

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Two-dimensional (2D) electron states at the surface of  $RT_2\text{Si}_2$  compounds ( $R$  = lanthanide,  $T$  = transition metal) with  $\text{ThCr}_2\text{Si}_2$  structure have proven to be ideal model systems for studying the joint action of spin-orbit (SOI) and exchange interactions on itinerant electrons [1-5]. Those surface states are predominantly situated in the  $\text{Si-T-Si-R}$  surface block and subject to Rashba-type spin splittings which can be manipulated by ordered  $4f$  moments.

Here, we present our combined angle-resolved photoelectron spectroscopy (ARPES) and density functional theory (DFT) studies on the Si-terminated surface of compounds with  $T=\text{Ir}$ , which are of particular interest because Ir leads to a large SOI. We found that in the paramagnetic phase the surface states are characterised by a huge energy splitting of the highly spin-polarised bands and an exotic triple-winding spin structure along the constant-energy contours induced by the so-called cubic Rashba effect [4]. Upon ordering of the  $4f$  moments below the Si-terminated surface, the emerging exchange coupling of the surface-state spins to the localised lanthanide moments modifies the spin structure, leading to pronounced asymmetries in the band dispersion. Surprisingly, these asymmetries were not only found for the antiferromagnet  $\text{GdIr}_2\text{Si}_2$  [5], but for the valence-fluctuating  $\text{EuIr}_2\text{Si}_2$ , too [3]. The latter allowed us to unveil unusual 2D ferromagnetic properties and related temperature scales of the iridium-silicide surface of  $\text{EuIr}_2\text{Si}_2$ , which is non-magnetic in the bulk. Moreover, a short overview on additional results from complementary experimental techniques like photoelectron diffraction and magnetic dichroism experiments on the  $4f$  shell is given [6].

[1] A. Chikina *et al.*, Nat. Comm. **5**, 3171 (2014)

[2] A. Generalov *et al.*, Nano Lett. **17**, 2 (2017)

[3] S. Schulz *et al.*, npj Quantum Mater. **4**, 26 (2019)

[4] D. Yu. Usachov *et al.*, Phys. Rev. Lett. **124**, 237202 (2020)

[5] S. Schulz *et al.*, Phys. Rev. B **103**, 035123 (2021)

[6] D. Yu. Usachov *et al.*, Phys. Rev. B **102**, 205102 (2020)

# Lifshitz transition-induced tuning of charge density waves in 2H-TaSe<sub>2</sub>

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2H-TaSe<sub>2</sub> is a metallic transition metal dichalcogenide which consists of weakly coupled sandwich-like layers in which an atomic plane of transition metals is embedded between two planes of seleniums. All the atoms are arranged in hexagonal lattices, with the chalcogen layers in each sandwich directly above/underneath each other. The consecutive sandwich-layers are rotated by 180 degrees and stacked so that the transition metals are placed on top of each other. Below 90 K, 2H-TaSe<sub>2</sub> exhibits a (3x3) charge density wave. As suggested by this high critical temperature, the electronic band reconstruction in this phase is quite strong, with the associated gap 50-100 meV. For this reason, 2H-TaSe<sub>2</sub> serves as a model to understand the mechanisms behind charge density wave formation in other materials (including other transition metal dichalcogenides).

We study the interplay between the charge density order and a Lifshitz transition by surface doping 2H-TaSe<sub>2</sub> with potassium. Using angle-resolved photoemission spectroscopy, we map out directly the electronic dispersion in the (3x3) charge density wave state and how it changes as the previously unoccupied electronic states in the topmost layers are filled so that the chemical potential crosses a saddle point in the dispersion. Based on calculations of generalized susceptibility within a minimal two-band model and symmetry arguments, we conclude that the change in the Fermi surface topology drives a change in the charge density order from a (3x3) to a (2x2) superlattice.



## Electronic structure of the $\text{Ce}_3\text{PdIn}_{11}$ heavy fermion system with two inequivalent Ce sites

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Heavy fermion superconductor  $\text{Ce}_3\text{PdIn}_{11}$  was investigated by means of angle-resolved photoemission spectroscopy (ARPES) at the CASSIOPEE beamline of the Soleil synchrotron. Spectra were collected at 6 K with photon energy tuned to the Ce  $4d$ - $4f$  resonant transition (122 eV), resulting in an increased Ce  $4f$ -electron spectral weight. The electronic structure of  $\text{Ce}_3\text{PdIn}_{11}$  was calculated using Korringa-Kohn-Rostoker (KKR) method within the single-particle Green function approach.

The experimentally obtained Fermi surface of  $\text{Ce}_3\text{PdIn}_{11}$  has a quite complex shape with certain structures similar to those found in related heavy fermion superconductors  $\text{Ce}_2\text{PdIn}_8$ ,  $\text{Ce}_2\text{RhIn}_8$ ,  $\text{Ce}_2\text{IrIn}_8$  and  $\text{CeCoIn}_5$ .  $4f$  electrons contribute to the ARPES spectra with well visible flat bands near the Fermi energy ( $E_F$ ). Hybridization effects between conduction band and Ce  $4f$  electrons are reflected in dispersion anomalies and enhanced effective mass in a vicinity of  $E_F$ . The calculations resolved different contributions to the electronic band structure due to Ce atoms located at the  $2g$  and  $1a$  crystal lattice sites. The structure of  $f^{1/2}$  final state exhibits ~50 meV energy splitting that may be attributed to crystal field effect. The observed spectral shape is characteristic of Fermi liquid state.

# Quantum Oscillations and ARPES Studies of Pd<sub>x</sub>Bi<sub>2</sub>Te<sub>3</sub> Topological Insulator

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Topological Insulators (TIs) are a novel quantum phase of matter with insulating bulk and conducting surface states, and these surface states are quite robust against backscattering and non-magnetic disorder, thus making them potential candidates for quantum computation, spintronic devices, and electronic devices.[1] Spin-orbit coupling, and time-reversal symmetry forms the basis of topological insulator. Bismuth chalcogenides based topological insulators have been of enormous interests, which comprises of single Dirac cone at the  $\Gamma$  point.[2] We present the intriguing results on Pd doped Bi<sub>2</sub>Te<sub>3</sub> using the detailed magnetotransport and angle resolved photoemission spectroscopy (ARPES) studies. The evolution of magnetoresistance, Shubnikov-de Haas quantum oscillations, and electronic band structure upon Pd doping has been discussed. The Pd doping in Bi<sub>2</sub>Te<sub>3</sub> leads to change in charge carrier density from *n*- to *p*-type which is evident from both Hall data and ARPES studies. ARPES studies shows the persistence of surface states upon 20% Pd doping, and consistent shift in the Dirac point of the topological surface states and bulk-derived valence bands to lower binding energy upon Pd doping in a rigid-band-like way up to  $x \sim 0.10$ . Furthermore, a comparison of parameters calculated from the transport and ARPES studies reveal reduction in Fermi wavevector ( $k_F$ ) value calculated in magnetotransport measurements is likely due to band bending induced by Schottky barrier.[3]

[1] Y. Ando, J. Phys. Soc. Jpn **82**, 102001 (2013).

[2] B. Yan and S.-C. Zhang, Rep. Prog. Phys. **75**, 096501 (2012).

[3] Shailja Sharma, Shiv Kumar, Girish C. Tewari, Girish Sharma, Eike F. Schwier, Kenya Shimada, A. Taraphder, and C.S. Yadav, Phys. Rev. B **105**, 115120 (2022).

## Planar Hall effect in Cu intercalated PdTe<sub>2</sub>

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The planar Hall effect (PHE) in topological semimetals have gained tremendous research interest lately. However, there is no clear picture about the origin of PHE in these systems due to the coexistence of chiral anomaly and orbital magnetoresistance (MR). PdTe<sub>2</sub> is a type-II Dirac semimetal with positive longitudinal MR, which makes it a good candidate to host topological superconducting states [1, 2]. It shows superconductivity below 1.7 K and exhibit topologically non-trivial surface states [3]. The intercalation of 5% Cu enhances the superconducting transition temperature to 2.6 K [4]. Recently there have been reports of PHE in PdTe<sub>2</sub> [5, 6]. This stimulated our interest in studying the PHE in the Cu intercalated compound; Cu<sub>0.05</sub>PdTe<sub>2</sub>. We observed positive longitudinal MR, linear field dependence of the amplitude of PHE, and the tilted prolate shaped orbits in parametric plot that point toward the importance of Fermi surface anisotropies in understanding the origin of PHE in a system like PdTe<sub>2</sub>. The existence of positive MR and PHE raises a doubt over the notion of chiral anomaly as an origin of PHE in the systems.

### References:

- 1) H. J. Noh *et al.*, Phys. Rev. Lett. 119, 016401 (2017).
- 2) F. Fei *et al.*, Phys. Rev. B 96, 041201 (2017).
- 3) Amit and Yogesh Singh, Physical Review B 97, 054515 (2018).
- 4) Ryu G., J. Supercond. Nov. Magn., 28 3275 (2015).
- 5) S. Xu *et al.*, arXiv:1811.06767 (2018).
- 6) J. Meng *et al.*, J. Phys.: Condens. Matter 32, 015702 (2020).

## Intriguing magnetism of the topological kagome magnet $\text{TbMn}_6\text{Sn}_6$

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Magnetic topological phases of quantum matter are an emerging frontier in physics and material science [1-6], of which kagome magnets appear as a highly promising platform. Here, we explore magnetic correlations in the recently identified topological kagome system  $\text{TbMn}_6\text{Sn}_6$  using muon spin rotation, combined with local field analysis and neutron diffraction [1,4]. Our studies identify an out-of-plane ferrimagnetic structure with slow magnetic fluctuations which exhibit a critical slowing down below  $T_{C1}^* \approx 120$  K and finally freeze into static patches with ideal out-of-plane order below  $T_{C1} \approx 20$  K. The appearance of the static patches sets in at a similar temperature as the appearance of topological transport behaviors. We further show that a hydrostatic pressure of 2.1 GPa stabilizes the static out-of-plane topological ferrimagnetic ground state in the whole volume of the sample. Therefore the exciting perspective arises of a magnetically-induced topological system whose magnetism can be controlled through external control parameters. The present results [4] will stimulate theoretical investigations to obtain a microscopic understanding of the relation between the low-temperature volume-wise magnetic evolution of the static  $c$ -axis ferrimagnetic patches and the topological electronic properties in  $\text{TbMn}_6\text{Sn}_6$ .

[1] J.-X. Yin *et al.*, Nature **583**, 533-536 (2020).

[2] Z. Guguchia *et al.*, Nature Comm. **11**, 559 (2020).

[3] N.J. Ghimire and I.I. Mazin, Nature Materials **19**, 137-138 (2020).

[4] C. Mielke III *et al.*, arXiv:2101.05763 (2021).

[5] C. Mielke III *et al.*, Phys. Rev. Materials **5**, 034803 (2021).

[6] C. Mielke III *et al.* ... Z. Guguchia, Nature **602**, 245-250 (2022).

## Temperature dependence of Dirac Fermions in SnTe

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Topological materials contain symmetry-protected surface states that produce spin-polarized currents with negligible dissipation. These surface states are robust against weak disorder and temperature changes, making them ideal for quantum computing and spintronics applications. SnTe is a topological crystalline insulator in which the surface states are protected by the mirror symmetry of its rock salt crystal structure at room temperature. It is known to distort to a less symmetric rhombohedral structure on cooling, which is believed to reduce the number of topological surface states. We attempted to examine this effect by growing a single crystal of SnTe using the modified Bridgman method. We did not find any signs of the rhombohedral transition in our extensive powder X-ray diffraction, magneto-transport, and specific heat measurements between 2-300 K [1]. We carried out angle-resolved photoemission spectroscopy on our sample at 22 K, 60 K, and 120 K. While we did not observe any qualitative signature of the structural transition, we did find a few anomalies [2]. On heating from 22 K to 60 K, the bulk bands shifted closer to the Fermi level, and the slope of the surface bands decreased. On further heating from 60 K to 120 K, these trends got reversed. Additionally, we observed a decrease in the surface state intensity near the Fermi level at 120 K. Our density functional theory calculations suggest that some of these anomalies can be attributed to the evolution of the hybridization physics with complex structural changes induced by temperature.

[1] A. Maiti *et al.*, Applied Physics Letters **120**, 112102 (2022).

[2] A. Maiti *et al.*, Physical Review B **104**, 195403 (2021).

# Imaging Chern mosaic and Berry-curvature magnetism in magic-angle graphene

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Magic angle graphene harbors eight flavors of charge carriers denoted by a combination of their spin, valley and sublattice polarizations. If either the substrate or strong interaction breaks the inversion and time reversal symmetries, the flavor-degeneracy is lifted and their corresponding bands are filled sequentially. Due to their non-trivial band topology and Berry curvature, each of the bands is classified by a topological Chern number, leading to the quantum anomalous Hall and Chern insulator states at integer fillings  $\nu$  of the bands. Using scanning superconducting quantum interference device (SQUID-on-tip) [1], we directly image nanoscale Berry-curvature induced equilibrium orbital magnetism the polarity of which is governed by the local Chern number, and detect its two constituent components associated with the drift and the self-rotation of the electronic wave packets [2]. At  $\nu = 1$ , we observe local zero-field valley-polarized Chern insulators forming a mosaic of microscopic patches of  $C = -1, 0$ , or  $1$ , governed by the local sublattice polarization. This, consistent with predictions that local atomic-scale arrangements of the graphene and the encapsulating hBN lattices makes the Chern number position dependent, leads to irreversible flips of local Chern number and magnetization. This in turn leads to formation of valley domain walls giving rise to hysteretic global anomalous Hall resistance.

[1] D. Vasyukov, Y. Anahory, L. Embon, D. Halbertal, J. Cuppens, L. Neeman, A. Finkler, Y. Segev, Y. Myasoedov, M. L. Rappaport, M. E. Huber, and E. Zeldov, *Nat. Nanotechnol.* 8, 639–644 (2013).

[2] S. Grover, M. Bocarsly, A. Uri, P. Stepanov, G. Di Battista, I. Roy, J. Xiao, A. Y. Meltzer, Y. Myasoedov, K. Pareek, K. Watanabe, T. Taniguchi, B. Yan, A. Stern, E. Berg, D. K. Efetov, E. Zeldov, arXiv:2201.06901 (2022).

# Magneto-resistance and quantum oscillations in thin ZrSiSe flakes

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Nodal line semi-metals (NLSMs) are materials in which the Dirac band crossing takes place along a one-dimensional line or loop in momentum space. NLSMs represent ideal platforms to investigate the properties of charge carriers with a linear dispersion relation and to study topological correlated matter. Among them, ZrSiSe has been reported to possess linearly dispersing Dirac bands over a wide energy range ( $\sim 2$  eV), as well as hybridized surface-bulk states [1, 2]. The non-symmorphic symmetry of the square lattice shared among the ZrSiX (X=Si, S, Te) family, in combination with the metallic nature of NLSMs, make ZrSiSe a candidate for the development of macroscopically ordered states such as superconductivity, magnetism, charge density wave or even excitonic order [3,4,5].

In this work, we present a thickness-dependent magnetotransport study on exfoliated high quality thin flakes of ZrSiSe with thicknesses ranging from 30 to 100 nm and up to 30 T. Changes in the magnetoresistance (MR) as well as in the onset and amplitude of the quantum oscillations (QOs), are observed as the flakes become thinner. In particular, we find that the MR in thin samples strongly deviates from the well-known quadratic MR for compensated systems. With the preparation of these high quality thin flakes, we pave the way to investigate the interplay of topology and correlated phases in highly mobile exfoliated layers of ZrSiSe by electrostatic gating.

[1] J. Hu *et al.*, Phys. Rev. Lett. **117**, 016602 (2016).

[2] S. Pezzini *et al.*, Nat. Phys. **14**, 178 (2018).

[3] J. Liu and L. Balents, Phys. Rev. B **95**, 075426 (2017);

[4] B. Roy, Phys. Rev. B **96**, 041113(R) (2017).

[5] M. M. Scherer, Phys. Rev. B **98**, 241112(R) (2018).

# Magnetotransport properties of half-Heusler antiferromagnets SmPtBi and DyPtBi

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Rare earth-based platinum bismuthides, belonging to the well-known family of half-Heusler (HH) phases, have been predicted to host topologically non-trivial electronic states [1]. After a decade of intense investigations, solid experimental proofs have been got for the existence of linearly-dispersed electronic states in several representatives of the HH family, including DyPtBi [2,3].

In this work, we performed comprehensive studies on magnetotransport properties of high-quality single crystals of two HH phases, viz. SmPtBi and DyPtBi, grown from Bi-flux. Both compounds were found to order antiferromagnetically below 2.2 and 3.4 K, respectively. Their electrical resistivity has a semiconducting-like character at high temperatures, while shows a metallic-like behavior at low temperatures. Transverse magnetoresistance (TMR) of both materials is large, positive, and does not saturate up to 14 T, the highest magnetic field studied. Longitudinal magnetoresistance (LMR) of SmPtBi is also positive, but it has smaller magnitude than TMR. Remarkably, LMR of DyPtBi is negative up to at least 50 K, possibly due to chiral magnetic anomaly, which is a unique and defining feature of topological semimetals.

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[1] S. Chadov *et al.*, *Nature Materials* **9**, 541 (2010).

[2] H. Zhang *et al.*, *Physical Review B* **102**, 094424 (2020).

[3] J. Chen *et al.*, *Advanced Functional Materials* **31**, 2107526 (2021).



# High-dimensional Hofstadter butterfly induced by aperiodic magnetic field in quasicrystalline topological insulator

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Motivated by the striking discoveries of quantum criticality [1] and superconductivity [2] in quasicrystals, physical properties in quasicrystals have recently attracted much attention from both experimental and theoretical points of view. Although essential differences of quasicrystals from uniform or random systems have been explored since the first discovery of quasicrystal, there still remain many unsolved problems, except for conventional one-body problem. Particularly, since effects of many-body interactions and topological features are intensively studied in both uniform and random systems, their quasicrystalline counterparts should become important to deepen our knowledge of physical properties in quasicrystals.

Here we extend a topological insulator to a quasicrystal lattice, the Ammann-Beenker lattice. With applied a magnetic field in uniform system, it is well known that there appears a complicated self-similar structure in energy spectrum, the so-called Hofstadter butterfly. This feature has already been reported in a quasicrystal [3]. Then, as an extension of this work, we apply an aperiodic magnetic field corresponding to the quasicrystalline lattice. By diagonalization of the tight-binding Hamiltonian with the vector potential, we obtain the ground-state energy and wavefunction. With the Bott index calculated with the wavefunction, we classify the topological phases appearing in the Hofstadter butterfly. More interestingly, as compared with the uniform magnetic field in quasicrystals, the aperiodic magnetic field brings a higher-dimensional complicity in energy spectrum, which we call higher-dimensional Hofstadter butterfly, reflecting the quasicrystalline structure.

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[1] K. Deguchi, S. Matsukawa, N. K. Sato, T. Hattori, K. Ishida, H. Takakura, and T. Ishimasa, *Nat. Mater.* **11**, 1013 (2012).

[2] K. Kamiya, T. Takeuchi, N. Kabeya, N. Wada, T. Ishimasa, A. Ochiai, K. Deguchi, K. Imura, and N. K. Sato, *Nat. Commun.* **9**, 154 (2018).

[3] C. W. Duncan, S. Manna, and A. E. B. Nielsen, *Phys. Rev. B* **101**, 115413 (2020).

## Is epitaxial germanene a two-dimensional topological insulator?

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Free-standing germanene (germanium analogue to graphene) is predicted to be a two-dimensional topological insulator with a topological gap of about 25 meV inside the material and two topologically protected spin-polarized conduction channels at the edges propagating in opposite directions. Using low-temperature scanning tunneling microscopy and spectroscopy, we explored the possibility of epitaxial germanene on Ge<sub>2</sub>Pt crystals to be a two-dimensional topological insulator. We have located a one-dimensional electronic state at about 150 meV above the Fermi level. The state is localized at the edges of germanene. It is very pronounced and does not depend on edge termination. Moreover, we demonstrate that the application of an electric field, by the close approach of the tip, leads to an electronic phase transition from a Dirac semimetal to the opening of a small gap in germanene.

# Topological insulating bilayers and related interface effects

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When a two unit cell thick perovskite layer is grown on a [111] oriented substrate, the bulk symmetry of the crystal is reduced to that of a buckled honeycomb lattice [1, 2]. A honeycomb lattice in combination with spin-orbit coupling gives rise to topological states [3]. We experimentally realized these systems in oxide heterostructures by depositing 2 unit cells of LaMnO<sub>3</sub> on different [111] oriented substrates with pulsed laser deposition. However, no signatures of topological properties were observed. Interface effects such as inversion symmetry breaking, interdiffusion and charge transfer are discussed as possible culprits. This discussion is supported with scanning tunneling electron microscopy data of LaMnO<sub>3</sub> thin films on different substrates.

[1] Xiao, D *et al.*, *Nature Communications*, **2**, 1. (2011).

[2] Doennig, D *et al.*, *Physical Review B*, **93**, 16 (2016).

[3] Kane, C. L., & Mele, E. J. *Physical Review Letters*, **95**, 22 (2005).

# Magnetic properties of the higher-order topological insulator $\text{EuIn}_2\text{As}_2$

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Bulk-boundary correspondence in a topological insulator (TI) results in gapped bulk states and gapless surface states, the latter being protected by the bulk band topology. In higher-order TI (HOTI), the gap is preserved both in the bulk and the surface, and only hinges or corners become gapless [1,2]. In HOTIs, new topological invariants become relevant, and such systems have been recognized as good platforms for the emergence of novel topological phenomena [3].

Recently, it has been predicted theoretically that the antiferromagnetic compound  $\text{EuIn}_2\text{As}_2$  can host at low temperatures both the HOTI and axion insulator (AI) features [4]. Preliminary experimental confirmation of this finding was obtained using angle-resolved photoemission spectroscopy [5,6].

The main objective of this work was to comprehensively experimentally characterize the anisotropic magnetic properties of single-crystalline  $\text{EuIn}_2\text{As}_2$  and to describe the measured data in the framework of the mean-field theory. In addition, complementary studies of the electrical transport properties, heat capacity, and magnetocaloric effect were performed.

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[1] M. Sitte, *et al.*, Phys. Rev. Lett. **108**, 126807 (2012).

[2] W. A. Benalcazar, *et al.*, Science **357**, 61 (2017).

[3] B. Xie, *et al.*, Nat. Rev. Phys. **3**, 520 (2021).

[4] Y. Xu, *et al.*, Phys. Rev. Lett. **122**, 256402 (2019).

[5] S. Regmi, *et al.*, Phys. Rev. B **102**, 165153 (2020).

[6] T. Sato, *et al.*, Phys. Rev. B **2**, 033342 (2020).

# Coulomb drag study of inhomogeneous dielectric medium: Hole-hole dynamic screening in 2D-GaAs DQW

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We measured drag resistivity ( $\rho_D$ ) numerically and analyzed analytically with the structure of non-homogeneous dielectric medium (NHDM). Drag resistivity ( $\rho_D$ ) is measured of double quantum well of 2D-GaAs bilayer systems at low temperature ( $T \ll T_F$ ), thick interlayer separation ( $1 \ll k_F d$ ) and weak screening regime ( $1 \ll \omega\tau$ ) for 2D hole-hole (h-h) dynamic screening using the random phase approximations (RPA) method. RPA is reliable method at high density regime ( $r_s \leq 1$ ), but not consistent at low density regime ( $r_s \gg 1$ ). In low density regime, exchange-correlation (XC) effects are considered for evaluating the drag resistivity, XC effects enhanced the interaction between the two layers. It is found that the drag resistivity is found enhanced on using the XC effects and holes, as hole has greater effective mass than electron. In general, drag resistivity is directly proportional to  $\frac{T^2 \epsilon_2^2}{n^3 d^4}$  at low temperature (T), high density (n) and large interlayer separation (d). We have found consistent results for h-h dynamic screening compare to e-e and/or static interactions.

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- [1] A. Kamenev and Y. Oreg, "Coulomb drag in normal metals and superconductors: Diagrammatic approach," *Phys. Rev. B*, vol. 52, no. 10, pp. 7516–7527, Sep. 1995, doi: 10.1103/PhysRevB.52.7516.
- [2] C. Jörger *et al.*, "Frictional drag between coupled 2D hole gases in GaAs/AlGaAs heterostructures," *Phys. E Low-dimensional Syst. Nanostructures*, vol. 6, no. 1, pp. 598–601, 2000, doi: [https://doi.org/10.1016/S1386-9477\(99\)00125-3](https://doi.org/10.1016/S1386-9477(99)00125-3).
- [3] S. M. Badalyan, C. S. Kim, G. Vignale, and G. Senatore, "Exchange and correlation effects on plasmon dispersions and Coulomb drag in low-density electron bilayers," *Phys. Rev. B*, vol. 75, no. 12, p. 125321, Mar. 2007, doi: 10.1103/PhysRevB.75.125321.
- [4] R. Asgari, B. Tanatar, and B. Davoudi, "Comparative study of screened interlayer interactions in the Coulomb drag effect in bilayer electron systems," *Phys. Rev. B*, vol. 77, no. 11, p. 115301, Mar. 2008, doi: 10.1103/PhysRevB.77.115301.
- [5] B. Scharf and A. Matos-Abiague, "Coulomb drag between massless and massive fermions," *Phys. Rev. B*, vol. 86, no. 11, p. 115425, Sep. 2012, doi: 10.1103/PhysRevB.86.115425.
- [6] S. K. Upadhyay and L. K. Saini, "Coulomb drag study in electron-electron bilayer system with a dielectric medium," *Phys. E Low-dimensional Syst. Nanostructures*, vol. 124, p. 114350, 2020, doi: <https://doi.org/10.1016/j.physe.2020.114350>.
- [7] S. K. Upadhyay and L. K. Saini, "Study of drag resistivity in dielectric medium with the correlations effect," *Appl. Phys. A*, vol. 127, no. 4, p. 276, Mar. 2021, doi: <https://doi.org/10.1007/s00339-021-04422-y>.
- [8] S. K. Upadhyay and L. K. Saini, "Drag resistivity in bilayer-graphene/GaAs coupled layer system with the effect of local field corrections," *Eur. Phys. J. Plus*, vol. 136, no. 4, p. 433, Apr. 2021, doi: 10.1140/epjp/s13360-021-01377-0.
- [9] S. K. Upadhyay and L. K. Saini, "Study of coulomb drag with the effect of local field correction and dielectric medium," *Phys. B Condens. Matter*, vol. 614, p. 412982, 2021, doi: <https://doi.org/10.1016/j.physb.2021.412982>.

# Exceptional Points in Fermi Liquids with multipolar interactions

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In the Landau Theory of Fermi liquids (FL) [1] collective modes are not a closed system, since they can exchange energy with individual quasi-particles. In this way, damped modes appear in the spectrum. This mechanism, known as “Landau damping”, trigger non-Hermitian degeneracies, called *exceptional points* (EP).

EPs are singularities of the Hilbert space characterized by a level degeneracy where not only the energy eigenvalues coalesce but also the eigenvectors. Therefore, at these special points, the Hamiltonian cannot be diagonalized [2].

Quasi-particle interactions are parametrized by a set of Landau parameters that codify different multipole channels. Most results of FL are based in the model with only density ( $F_0$ ) interactions. However, in Galilean invariant FL, dipolar interactions ( $F_1$ ) renormalizes the effective mass. So, systems with electron mass enhancement could have  $F_1 \neq 0$ . In addition, FL with quadrupolar interactions ( $F_2$ ) is the simplest model supporting an isotropic-nematic transition [3]. Nematic fluctuations play a crucial role in several systems, such as cuprates and Fe-based superconductors [4].

In this work, we show the existence of EPs in the collective mode spectrum of FL with multipolar interactions [5,6]. Using multidimensional bosonization [7] and a real space renormalization group approach we compute the dynamic quadrupolar susceptibility. We show that, in the weak attractive region, two stable collective modes coalesce to an EP. We completely characterize this singularity, showing its topological properties [6]. Experimental signatures are discussed in two set-ups: pump-probe spectroscopy; and in the AC conductivity of FL in a narrow slab [8].

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[1] P. Nozieres and D. Pines, *The Theory of Quantum Liquids* (Perseus Books, 1999), p. 48.

[2] W. D. Heiss and A. L. Sannino, *Journal of Physics A: Mathematical and General* **23**, 1167 (1990).

[3] V. Oganesyan, S. A. Kivelson and E. Fradkin, *Phys. Rev. B* **64**, 195109 (2001).

[4] E. Fradkin, S. A. Kivelson, M. J. Lawler, J.P. Eisenstein and A. P. Mackenzie, *Annual Review of Condensed Matter Physics*, **1**, 153 (2010).

[5] R. Aquino and D. G. Barci, *Phys. Rev. B* **100**, 115117 (2019).

[6] R. Aquino and D. G. Barci, *Phys. Rev. B* **102**, 201110 (R) (2020).

[7] M. J. Lawler, D. G. Barci, V. Fernández, E. Fradkin and L. Oxman, *Phys. Rev. B* **73**, 085101 (2006).

[8] R. Aquino and D. G. Barci, *Phys. Rev. B* **104**, 195150 (2021).

# Drastic Magnetic Anisotropy Change Under Electric Field in $\text{Fe}_n\text{GeTe}_2$ ( $n=3, 4$ ) Monolayers: Density Functional Theory Perspective

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Magnetic anisotropy energy (MAE) is one of the most important properties in two-dimensional magnetism since the magnetization in two dimension is vulnerable to the spin rotational fluctuations. Using density functional theory calculation, we show that perpendicular electric field dramatically enhances the in-plane and out-of-plane magnetic anisotropies in  $\text{Fe}_3\text{GeTe}_2$  and  $\text{Fe}_4\text{GeTe}_2$  monolayers, respectively, allowing the change of easy axis in both systems.

The changes of the MAE under the electric field are understood as the result of charge redistribution inside the layer, which is available due to the three-dimensional (3D) network of Fe atoms in the monolayers.[1] To support this mechanism, the convexity of the curve of MAE as charge doping was observed. The sign of the MAE change as doping in our study was identical to the previous study on bulk material.[2] Analysis based on spin direction dependent band structure was done to figure out the reason of convexity of the curve.

As a result, we suggest that due to the unique structure of  $\text{Fe}_n\text{GeTe}_2$  compounds composed by peculiar 3D networks of metal atoms, the MAE can be dramatically changed by the external perpendicular electric field.

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[1] J. Seo, D. Y. Kim, E. S. An et al., *Sci. Adv.* **17**, eaay8912 (2020).

[2] S. Y. Park, D. S. Kim, Y. Liu, J. Hwang, Y. Kim, W. Kim, J. -Y. Kim, C. Petrovic, C. Hwang, S. -K. Mo, H. -J. Kim, B. -C. Min, H. C. Koo, J. Chang, C. Jang, J. W. Choi and H. Ryu, *Nano Lett.* **9**, 9b03316 (2019).

## Structural and magnetic properties of LaFeO<sub>3</sub>/SrTiO<sub>3</sub> superlattices

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We report on structural and magnetic characterization of superlattices composed of antiferromagnetic LaFeO<sub>3</sub> and SrTiO<sub>3</sub>. We have fabricated superlattices consisting of a bilayer with 1, 2 or 3 unit cells of LaFeO<sub>3</sub> and 5 unit cells of SrTiO<sub>3</sub> that was repeated 10 times. The superlattices were grown by pulsed laser deposition on TiO terminated SrTiO<sub>3</sub> substrates and the growth was monitored by reflection high-energy electron diffraction. The structural properties of the superlattices were determined by X-ray diffraction and atomic force microscopy.

Magnetic properties of the superlattices were analyzed by low-energy muon spin rotation. The measurements in zero and weak transverse field indicate that LaFeO<sub>3</sub> remains antiferromagnetic in layers that are 3 and 2 unit cell thin, whereas it is suppressed down to 4 K in the superlattice with 1 unit cell of LaFeO<sub>3</sub>. The latter effect is probably caused by an enhancement of spin fluctuations in the two-dimensional limit.



# The energy of a two-dimensional electron gas with finite thickness

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An almost ideal two-dimensional electron gas [1,2] can be created in a heterostructure consisting of a thin layer of GaAs with a given finite thickness sandwiched between two thicker layers of AlGaAs. This setup provides the simplest realization of a quantum well. The electrons in the conduction band are confined on the GaAs layer which represents the well region. Such a region contains the electrons and is surrounded by the AlGaAs barriers. One can consider the infinitely deep square well approximation and assume that the electrons are frozen into the ground state of this dimension. However, this leaves the electrons free to move in the other transverse two dimensions. The net result is a quasi two-dimensional electron gas system [1,2] with a finite thickness. In this work, we consider such a model of electrons with an added jellium neutralizing background in order to make the whole system charge neutral. We study a spinless system of electrons and use the Hartree-Fock approximation to investigate the energy of the system as a function of the thickness the layer of electrons.

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[1] O. Ciftja, *Physica B* **458**, 92 (2015).

[2] O. Ciftja, *Sci. Rep.* **11**, 3181 (2021).

# Topological Dirac magnons in honeycomb ferromagnets

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The magnon band structures of honeycomb ferromagnets are analogous to the electronic band structure of graphene, which exhibits mode crossings with linear energy-momentum relations at the so-called Dirac wave vectors  $Q_K = \left(\pm\frac{1}{3}, \pm\frac{1}{3}\right)$ . Such linearly dispersive magnons are thus called Dirac bosons or even Dirac magnons in reference to the Dirac fermions in the graphene [1]. In the case of graphene's band structure, spin-orbit couplings across the next nearest neighbor bonds break the time reversal symmetry and open small energy gaps at the Dirac wave vectors causing the Dirac fermions to become massive in the bulk but not along the edges.

Similar spin-orbit-coupled topological gap openings were also predicted in magnon band structures of honeycomb ferromagnets, which were eventually observed in a series of Cr-based van der Waals honeycomb ferromagnets. In this talk, we will review the recent experimental works on Dirac magnons and topological gap openings in  $\text{CrX}_3$  ( $X = \text{Br}, \text{Cr}, \text{I}$ ) and  $\text{Cr}_2\text{Z}_2\text{Te}_6$  ( $Z = \text{Si}, \text{Ge}$ ) using inelastic neutron scattering [2-5]. We will discuss how the spin-orbit couplings, either as antisymmetric Dzyaloshinskii-Moriya or bond-directional Kitaev exchanges, can reproduce the observed magnon bands involving the gap openings at the Dirac wave vectors. Finally, we will see how the in-plane magnetic field dependence of the magnons rules out the Kitaev exchange and leaves the Dzyaloshinskii-Moriya exchange to be the only possible candidate [2].

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[1] J. Fransson *et al.*, Phys. Rev. B 94, 075401 (2016)

[2] L. Chen *et al.*, Phys. Rev. X 8, 041028 (2018); L. Chen, *et al.*, *ibid* 11, 031047 (2021)

[3] L. Chen *et al.*, 2D Materials 9, 015006 (2022)

[4] Z. Cai *et al.*, Phys. Rev. B 104, L020402 (2021)

[5] F. Zhu *et al.*, Sci. Adv. 7, eabi7532 (2021)

# Electronic and Magnetic Properties of Fe<sub>3</sub>GeTe<sub>2</sub> at High Magnetic Fields

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Magnetic van-der-Waals (vdW) materials, where planes of magnetic ions are sandwiched between van-der-Waals-bonded chalcogenide layers, are currently a hotbed of research with promising applications for spintronic devices [1]. Amongst them, the itinerant ferromagnet Fe<sub>3</sub>GeTe<sub>2</sub> (FGT) has received particular recent attention, with its high Curie temperature  $T_c = 220$  K and metallic behavior seldom seen in ferromagnetic vdW materials [2, 3]. FGT provides a promising platform to study the fundamental correlations between electronic structure and magnetic properties, as previous studies have shown competing antiferromagnetic interactions, meta-magnetic transitions and a topological Hall effect that may arise due to a skyrmion state [4, 5]. However, the number of high magnetic field studies on FGT is very limited and there is currently no knowledge of the nature of the Fermi surface and charge carriers. We have used pulsed-field magnets to measure the intra-layer magneto-transport properties of FGT up to 60 T. We report a negative linear MR that persists up to 60 T in addition to a complex field, temperature and angle dependence attributed to the electronic structure and anisotropic magnetism. Additionally, we infer further properties of the charge carriers through measurements of the Hall effect.

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[1] D. Duong *et al.*, *ACS Nano* **11**, 11803 (2017).

[2] I. Hwang *et al.*, *J. Phys.: Condens. Matter* **31**, 50LT01 (2019)

[3] H-J. Deiseroth *et al.*, *Eur. J. Inorg. Chem.* **2006**, 1561 (2006)

[4] J. Yi *et al.*, *2D Materials* **4**, 011005 (2016).

[5] Y. Wang *et al.*, *Phys. Rev. B* **96**, 134428 (2017)

# Single Crystal Studies of Charge Density Wave Physics in Quasi-1D Metals $RNiC_2$

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Ternary carbides  $RNiC_2$  ( $R$  = rare earths and Y) crystallize in the non-centrosymmetric orthorhombic  $CeNiC_2$ -type structure, space group  $Amm2$ . These compounds attracted attention, because of various interesting properties such as superconductivity, magnetism, multiple charge density wave (CDW) transitions related to quasi-one-dimensional electronic features of  $RNiC_2$ , and finally, a complex interplay of CDW order and rare earth magnetism in  $RNiC_2$  (see Ref. [1] for a review).

Here, we report on crystal growth, crystallographic characteristics explored via single crystal XRD, as well as magnetic, thermodynamic, and electronic properties studied by a variety of techniques revealing orientation dependent, anisotropic features of selected  $RNiC_2$  single crystals. Based on heat capacity, thermal expansion and electrical resistivity studies, we analyse the nature of multiple CDW transitions occurring in  $RNiC_2$  crystals (e.g., orthorhombic to incommensurate CDW and incommensurate to commensurate CDW transitions). We discuss their relations to electronic and crystal structure changes and, employing Clausius-Clapeyron and generalized Ehrenfest relations, we discuss resulting pressure and strain dependencies of the observed CDW phases.

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[1] V. Babizhetskyy, B. Kotur, V. Levytskyy, H. Michor, Chapter 298: Alloy systems and compounds containing rare earth metals and carbon, in: J.-C.G. Bünzli, V.K. Pecharsky (Eds.), Handbook on the Physics and Chemistry of Rare Earths, Vol. 52, North-Holland, Amsterdam, pp. 1-263. (2017).

## Single-crystal studies of the charge density wave and magnetism in TmNiC<sub>2</sub>

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Non-centrosymmetric, orthorhombic rare-earth nickel dicarbides RNiC<sub>2</sub> (R= rare earth) are a unique system offering an opportunity to tune their ground state with varying the R metal. LaNiC<sub>2</sub> is an unconventional superconductor [1], SmNiC<sub>2</sub> undergoes a ferromagnetic transition [2] and all other compounds, apart from nonmagnetic YNiC<sub>2</sub>, LuNiC<sub>2</sub> and PrNiC<sub>2</sub>, order antiferromagnetically below 25 K [3]. Charge density wave (CDW) formation has been reported for RNiC<sub>2</sub> with R = Pr – Lu and Y [4-6]. Recent investigations revealed an interplay of CDW and magnetic order parameters in several RNiC<sub>2</sub> compounds [2, 5, 7] as well as specific topological features of their electronic band structure [8].

TmNiC<sub>2</sub>, which is subject of this presentation, was reported to exhibit both, antiferromagnetic ordering [9,10] and CDW formation [4]. Recent studies of transport properties suggested the coexistence of CDW order with a field induced, saturated magnetic state [11] which stands in contrast to the rest of the RNiC<sub>2</sub> materials where magnetic order resulted in either a partial suppression of CDW modulations in NdNiC<sub>2</sub> and GdNiC<sub>2</sub> [5, 7] or in a complete suppression of superstructure reflections in SmNiC<sub>2</sub> [2].

Here, we present investigations of CDW and magnetism in single-crystalline TmNiC<sub>2</sub>, which includes a single-crystal X-ray diffraction study of CDW superstructure, isostructural to the commensurate CDW state of LuNiC<sub>2</sub> [12], as well as investigations of thermodynamic, transport and magnetic properties.

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[1] A. D. Hillier, J. Quintanilla, and R. Cywinski, Phys. Rev. Lett. **102**, 117007 (2009).

[2] S. Shimomura *et al.*, Phys. Rev. Lett. **102**, 076404 (2009).

[3] W. Schäfer *et al.*, Journal of Alloys and Compounds **180**, 251 (1992).

[4] M. Roman *et al.*, Phys. Rev. B **99**, 035136 (2018).

[5] S. Shimomura *et al.*, Phys. Rev. B **93**, 165108 (2016).

[6] H. Maeda, R. Kondo, and Y. Nogami, Phys. Rev. B **100**, 104107 (2019).

[7] K. K. Kolincio *et al.*, Phys. Rev. B **94**, 195149 (2016).

[8] R. Ray *et al.*, npj Quantum Materials **7**, 1 (2022).

[9] J. Yakinthos *et al.*, J. Magn. Magn. Mater. **89**, 299 (1990).

[10] Y. Koshikawa *et al.*, J. Magn. Magn. Mater. **179**, 72 (1997).

[11] K. K. Kolincio *et al.*, Phys. Rev. Lett. **125**, 176601 (2020).

[12] S. Steiner *et al.*, Phys. Rev. B **97**, 205115 (2018).

# Understanding the electronic structure of MoS<sub>2</sub>: Effect of chemical exfoliation and mechanical strain

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Polymorphism of 2D molybdenum disulphide (MoS<sub>2</sub>) with distinctly different electronic properties for different phases makes it a fundamentally interesting and technologically promising material. Chemical exfoliation of MoS<sub>2</sub> into few-layers form by Li-ion intercalation and applying a compressive strain on a monolayer of MoS<sub>2</sub> by stacking it between layers of other 2D materials such as graphene and boron nitride forming heterostructures, are two popular ways of tuning electronic properties of MoS<sub>2</sub>, where such metastable polymorphic forms are believed to play important roles [1,2]. However, the specific metastable phases and their electronic properties in each case have remained controversial [3]. Using spatially resolved photoelectron spectroscopy with ~120 nm resolution, complemented by micro-Raman experiments, we investigated the chemically exfoliated and mechanically strained MoS<sub>2</sub> samples. These results reveal that for chemically exfoliated MoS<sub>2</sub> samples, dominant metastable state is a distorted T' state with a small semiconducting gap [4]. Investigating two such samples with different extents of Li-residues present, we establish that Li-ions not only help to exfoliate MoS<sub>2</sub> into few-layer 2D forms but also contribute to enhancing the relative stability of the metastable state by doping the system with electrons, giving rise to a lightly doped conducting MoS<sub>2</sub> with the T' structure [5]. For the mechanically strained system, we establish that the compressive strain on the MoS<sub>2</sub> monolayer does not drive any structural phase transition. The graphene layer on MoS<sub>2</sub> only makes the system more electron-rich due to the hybridization between graphene and sulphur defect states in MoS<sub>2</sub>, thereby altering its transport properties significantly.

[1] G. Eda *et. al.*, Nano Lett. **11**, 5111 (2011)

[2] K. He *et. al.*, Nano Lett. **13**, 2931 (2013)

[3] D. Pariari and D. D. Sarma, APL Mater. **4**, 040909 (2020)

[4] B. Pal *et. al.*, Phys. Rev. B **96**, 195426 (2017)

[5] D. Pariari *et. al.*, Appl. Mater. Today **19**, 100544 (2020)

# First-principles study of intercalated transition metal dichalcogenides

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Recently, various interesting properties have been observed by inserting metallic elements between the layers of transition metal dichalcogenides (TMDs) and have been intensively studied. The various magnetic properties like noncollinear magnetism [1,2] and the anomalous Hall effect [3] are of practical importance, as they have been suggested to be applied to spintronics devices. Although there have been many studies of experimentally synthesized individual materials, systematic studies including those that have not been synthesized have been highly desired [4,5].

In our research, we performed first-principles calculations on a total of 48 materials with different composition ratios and intercalated transition metals and investigated their magnetic properties. The results were used to calculate the energy dependence of the exchange constants by the Liechtenstein formula [6]. In the Liechtenstein formula, the effective interaction ( $J_0$ ) is estimated by rotating a spin from the ferromagnetic state. Figure-1 shows Fermi level ( $E_F$ ) dependence of  $J_0$  in  $\text{CrNb}_3\text{S}_6$  and we estimate those of other elements simply by shifting the  $E_F$  for other elements. In our presentation, we discuss the origin of stable magnetic order and material dependence by comparing  $E_F$  dependence of  $J_0$  in other materials.

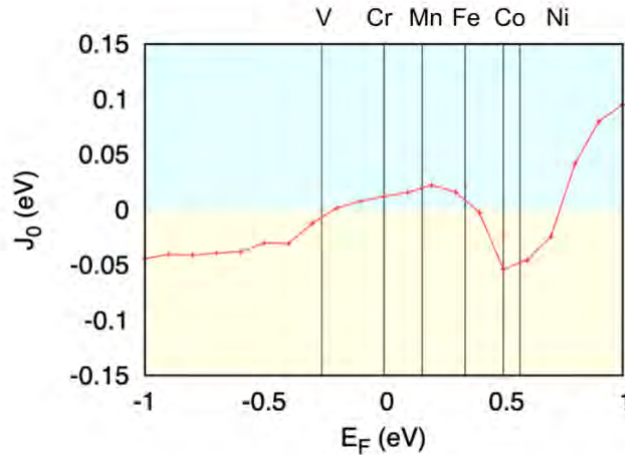


Figure 1:  $E_F$  dependence of the  $J_0$  of  $\text{MNb}_3\text{S}_6$  ( $M=\text{V, Cr, Mn, Fe, Co, Ni}$ )

- [1] Y. Togawa et al., Phys. Rev. Lett. 108, 107202 (2012)
- [2] H. Y. Lv et al., Phys. Rev. B 92, 214419 (2015)
- [3] Smejkal L, Gonzalez-Hernández R, Jungwirth T, Sinova J. Sci. Adv. 2020;6:eaaz8809.
- [4] H.Park et al , arXiv:2110.03029 [cond-mat.mtrl-sci]
- [5] O. Heinonen *et al* , arXiv:2109.13837v2 [cond-mat.mtrl-sci]
- [6] T.Nomoto *et al*, Phys. Rev. B 102, 014444 (2020)

# Signatures of Correlated Quantum Transport in Spintronic Heterostructures

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Spin current generation and detection have become the most intriguing areas of research in spintronics. Spin current generated through spin-Hall magnetoresistance (SMR) technique has been proved as a tool to probe the interfacial magnetic ordering in a Metal/Magnetic Insulator (MI) heterostructures, which otherwise requires sophisticated synchrotron facilities [1]. Strongly correlated oxides exhibit a plethora of exotic properties from unconventional superconductivity to existence of topological phases due to their strong interplay between the strong SOC ( $\zeta_{SO}$ ) and other interactions like the crystal field ( $\Delta$ ) and the electron correlation ( $U$ ), due to their comparable energy scales in these materials [2]. SrIrO<sub>3</sub> (SIO) has become one of the interesting perovskite compounds due to the high spin-orbit coupling and metallicity in Ruddlesden Popper series [3].

We explored the correlated quantum transport in 3d-5d heterojunctions comprising of the Dirac semi-metal, SrIrO<sub>3</sub> (SIO) as the spin transport layer and a topotactic oxide, SrCoO<sub>2.5</sub> (SCO) as the antiferromagnetic layer. SIO-SCO interfaces were fabricated by pulsed laser deposition on SrTiO<sub>3</sub> (STO) and LaAlO<sub>3</sub> (LAO) substrates to investigate the strain tuned spin transport behaviour and the underlying fundamental interactions. Transport characteristics revealed temperature dependent localization length, strain dependent electron-electron interactions and electron-boson scattering mechanisms. Further, the magnetoconductance data was fitted to well-known Hikami-Larkin-Nagaoka (HLN) equation to elucidate the transport mechanism. This work is a pragmatic approach towards realization of high-performance all-oxide spintronic circuits and sensors.

1. Frances Hellman et al. Reviews of Modern Physics 89, (2017)
2. Kondo, Takeshi, M. Nakayama, R. Chen, J. J. Ishikawa, E-G. Moon, T. Yamamoto, Y. Ota et al, *Nature communications* 6 (2015): 10042.
3. Tokiwa, Y., Ishikawa, J. J., Nakatsuji, S. & Gegenwart, P. Quantum criticality in a metallic spin liquid. *Nat. Mater.* 13, 356–359 (2014).



## Interplay of weak localization and magnetism in strongly correlated $\text{PrCo}_{0.5}\text{Ni}_{0.5}\text{O}_3$ thin films grown on $\text{SrTiO}_3$ substrates

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Strongly correlated oxides materials such as rare-earth metal oxides host a wide range of exotic properties including metal-insulator transitions, superconductivity and different topological phases. Metal-insulator transitions associated with complex antiferromagnetic ordering are observed in rare-earth nickel perovskites ( $\text{RNiO}_3$ ) [1]. Temperature dependent spin state excitations in rare earth cobalt oxides ( $\text{RCoO}_3$ ) [2] are equally intriguing as it traverses through the non-magnetic low spin to intermediate spin and then to high spin states with increase in temperature. These two systems combined exhibit spin glass behavior as in  $\text{PrCo}_{1-x}\text{Ni}_x\text{O}_3$  [3]. Further, when the dimensionality of these systems is reduced from bulk to ultrathin films, confinement and strain effects come into picture and further enhance the correlation among these electronic systems [4]. Here, we investigate the magnetic and transport properties of epitaxially grown thin films of  $\text{PrCo}_{0.5}\text{Ni}_{0.5}\text{O}_3$  on  $\text{SrTiO}_3$  substrate and studied the evolution of the spin states and electronic transport properties.  $\text{PrCo}_{0.5}\text{Ni}_{0.5}\text{O}_3$  favours a ferromagnetic ordering below 20 K which was evident from magnetization measurements. Strong electron correlation is observed in the temperature dependent electronic transport measurements where the electronic conduction follows Efros-Shklovskii type variable range hopping mechanism at low temperatures. An interplay of weak localization effects and ferromagnetism owing to strain and valence state modification will be discussed in detail.

[1] Sreedhar, K., *et al.* Phys. Rev. B **46**.10, 6382 (1992).

[2] Naiman, C. S., *et al.* J. Appl. Phys. **36**.3 1044-1045 (1965).

[3] P. Tomeš *et al.*, J. Phys. D. Appl. Phys. **44**, 305402 (2011).

[4] Millis, A. J., T. Darling, and A. Migliori. J. Appl. Phys. **83**.3, 1588-1591 (1998).

# Coexisting charge density wave and magnetic instabilities in monolayer InSe and Pb/Si(111) systems

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Coulomb interaction in two dimensions (2D) is often weakly-screened and long-ranged. The on-site Coulomb repulsion is usually responsible for the formation of magnetic fluctuations. At the same time, the strong non-local interaction may drive the system towards a charge density wave (CDW) instability. In this talk, I will discuss two particular examples of materials, where both these instabilities are present simultaneously. I will show that according to our theoretical predictions the monolayer InSe should exhibit a commensurate CDW ordering in a broad range of doping levels and temperatures [1]. Inside the CDW phase the considered system is expected to display a tendency to a ferromagnetic ordering. A similar physical picture can be found in a system of Pb adatoms disposed periodically onto a Si(111) surface. There, scanning tunneling microscopy and spectroscopy experiments observe a chiral spin texture in the CDW phase [2]. Investigating the phase diagram of this effective 2D system in the framework of the advanced many-body theoretical method allows us to reproduce this experimental result [3]. In addition, we illustrate that upon doping of the system the chiral spin texture changes from a row-wise-like to an antiferromagnetic-like structure. Moreover, we find that the CDW phase also consists of two types of orderings that are realized by means of a structural and a dynamical phase transitions, respectively.

[1] E. A. Stepanov, V. Harkov, M. Rösner, A. I. Lichtenstein, M. I. Katsnelson, A. N. Rudenko, arXiv:2107.01132 / to appear in npj Comput. Mater. (2022);

[2] C. Tresca *et al.*, Phys. Rev. Lett. **120**, 196402 (2018);

[3] M. Vandelli, A. Galler, A. Rubio, A. I. Lichtenstein, S. Biermann, E. A. Stepanov, to be published;

## Magnetism in strongly correlated twisted bilayers from first principles

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Twisted bilayer structures of van der Waals materials attract experimental and theoretical interest because of easy single layer exfoliation and processing and a variety of correlated states.<sup>1,2</sup> Magnetic twisted bilayers hosting skyrmions have recently been demonstrated.<sup>3</sup> Within first-principles approach, large supercells and tight convergence are required to compute magnetic interactions. Here we combine DFT and model simulations of Wannier function based tight-binding Hamiltonian to study the states in the twisted bilayer of CrI<sub>3</sub>.

\*This work is supported by the Program Committee.

[1] Xu *et al.*, Nature Nanotechnology **17**, 143–147 (2022)

[2] N. Sivadas., Nano Lett. **18**, 7658–7664 (2018)

[3] Shang *et al.*, ACS Appl. Nano Mater. **3**, 1282–1288 (2020)

# Pressure-induced structural phase transitions in 2D van der Waals material NiPS<sub>3</sub>

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The family of insulating antiferromagnets  $MPS_3$  ( $M = Ni, Fe, Mn$ ) at ambient pressure share a quasi-two-dimensional layered structure, with layers held together by van der Waals interactions. The interlayer spacing is an important component in the 2D nature of  $MPS_3$ . The application of hydrostatic pressure is a powerful tool for dimensionality control through the reduction of this interlayer spacing. High-pressure experiments with  $FePS_3$  have found two structural phase transitions, the second of which coincides with an insulator to metal transition [1]. Preliminary data and results reported by other groups suggest that  $NiPS_3$  goes through similar pressure-induced structural and insulator-metal transitions, but no consensus exists on what structures this material takes on nor at what pressure [2–4].

We use a combination of x-ray diffraction and theoretical predictions to characterize the structural phase transitions of  $NiPS_3$ . We observe up to two structural phase transitions in our x-ray diffraction data. At 10 GPa we observe sliding between layers with no change in the space group, and we are analyzing the possibility of a transition at 26 GPa. Further analysis is required to find the correct crystal structure of  $NiPS_3$  above 26 GPa.

We are also carrying out a series of density functional theory structural optimizations while increasing and decreasing pressure to confirm proposed structures or discover candidate structures. We are using our proposed structures as well as structures reported by other groups as starting points for these calculations. Finally, we will attempt to validate these proposed structures using diffraction data.

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[1] M. J. Coak et al., *Phys. Rev. X* **11**, 011024 (2021).

[2] X. Ma et al., *Sci. China Phys. Mech. Astron.* **64**, 297011 (2021).

[3] H. Cui et al., *Phys. Rev. Mater.* **5**, 124008 (2021).

[4] T. Matsuoka et al., *J. Phys. Soc. Jpn.* **90**, 124706 (2021).

# Atomic adsorbate identifying a correlated Mott insulator

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The Mott insulator is driven by strong electron-electron correlation in a half-filled metallic band. This correlated insulator is identified by the existence of an energy gap against the theoretical prediction of a gapless metallic state without considering the correlation [1]. However, the direct experimental way to identify the half-filled state in insulators has been missing, which sometimes causes a long debate in the origin of an insulator [2,3]. In this presentation, we show a simple and unambiguous experimental way to identify the Mott insulating state. We used scanning tunneling microscopy and observed two distinct insulating states with different energy gaps on a layered van der Waals material 1T-TaS<sub>2</sub> surface at low temperature, depending on the interlayer stacking of the surface layer. We deposited single-valent potassium (K) atoms on the surface and observed their distinguished adsorption behaviors on different insulating layers. Furthermore, the adsorbates have totally different effects in electronic states of the surface layer. On one insulating state, an extra electron from each K adatom is highly localized at its adsorption site and kills the empty state, while on the other insulating state, electrons from K adatoms are delocalized and induce the global doping. This can be straightforwardly understood from the fundamental difference between the Mott and band insulators: half-filled and full-filled electronic states, respectively. This work not only clarifies the dispute about the origin of the ground state in 1T-TaS<sub>2</sub> but also provides an atomic adsorbate as a simple and unambiguous Mott identifier.

[1] N. F. Mott, *Rev. Mod. Phys.* **40**, 677 (1968).

[2] P. Fazekas and E. Tosatti, *Philos. Mag. B* **39**, 229 (1979).

[3] T. Ritschel *et al.*, *Nat. Phys.* **11**, 328 (2015).

# Magnetic, electronic, and structural investigation of the strongly correlated $\text{Sm}_{1-x}\text{Y}_x\text{Co}_5$ system

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The investigation of hard magnets continues to be of enormous interest due to numerous high-tech applications where  $\text{SmCo}_5$  remains as one of the highest-performance hard magnets. The  $\text{YCo}_5$  compound is isostructural with the  $\text{SmCo}_5$  and it has a sufficiently high magnetocrystalline anisotropy to render the  $(\text{Sm},\text{Y})\text{Co}_5$  alloy [1,2] as an excellent candidate for a nanostructured permanent magnet.

Here we report a study of the effect of Y substitution for Sm in  $\text{Sm}_{1-x}\text{Y}_x\text{Co}_5$  ( $x=0.6, 0.7, 0.8, 0.9,$  and  $1$ ) on magnetic, electric, and structural properties. The X-ray diffraction (XRD) analysis reveals that the microstructure and single phase in  $\text{Sm}_{1-x}\text{Y}_x\text{Co}_5$  depends on the combination of heat treatment, quenching, and mechanical milling processes, setting a benchmark for the realization of pristine samples. In addition, electrical transport and magnetization measurements show an interplay between spin-density wave and Fermi-liquid behaviours to drive  $\text{Sm}_{1-x}\text{Y}_x\text{Co}_5$  system to a putative magnetic instability, a situation that recalls the competition between localized and itinerant  $f$ -electrons.

F. Passos acknowledges FAPESP grant process 2019/24711-0, J. L. J. and V. M. acknowledge FAPESP-Young Investigator Grants 2018/08845-3 and 2018/19420-3.

[1] M. Sakurai *et al.*, Phys. Rev. Materials **2**, 084410 (2018).

[2] P. Tozman *et al.*, AIP Advances **6**, 056016 (2016).

# Magnetic properties of a multicomponent intermetallic compound $Tb_{0.25}Dy_{0.25}Ho_{0.25}Er_{0.25}Al_2$

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Reports on multicomponent and high entropy alloys have motivated us to study the magnetic properties of a multicomponent  $RA_2$  system where R site is occupied by four equiatomic heavy rare earth elements. A polycrystalline multicomponent Laves phase intermetallic compound  $Tb_{0.25}Dy_{0.25}Ho_{0.25}Er_{0.25}Al_2$  has been synthesized by arc melting method and characterized using powder X-ray diffraction and magnetization experiments. The sample crystallizes in cubic structure with space group  $Fd\bar{3}m$  (MgCu<sub>2</sub>-type) and is found to be in single phase. The compound  $Tb_{0.25}Dy_{0.25}Ho_{0.25}Er_{0.25}Al_2$  undergoes paramagnetic to ferromagnetic transition around 50 K ( $T_C$ ), which is almost equal to the average of ferromagnetic ordering temperatures of individual  $RA_2$  (R= Tb, Dy, Ho, Er) compounds. Similar behaviour has been also observed for five-component Laves phase intermetallic compound  $Gd_{0.2}Tb_{0.2}Dy_{0.2}Ho_{0.2}Er_{0.2}Al_2$  [1]. Magnetization as a function of the field at a temperature of 15 K behaves like a soft ferromagnet and heat capacity in zero field shows a  $\lambda$ -type transition around  $T_C$  indicating its second order nature. Having multiple equiatomic rare earth elements at the rare earth site and obtaining single  $T_C$  suggests possible cooperative ordering rare earth moments in this multicomponent system. Since the multicomponent  $Tb_{0.25}Dy_{0.25}Ho_{0.25}Er_{0.25}Al_2$  is expected to have interesting magnetocaloric effect, we plan to study the magnetocaloric properties of the sample near the ferromagnetic transition.

[1] P. K. Jesla, J. Arout Chelvane, A. V. Morozkin, A. K. Nigam and R. Nirmala, IEEE Transactions on Magnetics **58**, 1 (2021).

## **Possible high temperature superconducting transitions in bulk twisted graphite**

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We have de-intercalated by soft chemistry at room temperature samples of  $KC_8$ . X-rays studies show mainly a  $KC_{72}$  structure, with orientational disorder. The six AB slabs have facing AA separations twisted at variable angles, certainly including "magic angles". The K atoms show only short-range order, implying a variable local doping. Thus the samples presumably scan both angles and dopings. Magnetization measurements show a ferromagnetic response at high temperature with  $T_0=420K$ . Tiny but clearly measurable transitions to diamagnetic states at  $T_c=110K$ ,  $T_c=240K$  and  $T_c=320K$  are observed. For all the transitions, we obtain at  $T < T_c$  diamagnetic hysteresis cycles similar to superconducting ones that decrease in size as the temperature increases, disappearing at  $T_c$ . For the 240K transition we observe a sharp 90% drop in the electrical resistance that shifts to lower temperatures under magnetic field, with an estimated critical field at zero temperature  $\sim 1000T$ . Reproducible measurements have been obtained for a dozen different preparations. Within a Moiré superconducting hypothesis it is obvious that a very small number of crystallites will have the magic angles, and that the volume of both the eventual superconductivity and ferromagnetism will be tiny. Thus more work is necessary to increase their fraction and confirm the existence of superconductivity in bulk twisted graphite.



# Exploration in new room temperature magnetocaloric materials: structure and magnetocaloric properties in $Mn_5(Si,P)B_2$ compounds

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The  $M_5XB_2$  materials system has been widely studied as permanent magnetic materials [1,2]. As permanent magnetic materials, their coercivity and magnetic energy product are lower than those of the mainstream permanent magnetic materials. Xie *et al.*[3] and Cedervall *et al.*[4] proposed that the  $Mn_5PB_2$  and  $(Fe_{1-x}Co_x)_5PB_2$  compounds have the prospect of being applied as magnetocaloric materials due to their near room temperature Curie temperature. In this work, the structure and magnetocaloric properties of the  $Mn_5(SiP)B_2$  compounds of the  $M_5XB_2$  material system were studied. According to a refinement of the XRD data the  $Mn_5(Si_{1-x}P_x)B_2$  compounds all crystallize in the  $Cr_5B_3$ -type body-centered tetragonal structure, with a small amount of  $Mn_2P$  as a secondary phase (less than 7%). The lattice parameters and the unit-cell volume of the compounds change linearly with the increase in P content. These experimental results are consistent with calculated DFT results. The Curie temperature of the compounds can continuously be adjusted between 305 and 411 K by changing the Si/P ratio. The introduction of P also caused a decrease in saturation magnetization. The magnetic phase transition of these compounds was determined using Arrot plots and the field exponent  $n$  for the magnetic entropy change based on Landau's theory. The studied compounds all show a second-order magnetic phase transition. Since the compounds show a second-order phase transition, the magnetic entropy change caused by the phase transition was not large: 1.9 and 1.4 J/kgK for  $Mn_5SiB_2$  and  $Mn_5PB_2$ , respectively. However, the advantage of this series of compounds is that the Curie temperature can be adjusted continuously around room temperature.

Keywords: magnetocaloric effect, magnetic phase transition, Curie temperature,  $Mn_5(Si,P)B_2$

References:

1. M. Kasaya, Sci. Rep. Tohoku Univ. LVIII (Supp. 2/37) (1975)
2. R. Wäppling, *et al.* J. Phys. Supp. 12/37 (1976) (C6-591-593)
3. Z. G. Xie *et al.* Appl. Phys. Lett. 97, 202504 (2010)
4. J. Cedervall. *et al.* Inorg. Chem. 57, 777–784(2018)

# Effects of Lead sulfate doping on the formation and superconducting properties of $(\text{Bi}_{2-x}\text{Pb}_x)\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_z$ superconductors

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The effects of Lead sulfate ( $\text{PbSO}_4$ ) doping on the formation and superconducting properties of  $(\text{Bi}_{2-x}\text{Pb}_x)\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_z$  ( $x = 0.3, 0.4$ ) samples prepared by using the solid-state reaction method were investigated. The samples were characterized by X-ray diffraction, levitation force density and resistivity measurements. X-ray diffraction patterns showed that the lead sulfate doping improved the formation the 2223 phase compared to that of the samples used  $\text{PbO}$  as the source of  $\text{Pb}$ . This results were accompanied by the increase in the levitation force density at liquid nitrogen temperature, although the transition temperature was nearly unchanged. The effects of different sources of lead/sulfur will be also dicussed.

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# Solid-state refrigeration with enormous heat absorption to less than 120 mK: Application of metallic magnetocaloric

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Adiabatic demagnetisation refrigeration (ADR) is an elegant approach to realise cryogenic systems without using depleting resources, being space-hungry or difficult to maintain. To overcome drawbacks associated with conventional refrigerants used in sub-Kelvin ADR, we have identified a new metallic magnetocaloric and designed a module to demonstrate its cooling properties. The functional phase of YbNi<sub>1.6</sub>Sn allows ADR from 1.8 K down to below 120 mK together with extraordinarily large heat absorption, meaning a substantial hold time even under high heat loads. Our set-up proves YbNi<sub>1.6</sub>Sn to be ideally suited for miniaturisation, providing powerful but energy-efficient and cryogen-free low-temperature platforms. Its use might be extended into the 10 mK range by combining it with paramagnetic salts, the recently discovered frustrated magnet KBaYb(BO<sub>3</sub>)<sub>2</sub> or a PrNi<sub>5</sub> nuclear demagnetisation stage within a dual system [1, 2].

The favourable cooling properties of YbNi<sub>1.6</sub>Sn as well as of some other metallic magnetocalorics indicate that these systems can display extreme local moment behaviour. They combine ultra-weak exchange interactions with good metallic conductivity and would in the classic Kondo lattice phase diagram be located to the far left, local moment side of the *magnetic dome*. This interpretation contrasts completely with earlier attempts to find good metallic magnetocalorics near magnetic quantum critical points. We discuss selection principles for metallic magnetocaloric materials based on relevant interactions and show that previously neglected areas in the generalised phase diagram of Kondo lattice materials suddenly become attractive for identifying optimal cooling materials.

[1] F. Pobell, *Matter and Methods at Low Temperatures* (2007), 3<sup>rd</sup> ed.

[2] Y. Tokiwa *et al.*, *Communications Materials* **2**, 42 (2021).

## Thermal Expansion and Magnetostriction of GdTe<sub>3</sub>

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Magnetic vdW layered materials are potential platforms for applications in heterostructures, spintronics, twistrionics and more. The family of rare-earth tritellurides (RTe<sub>3</sub>) consists of square net tellurium sheets, with vdW gaps, and rare earth - tellurium slabs [1]. The whole family hosts an incommensurate charge density wave phase and, with substitutions of some rare earth atoms (Gd, Tb, Dy), this structure hosts superconductivity under hydrostatic pressure.

The thermal expansion and magnetostriction are useful probes to map phase transitions over a phase diagram in temperature and field. These measurements are performed in a capacitive dilatometry setup suitable for high magnetic fields. The compound GdTe<sub>3</sub> has the highest carrier mobility of any magnetic vdW layered material [1].

The uniaxial expansion of this material is used to identify three magnetic transitions in the thermal expansion, at zero field two Neel transitions at 11.3 K and 9.8 K and another magnetic transition at 6.8 K. In the magnetostriction experiments up to 30 T and down to 1.3 K, a transition occurs around 17 T before the onset of quantum oscillations.

With the use of uniaxial stress up to 15 MPa these phenomena are further explored and discussed in the context of new high field experiments using the novel technique of stress dilatometry [2].

[1] S. Lei et al., Science Advances 6, eaay6407 (2020).

[2] R. Kuechler et al., Rev. Sci. Inst. 87, 073903 (2016).