KOND

Tuesday, 05.09.2023, Room Aula 033

Time	ID	KOND I: (Thermal) Transport in 2D systems *Chair: Ilaria Zardo, Universität Basel*
14:00	101	**Modern theory of thermal transport in solids** *Michele Simoncelli *, Nicola Marzari* *Theory and Simulation of Materials (THEOS) and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne* **Current address: Theory of Condensed Matter Group of the Cavendish Laboratory, University of Cambridge (UK)* We explore the atomistic mechanisms of thermal transport in solids, extending established formulations and developing the computational framework to solve them. Starting from a density-matrix formalism, we show how the phonon Boltzmann equation is missing a tunneling term that becomes pivotal in disordered or defective materials. Thus, we derive a unified 'Wigner formulation' that comprehensively describes heat conduction in crystals, glasses, and intermediate cases such as thermoelectrics. Also, we show how in crystalline conductors the microscopic transport equations can be coarse grained into a set of viscous heat equations that describe both Fourier diffusion and heat hydrodynamics; thus, we employ these to rationalize pioneering experiments, and to devise strategies to amplify and control heat hydrodynamics.
14:30	102	**Thermodynamic transport fingerprints in Twisted monolayer-bilayer graphene** *Jin Jiang [1], Sheng Chen [1], Zekang Zhou [1], Kenji Watanabe [2], Takashi Taniguchi [3], Mitali Banerjee [1]* *[1] Laboratory of Quantum Physics (LQP), Institute of Physics, EPFL, CH-1015 Lausanne* *[2] Research Center for Functional Materials, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan* *[3] International Center for Materials Nanoarchitectonics, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan* Twisted monolayer-bilayer graphene (TMBG) exhibits renormalized nearly flat bands harboring various exotic physical phenomena. Stacking an additional monolayer graphene on the TMBG paves a new way to extract single particle bandgap, the charge neutrality point (CNP) gap and bandwidth. The Dirac cone in the decoupled monolayer graphene serves as a perfect chemical potential sensor when the Landau levels (LLs) cross the bands, whereas the LLs are well separated and are not hybridized with flat bands. At D = 0.53 V /nm, the isospin flavor symmetry-broken correlated gap at flat-band filling v = 1 is largest and bandwidth is narrowest. This is a versatile tool which can be used in various similar systems to find thermodynamic properties.
14:45	103	**Electronic Poiseuille Flow in Hexagonal Boron Nitride Encapsulated Graphene FETs** *Tathagata Paul, Wenhao Huang, Mickael L. Perrin, Michel Calame, EMPA* In most conductors, diffusive scattering from defects and lattice vibrations results in Ohmic transport. Alternatively, transport is ballistic, when the channel dimensions are the smallest length scale. However, when electron-electron interactions are sufficiently strong, charge transport can mimic the viscous flow of fluids. In the current work, we explore this analogy and observe that the electrical signatures of viscous effects, characterized by measuring the differential resistance as a function of channel width and effective electron temperature, survives close to room temperature. Our findings open up new directions for designing devices exploiting viscous charge flow such as geometric rectifiers like a Tesla valve and charge amplifiers based on electronic Venturi effect.

15:00	**104**	**Dipole charge density ordering in bilayer semiconductors** *Joel Hutchinson, Jelena Klinovaja, Daniel Loss, Dmitry Miserev, University of Basel* Advances in the manipulation of van der Waals materials have shown that bilayers offer a unique platform for studying strongly correlated physics in two-dimensions (2D). Bilayers are importantly different from monolayers in that there exist long-range interactions between electrons in both the intra- and inter-layer channels, which differ only slightly. We show that the electronic charge susceptibility has peaks arising from scattering across the Fermi surfaces, not seen in the usual Lindhard function. In a bilayer system, these peaks give rise to an enhanced response of out-of-plane dipoles to local potential differences across the layers. This response is not diminished by screening and becomes larger in the low-density limit.
15:15	**105**	**Probing the electronic structure of chemically-induced van der Waals heterostructures in V_xTaS_2** *Wojciech Pudelko [1], Eduardo Bonini Guedes [1], Johan Chang [2], Ron Cohn-Wagner [2], Julia Küspert [2], Hang Li [1], Huanlong Liu [2], Francesco Petocchi [3], Nicholas Clark Plumb [1], Andreas Schilling [2], Philipp Werner [3], Karin von Arx [2]* *[1] Paul Scherrer Institut* *[2] Physik-Institut, Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich* *[3] University of Fribourg* Layered transition metal dichalcogenides exhibit numerous exotic electronic phases, which are known to be highly sensitive to minute changes in virtually any external parameter. We found that vanadium intercalation into the TaS_2 (V_xTaS_2) leads to intriguing changes in its properties. Upon increasing x, the electronic structure evolves from the pure 2H phase known for its charge density wave (CDW) and superconductivity to a pure 1T structure characterized by CDW and Mott interactions, with a clear coexistence of both at intermediate range. By exploiting V intercalation as a means to assemble 2H/1T layered heterostructures, we are granted a spectroscopic window into each layer type, as well as the interplay between them.
15:30	**106**	**Understanding pairing mechanism in magic angle twisted trilayer graphene** *Zekang Zhou [1], Jin Jiang [1], Kenji Watanabe [2], Takashi Taniguchi [3], Mitali Banerjee [1]* *[1] Laboratory of Quantum Physics (LQP), Institute of Physics, EPFL, CH-1015 Lausanne* *[2] Research Center for Functional Materials, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan* *[3] International Center for Materials Nanoarchitectonics, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan* Flat bands in twisted graphene systems offers plethora of strongly correlated states, among these, correlated insulator, superconductor and chern insulator are to name of few. Twisted trilayer graphene has shown robust superconductivity which drastically deviates from conventional weak-coupling BCS type superconductivity. In particular, twisted trilayer graphene may even host prag- matic example of strong coupling superconductivity – BEC type superconductivity. A full understanding of such superconductivity still needs more experimental works. In this talk, I will present our transport data of magic angle twisted trilayer graphene and highlight its unconventional nature.

15:45	**107**	**Origin and nature of defect states coupled to a van der Waals superconductor** *Paritosh Karnatak [1], Zarina Mingazheva [1], Kenji Watanabe [2], Takashi Taniguchi [3], Helmuth Berger [4], László Forró [4], Christian Schönenberger [1]* *[1] Department of Physics, University of Basel, CH-4056 Basel* *[2] Research Center for Functional Materials, National Institute for Material Science, 1-1 Namiki, Tsukuba 305-0044, Japan* *[3] International Center for Materials Nanoarchitectonics, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan* *[4] Institute of Condensed Matter Physics, EPFL, CH-1015 Lausanne* We perform tunnel spectroscopy on $NbSe_2$ by utilizing MoS_2 or hexagonal Boron Nitride (hBN) as a tunnel barrier. We observe subgap excitations and probe their origin by studying various heterostructure designs. We show that the edge of $NbSe_2$ hosts many defect states. By isolating the $NbSe_2$ edge and comparing MoS_2 and hBN tunnel barriers, we suggest defects in MoS_2 as the origin of the subgap features. We study the evolution of the subgap excitations and reveal both singlet and doublet type ground states, which indicates a competition of various energy scales. Based on nearly vanishing g-factors or avoided-crossing of subgap excitations we also highlight the role of strong spin-orbit coupling.
16:00	**108**	**Fabry-Perot interferometry in bi-layer graphene** *Mario Di Luca [1], Kenji Watanabe [2], Takashi Taniguchi [3], Mitali Banerjee [1]* *[1] Laboratory of Quantum Physics (LQP), Institute of Physics, EPFL, CH-1015 Lausanne* *[2] Research Center for Functional Materials, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan* *[3] International Center for Materials Nanoarchitectonics, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan* In solid-state systems, strong correlations cause the emergence of quasiparticles that are immune to local environmental perturbations. An example of such a system is the Quantum Hall Effect, in which electrons confined in two dimensions and subjected to a high perpendicular magnetic field give rise to fractionally charged quasiparticles (anyons) that are topologically protected. The statistics of anyons can be studied by interferometry techniques. To study the statistical behavior of anyons we use bilayer graphene in Fabry-Perot interferometer geometry. In this paper I will describe the techniques used in the fabrication process and some interferometry results.
16:15	**109**	**In-situ buried interface passivation enables efficient and stable inverted perovskite solar modules** *Virginia Carnevali, Lin Li, Mingyang Wei, Nikolaos Lempesis, Lorenzo Agosta, Mathias Dankl, Ursula Roethlisberger, Michael Graetzel, EPFL* Scaling-up perovskite solar cells (PSCs) is a prerequisite to the adoption of perovskite photovoltaics. However, the performance and stability of perovskite solar modules (PSMs) have lagged behind those of lab-scale PSCs. The development o PSMs requires interfacial passivation, yet this is challenging for the buried interface, owing to the dissolution of passivation agents during perovskite deposition. Here, we overcome this limitation with in-situ buried interface passivation – achieved via directly adding a cyanoacrylic acid-based molecular additive into the perovskite precursor solution. The preferential buried interface passivation results in facilitated hole transfer and suppressed surface recombination. We report a power-conversion efficiency (PCE) of 20.3% for inverted-structure PSMs.
16:30		***Coffee Break***

Time	ID	**KOND II: Cuprates** *Chair: Henrik Rønnow, EPF Lausanne*
17:00	**111**	**Uniaxial Control of Quantum Matter. Application to Cuprates** *Gediminas Simutis, Paul Scherrer Institut, 5232 Villigen PSI* Quantum matter is characterised by competing and intertwined orders. Here we will present our recent advances in using uniaxial pressure as a clean "surgical" tool to tune quantum phases while simultaneously obtaining microscopic insights via scattering experiments. To achieve the fine-tuning, we have designed a new in-situ uniaxial device for large-scale facility research based on an actuator-motor mechanism, efficient feedback loops and the sample-holder design enabling rapid exchange of the samples. I will demonstrate the advanced capabilities of this device by reporting the control of charge and structural degrees of freedom in an archetypical cuprate.
17:15	**112**	**A strong-coupling mechanism for the pseudogap from spin fluctuations** *Friedrich Krien, Patrick Chalupa-Gantner, Karsten Held, Alessandro Toschi, Paul Worm, TU Wien* The mechanism of the pseudogap observed in hole-doped cuprates remains one of the central puzzles in condensed matter physics. We analyze this phenomenon via a Feynman-diagrammatic inspection of the Hubbard model. Our approach captures the pivotal interplay between Mott localization and Fermi surface topology *beyond* weak-coupling spin fluctuations. Our analysis naturally explains puzzling features of the pseudogap observed in experiments, such as Fermi arcs being cut off at the antiferromagnetic zone boundary and the subordinate role of hot spots.
17:30	**113**	**Investigating the periodic electronic modulations in $Bi_2Sr_2Ca_1Cu_2O_{8+\delta}$ by Scanning Tunneling Microscopy** *Tejas Parasram Singar [1], Genda Gu [2], Ivan Maggio-Aprile [1], Christoph Renner [1]* *[1] University of Geneva, [2] CMPMS Division, Brookhaven National Laboratory* In this work, we will discuss our latest investigations of the $Bi_2Sr_2Ca_1Cu_2O_{8+\delta}$ cuprate superconductor using Scanning Tunneling Microscopy (STM). We focus on the atomic scale periodic charge modulations as a function of doping and magnetic field. Specifically, we try to address the nature and origin of the $4a_0 \times 4a_0$ and $(4/3)a_0 \times (4/3)a_0$ modulations (a_0: crystallographic unit cell) using different acquisition modes of STM. The periodic conductance modulations we observe do not reveal the characteristic features usually associated with charge density waves in STM experiments, suggesting they are rather quasiparticle interferences.
17:45	**114**	**High-T_c cuprates – story of two electronic subsystems** *Neven Barisic, TU Wien, Austria & PMF Zagreb, Croatia* Based on now well-established universal transport and optical conductivity properties, we show that the phenomenology of cuprates across the phase diagram is fully captured by the charge conservation relation: $1 + p = n_{loc} + n_{eff}$ with the superfluid density that simply corresponds to: $\rho_S = n_{eff} \cdot (O_S \cdot n_{loc})$ where p is doping, n_{eff} is the carrier density, which can be directly determined experimentally, while O_S is a compound-dependent constant. We attribute the distinction between low- and high-T_c cuprates to the fine-tuning of the p–d–p fluctuation of the Cu-localized hole (n_{loc}) visiting the neighboring planar–oxygen atoms, which is the reason for the material-dependence embodied in the constant O_S.

18:00	**115**	**Murunskite: A Bridge Between Cuprates and Pnictides** *Trpimir Ivsic [1], Davor Tolj [2], Ivica Zivkovic [2], Konstantin Semeniuk, Eduardo Martino, Ana Akrap [3], Priyanka Reddy [4], Benjamin Klebel-Knobloch [1], Ivor Loncaric [4], László Forró [2], Neven Barisic [1,4], Henrik Rønnow [2], Denis Sunko [4]* *[1] Technische Universitat Wien, [2] EPFL, [3] University of Fribourg, [4] University of Zagreb* Exploring novel materials as the candidates for unconventional superconductors can help to understand the mechanism of this exotic phenomenon but also lead to synthesis of compounds with important technological applications. The main compound of interest is murunskite, a material isostructural to iron-based superconductors with iron and copper occupying the same crystal site. I will discuss the synthesis methods of single crystals and measurements of structural, electronic and magnetic properties. Murunskite structure has been successfully altered by substitution and doping on all three crystallographic positions. Effects on the electronic and magnetic properties towards the metallization will be discussed.
	~~116~~	*cancelled*
18:15	**117**	**Cuprates in Magnetic Field** *Benjamin Klebel-Knobloch [1], Neven Barisic [1,2], Osor S. Barisic [3], C. M. N. Kumar [1], Petar Popcevic [3], Wojtek Tabis [4,1]* *[1] TU Wien, [2] PMF Zagreb, Croatia, [3] Institute of Physics, Zagreb, Croatia* *[4] AGH University of Science and Technology, Krakow, Poland* We investigate the magnetic response on transport properties in cuprates. Firstly, we show that the Hall coefficient in the low-field/high-temperature regime is accurately described by Boltzmann transport equations. Secondly, we validate Kohler's rule for the magnetoresistance across the phase diagram. Thirdly, we determine that field promoted charge density wave correlations at $p \sim 0.12$ doping reconstruct the Fermi surface from arcs to a pocket. Remarkably, the high-field/low-temperature transport properties agree with those calculated for the Fermi surface determined by quantum oscillations. Finally, Umklapp scattering emerges as the dominant process in cuprates' phase diagram.
18:30	**118**	**Ionic effects in cuprates: from Fermi arcs to superconductivity** *Denis Sunko, Department of Physics, Faculty of Science, University of Zagreb* Extensive experimental evidence indicates that the mobile carriers in the normal state of high-T_c superconducting cuprates are a Fermi liquid with practically the same transport parameters for all compounds and dopings. A comprehensive theoretical framework is laid out to explain such an outcome, despite the large Coulomb scales affecting the mobile carriers, and despite the superconducting planes being two-dimensional. Conduction occurs via the O 2p and Cu 4s orbitals, and NOT through the Cu 3d orbital. Fermi arcs are a simple kinematic projection effect of the local ionic disorder in cuprates, and have nothing to do with carrier interactions at the Fermi energy.
18:45		
19:00		***Postersession with Apéro***

Time	ID	**KOND III: Devices and Applications** *Chair: Aswathi K. Sivan, Universität Basel*
14:30	**121**	**High performance bifacial $Cu(In,Ga)Se_2$ solar cells with silver promoted low-temperature process** *Shih-Chi Yang, Empa & ETHZ* Bifacial photovoltaic (PV) systems have shown great promise in generating higher annual energy yields compared to conventional monofacial-based PV systems. They offer advantages in building-integrated PVs, vertically mounted bifacial PVs, and agrivoltaics, with low-carbon emissions and a cost-effective levelized cost of electricity. However, bifacial thin-film solar cells, specifically bifacial $Cu(In,Ga)Se_2$ (CIGS) cells, have not kept pace with their monofacial counterparts. The efficiencies of bifacial CIGS cells remain low, hindering their adoption in various applications. Challenges such as the detrimental GaO_x interlayer formation at the CIGS/TCO (transparent conductive oxide) interface during high-temperature deposition have degraded device performance, leading to stagnation in the development of TCO-based CIGS devices. To overcome these limitations, a groundbreaking study introduced an Ag-promoted low-temperature CIGS deposition process. This innovative approach enabled high-quality CIGS growth at lower temperatures, preventing oxidation reactions at the CIGS/TCO interface. It resulted in higher Ga gradings, enhancing carrier collection under rear illumination. Optimizing the substrate temperature achieved a record bifacial CIGS solar cell with efficiencies of 19.77 % (front) and 10.89 % (rear) under one-sun illumination, independently certified by Fraunhofer ISE. Additionally, the study directly fabricated bifacial CIGS solar cells on flexible substrates without lift-off process, offering scalability and cost reduction for larger-scale production. Furthermore, the demonstration of the first-ever bifacial perovskite/CIGS tandem solar cell in a 4-terminal configuration achieved a power generation density of 28.0 mW/cm^2 BiFi300, opening possibilities for various device architectures. These advancements hold great potential for the photovoltaic community, offering high performance and expanding the range of clean and sustainable energy applications.
	~~122~~	*cancelled*
15:00	**123**	**Thermal circuit elements with Telescopic nanowires** *Yashpreet Kaur [1], Ilaria Zardo [1], Saeko Tachikawa [1], Milo Yaro Swinkels [1], Matteo Camponovo [1], Miquel Lopez-Suarez [2], Anna Fontcuberta I Morral [3], Riccardo Rurali [2]* *[1] University of Basel* *[2] Institut de Ciencia de Materials de Barcelona (ICMAB–CSIC)* *[3] Laboratory of Semiconductor Materials, Institute of Materials, EPFL* Heat dissipation has become a critical problem in the performance of electronic devices, thus, reducing their lifespans. Therefore, to manipulate and control heat, thermal circuit elements analogous to electronic ones like thermal diodes, transistors, and thermal logic gates are needed. In our current research, we have experimentally studied telescopic nanowires for their thermal rectification capabilities giving a rectification ratio of up to 8 % as a function of applied temperature bias, thus, exhibiting the thermal diode effect. This is the first experimental study on telescopic nanowires indicating rectification and an important contribution towards the development of thermal circuit elements.

15:15	**124**	**Chemical and structural characterization of tannin-furanic foams using X-Ray micro-CT, FTIR imaging and UV Resonant Raman scattering** *Maurizio Musso [1], Diana Bedolla [2], Raphael J. F. Berger [1], Francesco D'Amico [2], Giulia Saccomano [2], Thomas Schnabel [3], Thomas Sepperer [3], Lisa Vaccari [2]* *[1] University of Salzburg, Department of Chemistry and Physics of Materials* *[2] Elettra - Sincrotrone Trieste S.C.p.A.* *[3] Forest Products and Timber Construction Department, Salzburg University of Applied Sciences* Tannin-furanic foams are green lightweight materials, presenting quite good compression resistance and thermal insulation, and being suitable as a wastewater treatment agent, therefore getting more attention as alternatives to oil-based lightweight materials. Within the Interreg V-A Italy-Austria project ITAT1059 InCIMa4, and within the CERIC proposal 20217081, mechanically and structurally improved tannin-furanic foams have been characterized by the complementary use of infrared spectroscopy and UV Resonance Raman spectroscopy to study similarities and differences in their chemical structures. Additionally, their internal tridimensional micro-architecture was investigated by synchrotron radiation computed micro-tomography (SRµCT) to assess porosity based on the relative abundance of voids, demonstrating differences in pore network and pore size distribution.
15:30	**125**	**Understand the photoinduced phase transition of the monoclinic VO_2 with the nonequilibrium DMFT** *Jiyu Chen, Francesco Petocchi, Philipp Werner, University of Fribourg* The ultrafast dynamics in the quantum many-body systems introduces the novel photoinduced phase transition (PIPT) to the family of quantum phase transitions. In the VO_2, although the thermal-induced metal-to-insulator transition due to the lattice distortion has been explained with cluster DMFT since 2005, it was verified only a few years ago in the experiment that the photoexcitation is also able to induce the PIPT from the insulating phase to a transient metal state without crystallographic change. In our work, with the state-of-the-art realistic nonequilibrium DMFT simulation, we consistently demonstrated the strategies of the ultrafast in-gap charge carriers, which are sensitive to the frequency and polarization of the laser pump.
15:45	**126**	**3D Magnonic Conduits by Direct Write Nanofabrication** *Sebastian Lamb-Camarena [1,2], Fabrizio Porrati [3], A. Kuprava [3], Qi Wang [4], Michal Urbánek [5], Sven Barth [3], Denys Makarov [6], Michael Huth [3], Oleksandr V. Dobrovolskiy [1]* *[1] Nanomagnetism and Magnoniocs, Faculty of Physics, University of Vienna, Boltzmanngasse 5, AT-1090 Vienna* *[2] Vienna Doctoral School in Physics, University of Vienna, Boltzmanngasse 5, AT-1090 Vienna* *[3] Physikalisches Institut, Goethe-Universität, Max-von-Laue-Str. 1, DE-60438 Frankfurt am Main* *[4] School of physics, Huazhong University of Science and Technology, Wuhan 430074, China* *[5] CEITEC BUT, Brno University of Technology, CZ-61200 Brno* *[6] Helmholtz-Zentrum Dresden-Rossendorf e.V., Institute of Ion Beam Physics and Materials Research, Bautzner Landstrasse 400, Dresden, Germany* Magnonics is a rapidly developing domain of nanomagnetism, with application potential in information processing systems. Realisation of this potential and miniaturisation of magnonic circuits requires their extension into the third dimension. However, so far, magnonic conduits are largely limited to thin films and 2D structures. Here, we introduce 3D magnonic nanoconduits fabricated by the direct write technique of focused-electron-beam induced deposition (FEBID). We use Brillouin light scattering (BLS) spectroscopy to demonstrate significant qualitative differences in spatially resolved spin-wave resonances of 2D and 3D nanostructures, which originates from the geometrically induced non-uniformity of the internal magnetic field. This work demonstrates the capability of FEBID as an additive manufacturing technique to produce magnetic 3D nanoarchitectures and presents the first report of BLS spectroscopy characterisation of FEBID conduits.
16:00		
16:30		***Coffee Break***

Time	ID	**KOND IV: Varia** *Chair: Maurizio Musso, Universität Salzburg*
17:00	**131**	**Non-thermal superconductivity in photo-doped multi-orbital Hubbard systems** *Sujay Ray, Philipp Werner, University of Fribourg* Superconductivity in laser-excited correlated electron systems has attracted considerable interest due to reports of light-induced superconducting-like states. We explore the possibility of non-thermal superconducting order in strongly interacting multi-orbital Hubbard systems, using non-equilibrium dynamical mean field theory. We find that a staggered η-type superconducting phase can be realized on a bipartite lattice in the high photo-doping regime, if the effective temperature of the photo-carriers is sufficiently low. The η superconducting state is stabilized by Hund coupling – a positive Hund coupling favors orbital-singlet spin-triplet η-pairing, whereas a negative Hund coupling stabilizes spin-singlet orbital-triplet η pairing.
17:15	**132**	**Pressure dependence of unconventional superconductivity in rare-earth nickel oxides** *Simone Di Cataldo [1], Paul Worm [1], Liang Si [2], Karsten Held [1]* *[1] TU Wien, [2] School of Physics, Northwest University* Superconductivity in nickelates was discovered only four years ago, and sparked great interest in this family of superconductors. Although the underlying mechanism for superconductivity is still under debate, DΓA could successfully predict the occurrence of a superconducting dome. In short, the T_c is inversely proportional to the ratio between the Hubbard interaction *U* and the hopping *t*, and might be optimized by a careful tuning of this ratio. Using first-principles calculations, we explore the effect of pressure and doping on the $Pr_{1-x}Sr_xNiO_2$ nickelate superconductor. While pressure does not change the interaction *U*, it increases *t* up to a factor of two, which has a significant effect on the superconducting T_c.
17:30	**133**	**First-principles modelling of the metal-insulator transition in vanadium dioxide using a bond-centered orbital basis** *Peter Mlkvik, Claude Ederer, Nicola Spaldin, ETH Zürich* Vanadium dioxide (VO_2) is a prototypical metal-insulator transition (MIT) material, hosting both intriguing physical phenomena and industrial application potential. The VO_2 MIT originates from a complex interplay between Peierls-like dimerization and Hubbard-Mott correlations that is difficult to capture with standard theoretical models or computational techniques. Here, we present simulations of VO_2 using an unconventional set of bond-centered basis functions. Combining density-functional theory (DFT) and dynamical mean-field theory (DMFT) with these orbitals, we provide a complementary view on the interplay of dimerization and electronic correlation in VO_2 that treats both effects on the same footing.
17:45	**134**	**Mapping out phase diagrams with generative classifiers** *Julian Arnold [1], Frank Schäfer [2], Christoph Bruder [1]* *[1] Department of Physics, University of Basel, [2] CSAIL, Massachusetts Institute of Technology* One of the central tasks in condensed matter physics is the characterization of phase diagrams. Traditionally, this is done by a physicist who identifies a small set of characteristic quantities, like response functions or order parameters, guided by his human intuition. This process can be automated by casting the problem of mapping out a phase diagram as a classification task. We show that such classification tasks are naturally suitable to be solved using generative classifiers. This constitutes an alternative approach compared to discriminative classifiers and benefits from generative modeling concepts native to the realm of statistical and quantum physics, as well as recent advances in machine learning.

18:00 **135**

Probing ferroelectricity in Zr/Nb-substituted barium titanate relaxors by PFM

Philipp Münzer [1], Marco Deluca [2], Markus Kratzer [1], Christian Maier [3], Klaus Reichmann [3], Christian Teichert [1]
[1] Institute of Physics, Montanuniversität Leoben, [2] Materials Center Leoben
[3] Institute for Chemistry and Technology of Materials, TU Graz

$BaTiO_3$-relaxors are promising materials for energy storage applications in microelectronics. These lead-free dielectrics are thermally stable and suitable for high-temperature operation due to their broad and high permittivity response and low electric coercivity. Relaxor behaviour is induced by homo- or heterovalent substitution of the central Ti^{4+} ions, which disrupts the long-range ferroelectric order. We investigated ferroelectricity in homovalent (Zr^{4+}) and heterovalent (Nb^{5+}) substituted polycrystalline $BaTiO_3$ relaxors utilizing Piezoresponse Force Microscopy (PFM). We probed spontaneous polarization, conducted local polarization switching, and recorded PFM-hysteresis loops utilizing Switching-Spectroscopy-PFM. The results suggest that indicators of ferroelectricity vanish at different substitution levels and that traces of ferroelectricity can even be found in highly substituted systems.

18:15 **136**

Spin-polarized electron-hole pair excitations in $Co_3Sn_2S_2$ studied by magnetic circular dichroism resonant inelastic X-ray scattering

Tianlun Yu, Wenliang Zhang, Yuan Wei, Dariusz Jakub Gawryluk, Loïc Roduit, Vladimir Strokov, Gabriel Aeppli, Thorsten Schmitt, Yona Soh, Paul Scherrer Institute

$Co_3Sn_2S_2$ is a Weyl ferromagnet ($T_c \sim 177$ K) with kagome layers stacked along its c-axis. A recent resonant inelastic X-ray scattering (RIXS) study with linear polarized X-rays reported correlation driven near-flat band Stoner excitations. However, our RIXS measurements employing a magnetic circular dichroism (MCD) analysis suggests that the reported “near-flat band” is dispersive and its intensity reduces upon approaching T_c. We suggest these excitations correspond to the electron-hole pair excitations between spin-polarized occupied and unoccupied bands that are s directly related to the magnetic order. Furthermore, the MCD RIXS spectrum shows opposite sign compared to spin waves in the ferromagnetic topological metal Fe_3Sn_2 due to the orbital moment involvement.

18:30 **137**

Tensor network investigation of the finite temperature behaviour of the $J_1 - J_2 - J_3$ Kagome Ising Antiferromagnet

Afonso dos Santos Rufino, Jeanne Colbois, Frédéric Mila, Samuel Louis Nyckees, EPFL

The finite temperature behavior of the Kagome Ising Antiferromagnet with farther neighbor interactions (J_1, J_2, J_3) is investigated with the Corner Transfer Matrix Renormalization Group (CTMRG) algorithm. In the parameter region $J_1 > J_3 > J_2 > 0$, the system breaks a $\mathbb{Z}_3$ rotation symmetry and a $\mathbb{Z}_2$ translation symmetry in the ground state. These symmetries are restored at higher temperature either in a single first-order transition or through a couple of transitions separated by an intermediate nematic phase, depending on the value of J_2.
In the limit $J_1, J_3 >> J_2$, the rotational symmetry is restored in a sequence of first-order transitions whose discrete character can be understood from the quantisation of the density of extended defects (Domain Walls).

18:45 **138**

Spin-orbital excitations encoding the magnetic phase transition in the van der Waals antiferromagnet $FePS_3$

Yuan Wei [1], Yi Tseng [1], Hebatalla Elnaggar [2], Wenliang Zhang [1], Teguh Citra Asmara [1], Eugenio Paris [1], Gabriele Domaine [1], Vladimir Strokov [1], Luc Testa [3], Virgile Favre [3], Andrew Wildes [4], Henrik Rønnow [3], Frank Groot [5], Thorsten Schmitt [1]
[1] Paul Scherrer Institut, [2] Sorbonne Université, [3] EPFL, [4] ILL, [5] Utrecht University

Magnetic van der Waals (vdW) materials offer exciting opportunities to study exotic magnetic phases and collective behavior in two-dimensional limits. $FePS_3$ is an S = 2 zig-zag quasi-two-dimensional antiferromagnetic insulator with a honeycomb lattice, making it an ideal candidate for investigating dimensionality and interlayer coupling on magnetic behavior. In this talk, Resonant inelastic X-ray scattering (RIXS) was used to study spin-orbital excitations in $FePS_3$ and their relation to magnetism, revealing the essential role of the trigonal lattice distortion and negative metal-ligand charge transfer. This approach provides a perspective of studying low-energy electronic properties in relation to the magnetic state.

19:00	139	**Quantum transport theory in disordered interacting systems: A dynamical mean-field approach** *Jiawei Yan, Philipp Werner, University of Fribourg* We introduce a non-equilibrium dynamical mean-field theory (DMFT) for studying an inhomogeneous Anderson-Hubbard lattice that contains both electron-electron interactions and chemical disorders, which are treated on an equal footing. The theory reduces to conventional DMFT in the presence of only electron interactions and to coherent potential approximation (CPA) with only disorders. An 8-site cube is employed to benchmark our method, showing high agreement in the spectral function in both weak and strong coupling cases. A serial double quantum dot sandwiched by two leads under a step-shaped voltage bias is also studied. Our method provides a generic framework for studying quantum transport problems with both interaction and disorder degrees of freedom.
19:15		

Thursday, 07.09.2023, Room Aula 033

Time	ID	**KOND V: Superconductivity** *Chair: Ding Peng, PSI Villigen*
14:00	141	**Driven-dissipative engineering: A generalized fitness criterion for the superconducting transition temperature** *Aline Ramires [1], Ramasubramanian Chitra [2], Rui Lin [2]* *[1] Paul Scherrer Institut, [2] ETH Zürich* Floquet engineering has attracted significant interest given the recent developments in experimental techniques such as ultrafast spectroscopy and the potential to enhance the stability of phases of matter such as superconductivity. Here we explore how an external drive and intrinsic dissipation jointly affect superconductivity. Inspired by the fitness criterion for static superconductors, we recognize the distinct effects of external drives on superconductors based on their commutativity or anticommutativity with the superconducting order parameter within the Floquet-Keldish formalism. Our proposal goes beyond standard mechanisms, such as phonon squeezing and dynamical localization. It opens the door for further studies toward driven-dissipative engineering of exotic phases of complex matter in solid-state systems.
14:15	142	**Vortex Counting and Velocimetry for Slitted Superconducting Thin Strips** *Barbora Budinská [1], Volodymyr Bevz [2], Mikhail Mikhailov [3], Sebastian Lamb-Camarena [1], Stanislava Shpilinska [1], Andrii Chumak [1], Michal Urbánek [4], Markus Arndt [1], Wolfgang Lang [1], Oleksandr Dobrovolskiy [1]* *[1] University of Vienna, AT-1090 Vienna* *[2] V. Karazin Kharkiv National University, Kharkiv 61022, Ukraine* *[3] B. Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine, Kharkiv 61103, Ukraine* *[4] CEITEC, Brno University of Technology, Brno 61200, Czech Republic* At low magnetic fields, the approach to deduce the energy relaxation times from current-voltage curves fails. The problem arises given the fact that the number of vortices, deduced from the applied magnetic field only, is in fact larger. Here, we provide a method to count the number of vortices in samples at zero magnetic field. Experiments were performed on MoSi samples with focused ion beam milled-out slits. Every time the number of vortices crossing the sample is increased by one, a current-voltage kink appears. The number of kinks corresponds to the number of vortices. This information allows one to correct the previously unphysical energy relaxation times at low magnetic fields.

14:30	**143**	**Particle-hole symmetry in the 5/2 Quantized Hall State at small magnetic field** *Loic Herviou, Frédéric Mila, École Polytechnique Fédérale de Lausanne* The nature of the experimentally-measured fractional conductance plateau at filling 5/2 in Quantum Hall states remains an open question. After a decade of debate, the theoretical consensus settled on the non-Abelian Antipfaffian while recent experimental results measured an incompatible quantized thermal conductance of 5/2. We revisit previous theoretical approaches with a more careful treatment of the Landau level mixing, the parameter controlling the interaction between different Landau levels. I will present the challenges behind this approach, and our main results: an inversion of the gaps at mixings well below the experimental regime and the important role of frozen spin degrees of freedom.
14:45	**144**	**Coupled chain construction for a fractional spin quantum Hall effect** *Pierre Fromholz [1], Even Thingstad [1], Flavio Ronetti [2], Daniel Loss [1], Jelena Klinovaja [1]* *[1] University of Basel, [2] ix Marseille Univ, Universite de Toulon, CNRS, CPT* While the topological classification of non-interacting spin excitation band structures has successfully been applied to understand many magnetic insulators, intrinsic magnon-magnon interactions can modify the topological properties significantly. Using a coupled wire approach, we show that the system of weakly coupled spin chains with modulated Dzyaloshinskii-Moriya coupling strengths can be engineered to host Abelian and non-Abelian fractional spin quantum Hall effects controlled by tuning the chain magnetizations. The associated spin fractionalization can be detected through the spin conductance. We argue that these phases can be realized in systems of synthetic spin chains and ultracold atoms.
15:00	**145**	**Characterizing fractional quantum Hall states using isometric tensor networks** *Bartholomew Andrews, Zhehao Dai, Yantao Wu, Michael Zaletel, UC Berkeley* The simulation of strongly-correlated quantum many-body systems is a long-standing numerical challenge. Although the ground-state properties of one-dimensional systems may be efficiently distilled using the density matrix renormalization group, now understood in the framework of matrix product states, generalizing this procedure to higher dimensions is problematic, since the exact evaluation of tensor network states becomes exponentially expensive. In this talk, we remedy this by employing isometric tensor networks (isoTNS), a recently-proposed restriction of the projected entangled pair state ansatz. We evaluate isoTNS algorithms for bosons and fermions, and present current progress in applying them to characterize fractional quantum Hall states.
15:15	**147**	**Topological interlayer superconductivity mediated by magnons** *Even Thingstad, Joel Hutchinson, Jelena Klinovaja, Daniel Loss, University of Basel* Most proposals to realize topological superconductivity rely on exploiting the properties of a topologically trivial superconductor through the proximity effect. An alternate route is to search for systems where the pairing interaction directly gives rise to topologically non-trivial superconductivity. We show that magnon-mediated superconductivity in heterostructures of transition metal dichalcogenides coupled to magnetic insulators provides a promising route to this end. Considering a trilayer heterostructure consisting of an antiferromagnetic insulator sandwiched between two transition metal dichalcogenides, we show that magnons can mediate topologically non-trivial interlayer superconductivity.

15:30 | **148**

Tunable unconventional kagome superconductivity in charge ordered RbV_3Sb_5 and KV_3Sb_5

Zurab Guguchia [1], Charles Mielke III [2], Debarchan Das [1], Ritu Gupta [1], J.-X. Yin [3], H. Liu [4], Q. Yin [5], M. H. Christensen [6], Z. Tu [5], C. Gong [5], N. Shumyia [7], Md. S. Hossain [7], Ts. Gamsakhurdashvili [1], M. Elender [1], P. Dai [8], Alex Amato [1], Youguo Shi [4], Hechang Lei [5], R. M. Fernandes [9], M. Z. Hasan [7], Hubertus Luetkens [1], Rustem Khasanov [1]
[1] Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute
[2] Laboratory for Multiscale materials eXperiments, Paul Scherrer Institute
[3] Department of physics, Southern University of Science and Technology, Shenzhen, China
[4] University of Chinese Academy of Sciences, Beijing 100049, China
[5] Department of Physics and Beijing Key Laboratory of Opto-electronic Functional Materials and Micro-nano Devices, Renmin University of China, Beijing 100872, China
[6] Niels Bohr Institute, University of Copenhagen, 2100 Copenhagen, Denmark
[7] Laboratory for Topological Quantum Matter and Advanced Spectroscopy (B7), Department of Physics, Princeton University, Princeton, New Jersey 08544, USA)
[8] Department of Physics and Astronomy, Rice Center for Quantum Materials, Rice University, Houston, TX, USA
[9] School of Physics and Astronomy, University of Minnesota, Minneapolis, MN 55455, USA

We utilized pressure-tuned and ultra-low-temperature muon-spin spectroscopy to uncover the unconventional nature of superconductivity in kagome metals $(Rb,K)V_3Sb_5$. At ambient pressure, the superconducting state displays a nodal energy gap and a reduced superfluid density, which is attributed to the competition with the charge order. Upon applying pressure, the charge-order is suppressed, the superfluid density increases, and the superconducting state evolves from nodal to nodeless. Once optimal superconductivity is achieved, we find a superconducting pairing state that is not only fully gapped, but also spontaneously breaks time-reversal symmetry. Our results offer unique insights into the nature of the pairing state.

15:45 | **146**

Magnetic Impurity Effect in the Kagome Superconductor $LaRu_3Si_2$

Zurab Guguchia [1], Charles Mielke III [1], Jonathan Spring [2], Dariusz Jakub Gawryluk [1], H. Nakamura [3], Soohyeon Shin [1], Huanlong Liu [2], Vahid Sazgari [1], Jike Lyu [1], Toni Shiroka [4], Marisa Medarde [1], Alex Amato [1], Satoru Nakatsuji [3], Rustem Khasanov [1], Hubertus Luetkens [1], Debarchan Das [1]
[1] Paul Scherrer Institut, [2] University of Zürich, [3] ISSP Tokyo, [4] ETH Zürich

The rich interplay of unconventional superconductivity and symmetry-breaking states lies at the frontier of physics and materials science. Here we report muon spin rotation (μSR) experiments of the magnetic impurity effect on the superconducting and normal state properties in the prototypical kagome superconductor $LaRu_3Si_2$. In the normal state, zero-field μSR experiments reveal a hidden magnetism in the undoped system which is enhanced by Fe-doping. From measurements of magnetic penetration depth λ, doping induces a change of gap structure from nodeless s-wave to nodal gap symmetry. The T_c/λ_{-2} ratio is comparable to that of unconventional superconductors. Taken together, these results suggest unconventional superconducting and normal states in this kagome system.

16:00 | **149**

Two-dimensional Shiba lattices as a platform for crystalline topological superconductivity

Titus Mangham-Neupert, Martina Soldini, Glenn Wagner, University of Zürich

Localized or propagating Majorana boundary modes are the key feature of topological superconductors. Lattices of Yu-Shiba-Rusinov bound states – Shiba lattices – that arise when magnetic adatoms are placed on the surface of a conventional superconductor can be used to create topological bands within the superconducting gap of the substrate. I will discuss results using scanning tunnelling microscopy to create and probe adatom lattices with single atom precision.Our results highlight the potential of Shiba lattices as a platform to design the topology and sample geometry of 2D superconductors.

16:15	**150**	**Mechanisms for π phase shifts in Little-Parks experiments on single crystals** *Mark Fischer, Universität Zürich, Patrick A. Lee, MIT, Jonathan Ruhman, Bar Ilan University* The Little-Parks effect, the periodic change in the critical temperature upon threading magnetic flux through a superconducting cylinder, exhibits a maximum or a minimum at zero flux in the presence of time-reversal symmetry. The latter situation, referred to as π rings, is only expected for polycrystalline rings of an unconventional superconductor. Interestingly, recent measurements of the Little-Parks effect in single-crystal rings of 4Hb-TaS_2 show zero and π rings and have been interpreted as evidence of exotic superconductivity. We discuss two scenarios for this unconventional behavior, namely a two-component order parameter and negative interlayer Josephson coupling in a s-wave superconductor, as well as both scenarios' reliance on crystal defects.
16:30		***Coffee Break***
		KOND VI: METHODS *Chair: NN*
17:00	**151**	**Entanglement and thermo-kinetic uncertainty relations in coherent mesoscopic transport** *Kacper Prech [1], Philip Johansson, Gabriel Landi [2], Elias Nyholm, Patrick Potts [1], Peter Samuelsson [3], Claudio Verdozzi [3]* *[1] University of Basel, [2] University of Rochester, [3] Lund University* Some aspects concerning coherence in open quantum systems remain poorly understood. On the one hand, coherence leads to entanglement and nonlocality. On the other, it leads to a suppression of fluctuations, causing violations of classical thermo-kinetic uncertainty relations. These represent its different manifestations, one depending only on the state of the system and one depending on two-time correlation functions. We employ these manifestations to determine when mesoscopic quantum transport through a double quantum dot can be captured by a classical jump model, and when such model breaks down implying nonclassical behavior. Quantum tunneling induces Rabi oscillations and results in both manifestations of coherence, indicating the breakdown of a classical description.
17:15	**152**	**Weak-signal extraction enabled by deep-neural-network denoising of diffraction data** *Jens Oppliger [1], Michael Denner [1], Julia Küspert [1], Ruggero Frison [1], Qisi Wang [1], Alexander Morawietz [1], Oleh Ivashko [2], Ann-Christin Dippel [2], Martin von Zimmermann [2], Izabela Biało [1], Leonardo Martinelli [1], Benoît Fauqué [3], Jaewon Choi [4], Mirian Garcia-Fernandez [4], Kejin Zhou [4], Niels B. Christensen [5], Tohru Kurosawa [6], Naoki Momono [6], Migaku Oda [6], Fabian Donat Natterer [1], Mark Hannes Fischer [1], Titus Neupert [1], Johan Chang [1]* *[1] Physik-Institut, Universität Zürich* *[2] Deutsches Elektronen-Synchrotron DESY, Hamburg* *[3] JEIP, USR 3573 CNRS, College de France, PSL University* *[4] Diamond Light Source, Oxfordshire* *[5] Department of Physics, Technical University of Denmark* *[6] Department of Physics, Hokkaido University* We show how data can be denoised via a deep convolutional neural network such that weak signals appear with quantitative accuracy. In particular, we study X-ray diffraction on crystalline materials. We demonstrate that weak signals stemming from charge ordering, insignificant in the noisy data, become visible and accurate in the denoised data. This success is enabled by supervised training of a deep neural network with pairs of measured low- and high-noise data. This way, the neural network learns about the statistical properties of the noise. We demonstrate that using artificial noise does not yield such quantitatively accurate results.

17:30	**153**	**A Versatile Ultrasonic Setup for Quantum Matter Research** *Xuan Dang Dang, Marek Bartkowiak, Marc Janoschek, Paul Scherrer Institut* Ultrasound techniques offer a simple and efficient method for studying quantum matter as they are able to detect subtle changes to symmetry and are also sensitive to lattice-spin/charge coupling. There are two distinct measurement paradigms used for ultrasonic studies: Whereas RUS provides a comprehensive view of the elastic tensor of solids, PEUS measures changes in sound wave attenuation and velocity, revealing the coupling of the lattice to spin or charge degrees of freedom. Here we will present versatile ultrasonic setup, which is using the same electronic system and allowing for efficient switching between both methods. The setup is further optimized for studying quantum systems in low-temperature and magnetic field environments.
17:45	**154**	**Infrared ellipsometry study of the charge dynamics in K_3p-terphenyl** *Qi He [1], Dionys Baeriswyl [1], Christian Bernhard [1], Florian le Mardelé [2], Sharma Meenakshi [2], Premysl Marsik [1], Bing Xu [1], Andrea Perali [2], Claudio Pettinari [2], Nicola Pinto [2]* *[1] University of Fribourg, [2] Università di Camerine* We report an infrared ellipsometry study of the charge carrier dynamics in polycrystalline K_xp-terphenyl samples with nominal x = 3, for which signatures of high-temperature superconductivity were previously reported. A dc resistivity of about 0.3 Ω·cm at 300 K is deduced from the IR data, comparable to values measured by electrical resistivity on a twin sample. Our data might still be compatible with a filamentary superconducting state with a volume fraction well below the percolation limit for which the spatial confinement of the condensate can result in a plasmonic resonance at finite frequency.
18:00	**155**	**Electronic properties of single layer molybdenum disulphide-on-gold heterostructure as a function of twist angle** *Ishita Pushkarna, Árpád Pásztor, Christoph Renner* *Department of Quantum Matter Physics, University of Geneva, 24 Quai Ernest-Ansermet, CH-1211 Geneva* Transition metal dichalcogenides like molybdenum disulphide (MoS_2) have been studied on metal surfaces, but little is known about twist angle-dependent electronic properties of these simple heterostructures, which indeed offers tremendous opportunities to design functional quantum materials. In this talk, we present a detailed scanning tunnelling microscopy and spectroscopy investigation of electronic properties of monolayer MoS_2 on gold as a function of twist angle. We find that the semi-conducting band edges and hence the band gap are modulated at the moiré wavelength (moiré between MoS_2 and gold) and this modulation progressively vanishes with increasing twist angle.
18:15	**156**	**Field-induced bound-state condensation and spin-nematic phase in $SrCu_2(BO_3)_2$ revealed by neutron scattering up to 25.9 T** *Mithilesh Nayak [1], Ellen Fogh [1], Maciej Bartkowiak [2], Hiroshi Kageyama [3], Kazuhisa Kakurai, Frédéric Mila [1], Koji Munakata [4], Hiroyuki Nojiri [5], Bruce Normand [6], Ekaterina Pomjakushina [6], Oleksandr Prokhnenko [2], Henrik Rønnow [1], Jian-Rui Soh [1], Alexandra Angeline Turrini [6], Mohamed E. Zayed [7]* *[1] EPFL, [2] Helmholtz-Zentrum Berlin für Materialien und Energie, [3] University of Tokyo* *[4] Neutron Science and Technology Center, Comprehensive Research Organization for Science and Society (CROSS)* *[5] Tohoku University, [6] Paul Scherrer Institute, [7] Carnegie Mellon University in Qatar* High-field Inelastic Neutron Scattering experiments have been conducted on $SrCu_2(BO_3)_2$ up to 25.9 T and we find a rich set of excitations whose energies and spectral intensities have been measured as a function of magnetic field. Using cylinder matrix-product-states calculations on the Shastry-Sutherland model with Dzyaloshinskii–Moriya interactions, we reproduce experimental spectra. Multiple unconventional spectral features such as the gradients of the one-triplet branches and the persistence of the single-triplet gap point to a condensation of spin-2 bound states, thus realizing a spin-nematic phase. The single-triplet gap reflects a direct analogy with superconductivity, suggesting that the spin-nematic phase in $SrCu_2(BO_3)_2$ is best understood as a condensate of Cooper pairs of hardcore bosons.

18:30	**157**	**3D ptychography reconstruction** *Ding Peng, Tatiana Latychevskaia, Sara Mustafi, Paul Scherrer Institut* Electron ptychography has demonstrated the world-record highest resolution in imaging two- dimensional materials such as transition metal dichalcogenides (TMD). We are investigating the possibility of applying electron ptychography-related techniques for three-dimensional reconstruction of atomic positions and the associated resolution limits.
18:45		
19:00		***Transfer to Dinner***
19:30		***Conference Dinner***

Friday, 08.09.2023, Room Aula 033

Time	**ID**	**KOND VII: Diffraction and Spectroscopy** *Chair: Ilaria Zardo, Universität Basel*
12:00	**161**	**Raman spectroscopy as an ideal tool for probing phonon-carrier interactions in low dimensional materials** *Mirjana Dimitrievska, Angel Labordet Alvarez, Gabriela Borin Barin, Roman Fasel, Michel Calame, EMPA* Low dimensional materials (1D and 2D) are promising candidates as building blocks of future electronics and optoelectronics. Controllable bandgap, strong light-matter interaction, sub-nanometer thickness, and high carrier mobility are among their favorable properties for electronic and optical applications. Comprehensive characterization of these materials is a crucial learning step toward their reliable incorporation in devices. In this work, we will discuss how temperature-dependent, multiwavelength excitation Raman spectroscopy could be effectively used to probe the interaction between the 1D graphene nanoribbons and various substrates (metal, oxides, semiconductors), including the effects on the phonon-carrier interaction, which are crucial for the device performance.
12:15	**162**	**Three-dimensional microstructural investigation of Silicon Carbide composite materials using synchrotron radiation** *Fareeha Hameed [1], Lucia Mancini [2], Andrea Moriani [3], Halit Tatlisu [4], Silvano Tosti [3]* *[1] Forman Christian College University* *[2] Slovenian National Building and Civil Engineering Institute ZAG* *[3] ENEA, Italian National Agency for New Technologies* *[4] ATI, Vienna University of Technology* Fiber-reinforced silicon carbide composite materials are promising candidates for applications in the aerospace industries as well as future energy sources (fusion and fission). They have structural as well as functional applications. These composites were previously analyzed by methods of neutron scattering and neutron tomography. Recently synchrotron X-ray phase contrast micro-tomography has been performed to get three-dimensional information on the porosity and morpho-textural properties. Porosity plays a major role in their safety and reliability. The length scale of the porosity ranges from macro to micropores. Hence advanced techniques have to be employed to get a complete qualitative and quantitative analysis.

12:30	**163**	**Shape Transformation of Nanocrystals investigated by Model Free X-Ray Scattering Analyses** *Rainer Lechner [1], Max Ritter [2], Agnes Weimer [3], Artur Feld [3]* *[1] Montanuniversität Leoben, [2] Wood Materials Science, ETH Zürich* *[3] Institute of Physical Chemistry, Hamburg University* Chemical synthesis of colloidal nanocrystals (NCs) can produce particles with controlled sizes and complex shapes, which influence their physical properties. For controlling the NCs' morphology, the 3D shape analysis of NCs is a key issue. Small angle X-ray scattering (SAXS) is a leading technique for analyzing NCs in sub-nanometer resolution. From SAXS data the 3D mean shape can be retrieved using model-free techniques. In this study the varying morphology during growth of iron oxide nanocrystals is analyzed. The FeO NCs transform from nanostars to nearly perfect nanocubes. X-ray diffraction experiments link the derived NC-shape to crystallographic directions. The congruence of the results is demonstrated by comparison to TEM analysis.
12:45	**164**	**Phonon engineering in GaAs-GaP Superlattice Nanowires** *Aswathi Kanjampurath Sivan [1], Begoña Abad [1], Tommaso Albrigi [2], Omer Arif [3], Johannes Trautvetter [1], Alicia Ruiz Caridad [1], Chaitanya Arya [1], Valentina Zannier [3], Lucia Sorba [3], Riccardo Rurali [2], Ilaria Zardo [1]* *[1] University of Basel* *[2] Institut de Ciència de Materials de Barcelona, ICMAB-CSIC, Campus UAB, 08193 Bellaterra* *[3] NEST, Instituto Nanoscienze-CNR and Scuola Normale Superiore, Pisa, Italy* Designing materials with tailormade thermal properties is crucial in developing energy-efficient devices. Superlattices (SLs), which are artificially layered superstructures with periodic repetition of two or more materials, offer a promising approach for controlling thermal properties through the modification of the phonon spectrum. To control heat flow, we must manipulate the phonons at the nanoscale. Nanowires (NWs) offer the possibility to combine a wide range of materials at the nanoscale in the form of SLs. In this work, we demonstrate the continuous tuning of the phononic properties of GaAs/GaP SL NWs as a function of SL periodicity through inelastic light scattering experiments corroborated by ab initio calculations.
	~~**165**~~	*cancelled*
13:00	**166**	**Squaraine molecular crystals: Femtosecond dynamics and Davydov splitting** *Robert Schwarzl [1], Davide Giavazzi [2], Pascal Heim [1], Maximilian Jeindl [1], Markus Koch [1], Peter Puschnig [3], Manuela Schiek [4], Frank C. Spano [5], Andreas Windischbacher [3]* *[1] TU Graz, [2] University of Parma, [3] University of Graz,* *[4] Center for Surface and Nanoanalytics (ZONA), Institute for Physical Chemistry (IPC) & Linz Institute for Organic Solar Cells (LIOS), Johannes Kepler University Linz* *[5] Temple University, Philadelphia* Squaraines are a class of organic chromophores which are particularly well-suited as molecular aggregates. Their structure-functionality relationship allows one to manipulate optical properties through the adjustment of side chains. SQIB is investigated via femtosecond transient absorption microscopy in an amorphous PMMA matrix and in its orthorhombic molecular crystal form with four molecules per unit cell in a non-parallel molecular arrangement. This results in multiple Davydov splitting of the excited states. We combine our measurements with simulations based on the essential states model and TD-DFT in order to explain all contributions to the absorption spectrum. The influence of molecular aggregation on dynamics is studied via femtosecond transient absorption microscopy.

13:15	**167**	**Non-adiabatic Lifshitz transition in High T_c superconductor Bi2212** *Siham Benhabib, Laboratoire de physique des solides, université Paris Saclay, France* The equilibrium tunning of doping generates substantial changes in the electronic states of cuprates. They undergo a gradual transition from Mott insulator to Fermi liquid, crossing d-wave superconductivity. Usually, these changes are accompanied by an abrupt transformation in Fermi surface topology, the so-called Lifshitz transition. Here in this work, we address the effect of ultrashort pulses on the Fermi surface topology of cuprates $Bi_2Sr_2CaCu_2O_{8+\delta}$ by means time-resolved-Angle resolved Photoemission Spectroscopy with pump energy of 1.55 eV. For the first time, we demonstrate that high fluence pulses are significantly efficient in supplying the Fermi level with additional carriers through the photodoping process, driving non-adiabatically the Fermi surface from hole-like to electron-like.
13:30	**168**	**Phase transition driven by ultrashort laser pulses in the charge-density-wave material $K_{0.3}MoO_3$** *Rafael Winkler [1], Larissa Boie [1], Yunpei Deng [2], Matteo Savoini [1], Serhane Zerdane [2], Abhishek Nag [2], Sabina Gurung, Davide Soranzio [1], Tim Suter [1], Vladimir Ovuka [1], Janine Dössegger [1], Elsa Souto Gonçalves de Abreu [1], Simone Biasco, Roman Mankowsky [2], Edwin J. Divall [2], Alexander R. Oggenfuss [2], Mathias Sander [2], Christopher Arrell [2], Danylo Babich [2], Henrik T. Lemke [2], Paul Beaud [2], Urs Staub [2], Jure Demsar [3], Steven Johnson [1]* *[1] ETH Zürich, [2] SwissFEL, Paul Scherrer Institute, Villigen* *[3] Faculty Institute of Physics, Johannes Gutenberg-University Mainz* Blue Bronze ($K_{0.3}MoO_3$) is a quasi 1D material exhibiting a charge density wave with a periodic lattice distortion (PLD). In a time resolved x-ray experiment at SwissFEL, we study the dynamics of the PLD by pumping $K_{0.3}MoO_3$ with short laser pulses and probing it using x-ray diffraction. We construct reciprocal space maps (RSM) of superlattice reflections at different delays. The RSM along the surface normal gets broader at the delay equal to half the amplitude mode oscillation period, indicating a transient inversion of the PLD. For longer delays, this broadening is not visible. However, the diffracted x-ray intensity drops below the unpumped value indicating a molten CDW near the surface.
13:45	**169**	**Band structure measurements on the topological magnet PrGeAl** *Ola Kenji Forslund [1], Johan Chang [1], Masafumi Horio [1], Kevin Kramer [1], Xiaoxiong Liu [1], Titus Neupert [1], Ekaterina Pomjakushina [2], Pascal Puphal [2], Yasmine Sassa [3], Qisi Wang [1], Jonathan White [4]* *[1] Physik-Institut, Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich* *[2] Laboratory for Multiscale Materials Experiments (LMX), Paul Scherrer Institut (PSI), CH-5232 Villigen PSI* *[3] Department of Physics, Chalmers University of Technology, SE-412 96 Göteborg* *[4] Laboratory for Neutron Scattering and Imaging (LNS), Paul Scherrer Institut (PSI), CH-5232 Villigen PSI* None zero Berry curvature in condensed matter is the fundamental concept behind the unique responses topological materials exhibit. We report intrinsic spin fluctuations to be enough to realise anomalous hall effect (AHE) in PrGeAl. PrGeAl is a topological ferromagnet and is stabilised in a none centosymmetric structure. Based on muon spin relaxation, transport, angle resolved photo emission spectroscopy (ARPES) measurements and density functional theory calculations, we show AHE in the paramagnetic phase. Our study show that long-range magnetic order and spontaneous time-reversal symmetry breaking are not essential requirements for AHE and can emerge in a wider range of condensed matter systems than previously thought.

14:00	**170**	**Interplay between phonon and charge density wave in Superconducting $La_{1.675}Eu_{0.2}Sr_{0.125}CuO_4$** *Xunyang Hong [1], Johan Chang [1], Jaewon Choi [2], Mirian Garcia-Fernandez [2], S. Pyon [3], Yasmine Sassa [4], H. Takagi [3], T. Takayama [3], Qisi Wang [5], Kejin Zhou [2], Karin von Arx [1]* *[1] Physik-Institut, Universität Zürich, [2] Diamond Light Source, Oxfordshire* *[3] Department of Advanced Materials, University of Tokyo* *[4] Department of Physics, Chalmers University of Technology, SE-412 96 Göteborg* *[5] Chinese University of Hong Kong* We conducted a resonant inelastic X-ray scattering (RIXS) experiment at the O-K edge on $La_{1.675}Eu_{0.2}Sr_{0.125}CuO_4$, leveraging RIXS's high resolution to study charge density wave (CDW) and its interaction with phonons in cuprate superconductor. Three phonon modes are detected in the RIXS spectra, which are assigned to the bond-stretching, bond-buckling, and an acoustic phonon mode respectively. The low-lying acoustic mode displays a sharp peak of spectral weight at q ~ 0.25, slightly larger than the CDW wavevector Q_{CDW} ~ 0.23. Meanwhile, no significant softening of this phonon mode is observed, suggesting a weak interaction between charge and phonon excitation. These results are well explained by our theoretical model within the weak-coupling framework.
14:15		***END***

ID	KOND POSTER
181	**RIXS study of Cu-O-Mn superexchange coupling at $YBa_2Cu_3O_7$ / manganite interfaces** *Subhrangsu Sarkar [1], Roxana Gaina Capu [1,2], Yurii Pashkevich [1], Davide Betto [3], Kurt Kummer [3], Roberto Sant [3], Claude Monney [1], Christian Bernhard [1]* *[1] University of Fribourg, [2] West University of Timisoara, RO* *[3] European Synchrotron Radiation Facility, B.P. 220, FR-38043 Grenoble* Here we study the anomalous interface magnetic excitations in the $YBa_2Cu_3O_7$/ manganite heterostructures. Detailed analysis of the inelastic part of the high-resolution Resonant Inelastic X-ray Scattering (RIXS) signal in conjunction with polarimetry show the presence of two magnon modes in the cuprate, including a unique, non-dispersive interface magnon, that appears only due to the interfacial proximity of the manganite layer. We demonstrate that this low energy magnon originates from the interface copper layer in which intralayer exchange decreases due to Cu orbital reconstruction in favor of 3dz2-r2, instead of usual 3dx2-y2. Our work contributes to future studies of oxide interfaces offering perspectives for the design of artificial magnetic meta-materials.
182	**Magnetostriction and heat capacity measurements of quantum spin ice materials at ultra-low temperatures** *Ilaria Villa, Marek Bartkowiak, Romain Sibille* *Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut, CH-5232 Villigen PSI* In the search for Quantum Spin Liquid (QSL) phases, Rare-Earth pyrochlores are of interest to stabilize Spin Ice states. In QSL candidates, magnetic neutron scattering is a well-established probe for studying magnetic order and interactions. However, in rare-earth elements, degrees of freedom can include magnetic and electric multipoles, which are elusive in scattering experiments. Then, bulk techniques like specific heat and magnetostriction, especially at ultra-low temperatures (ULTs), are crucial to detect phase transitions “hidden” in scattering experiments. We present magnetostriction measurements on Quantum Spin Ice candidates and the development of a heat capacity probe at ULTs.

183 **Thermoelectric properties of individual silicon nanotubes**

Jose Manuel Sojo Gordillo [1], Saeko Tachikawa [1], Yashpreet Kaur [1], Giulio de Vito [1], Alex Morata [2], Ilaria Zardo [1]
[1] University of Basel, [2] Catalonian Institute for Energy Research

Large amounts of waste heat generated in our economy could be converted into useful electric power using thermoelectric generators. However, the low efficiency, scarcity, high cost, and poor production scalability of conventional thermoelectric material hinder their mass deployment. Nanoengineering has proven an excellent approach for enhancing the thermoelectric properties of abundant and cheap materials such as silicon. Recently, a family of nano-enabled materials in the form of large-area paper-like fabrics made of nanotubes has been developed as a cost-effective and scalable solution for thermoelectric generation. In this project, the thermoelectrical properties of the described nanotubes will be measured using different techniques (such as self-heating, nano calorimeters, and Raman thermography).

184 **Neutron scattering on a new organo-metallic quantum magnet**

Oksana Shliakhtun, Marc Janoschek, Jonas Philippe, Gediminas Simutis, Paul Scherrer Institut

Quantum spin ladders are fascinating systems with complex excitation spectra that depend on the relative strengths of the leg and rung exchange interactions. Here we report the magnetic properties of a new strong-leg spin ladder obtained by using magnetization, specific heat and neutron scattering measurements. In particular, we performed comprehensive inelastic neutron scattering experiments using both triple-axis and neutron time-of-flight techniques. Our results reveal a gapped excitation spectrum, consistent with the spin-ladder model. In addition, we will also show our magneto-thermodynamic experiments to demonstrate how the system transforms from a quantum paramagnet into a partially spin-polarized state.

185 **H_{c2} as a function of the order parameter in unconventional superconductors**

Bernhard Lüscher, Mark Fischer, Universität Zürich

The exact symmetries and form of the cooper pair wave function in many unconventional superconductors remains subject of ongoing debate. A possible way to shed some more light upon the matter is by explicitly computing thermodynamic properties given a functional form of the order parameter as well as a microscopic description of the normal state of a material. One such quantity is the upper critical field H_{c2}.
We develop a numerical pipeline interfacing between a normal-state description including a microscopic interaction and thermodynamic quantities such as the upper critical field. This allows us to draw conclusions on the microscopic structure of an unconventional superconductor considering its experimental H_{c2} signature.

186 **Emergent U(1) symmetry in non-particle-conserving 1D models**

Zakaria Jouini, Natalia Chepiga, Loic Herviou, Frédéric Mila, EPFL

The properties of stable Luttinger liquid phases in models with a non-conserved number of particles are investigated. We study Luttinger liquid phases in one-dimensional models of hard-core boson and spinless fermion chains where particles can be created and annihilated three by three on adjacent sites. We provide an intuitive and systematic method based on the flow equation approach, which accounts for additional terms in the correlations generated by the Z_3-symmetric interactions. We find that despite the emergence of U(1) symmetry under renormalization, the observables are still affected by its breaking in the bare Hamiltonian. In particular, the standard bosonization mapping becomes insufficient to capture the full behavior of correlation functions.

187 **Critical line of the triangular Ising antiferromagnet in a field from a C3-symmetric corner transfer matrix algorithm**

Samuel Louis Nyckees, Jeanne Colbois, Afonso Dos Santos Rufino, Frédéric Mila, EPFL

We propose a variant of the corner transfer matrix renormalisation group algorithm that contracts infinite tensor networks on the honeycomb lattice. We then apply the algorithm to the conceptually simple yet numerically challenging problem of the triangular lattice Ising antiferromagnet in a field at low temperatures and magnetic fields. We study how the finite temperature three-state Potts critical line in this model approaches the ground-state Kosterlitz-Thouless transition driven by a reduced field (h/T).

188 Convergent beam electron diffraction of adsorbates on graphene

Sara Mustafi, Tatiana Latychevskaia, Ding Peng, Paul Scherrer Institut

Convergent beam electron diffraction (CBED) on 2D materials provides a method for high-resolution imaging of individual particles deposited on a 2D material. A single-shot CBED pattern combines a diffraction pattern and a defocused image of the sample. We are investigating the optimal experimental imaging conditions for CBED of nanoparticles deposited on graphene. CBED allows regulating the radiation dose deposited into the sample by moving the sample within the probing convergent beam. This allows us to establish the resolution limits of the technique as a function of the required radiation dose.

189 Finite temperature investigation of the ferroJ1-J2 model

Olivier Gauthé, Frédéric Mila, EPFL

We study the spin-1/2 Heisenberg model on the square lattice with ferromagnetic nearest-neighbor coupling J1 < 0 and frustrated antiferromagnetic next-nearest coupling coupling J2 > 0. For spin- 1/2, the zero-temperature phase diagram differs from the J1 < 0 case, with a first order transition to the ferromagnetic state. By combining tensor network methods and spin wave theory, we draw the finite temperature phase diagram of the model. We locate the critical point ending the first order line in addition to the Ising transition at large J2. Our results support the absence of a spin nematic phase in the intermediate region at zero field.