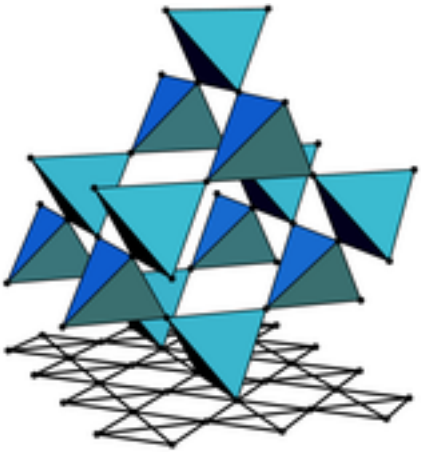

3rd Symposium of the PhD-program in Correlated Magnetism (SFB1143)

IFW Dresden, 5 Apr. 2022

Contents

About the Symposium

Correlated Magnetism: From Frustration to Topology (SFB 1143)

The Collaborative Research Center (CRC) 1143 “Correlated Magnetism: From Frustration to Topology” is devoted to the study of a class of magnets where competing (frustrated) interactions prevent the establishment of a simple conventionally ordered state, leading to a plethora of alternative and highly non-trivial behaviors, the most remarkable of which involve either topological phases of matter or proximity to them. The CRC aims to identify, produce, and understand magnetic materials exhibiting these.

The PhD Symposium is an annual event within the SFB which aims to bring together Doctoral researchers from the various theoretical and experimental groups. Students have the opportunity to present their projects with short oral as well as poster presentations. Associated doctoral researchers of SFB project partners are also invited to participate.

Besides the opportunity to present their research projects, the Symposium offers the opportunity to get to know the research of other groups in the SFB, and to discuss different scientific approaches. Additionally, an invited speaker from outside the SFB is invited to open the symposium with a keynote talk.

Organizing committee

Kerstin Brankatschk
David Moser
Christos Kourris

Timetable

8:30–9:00	**Registration**		
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10:00–10:20	CT	**Maria A. Hertz**	Design of High-Temperature Syntheses on the Example of $Sn[PtBi_6I_{12}]$
10:20–10:40	CT	**Andy Knoll**	Classification of Weyl points and nodal lines based on magnetic point groups for spin-$\frac{1}{2}$ quasiparticles
10:40–11:00	**Coffee Break**		
11:00–11:20	CT	**Sukriti Singh**	Anisotropic Nodal-Line-Derived Large Anomalous Hall Conductivity in ZrMnP and HfMnP
11:20–11:40	CT	**Erik Wagner**	Series expansion studies of the J_1-J_2-Heisenberg bilayer
11:40–12:00	CT	**Tom Klaproth**	Tuning the electronic structure of the trichloride honeycomb lattice by transition metal substitution
12:00-12:20	CT	**Andreas Hauspurg**	Investigation of the magnetoelastic properties of α-$RuCl_3$
12:20–13:30	**Lunch Break**		
13:30–13:50	CT	**Bastian Rubrecht**	Power-law and scaling behaviour in double perovskite system
13:50–14:10	CT	**Willi Roscher**	Microscopic modeling of the Kitaev spin liquid candidates $Na_3Co_2SbO_6$ and $Li_3Co_2SbO_6$ under uniaxial strain
14:10–14:30	CT	**Ellen Häußler**	Diluting a triangular-lattice spin liquid: Synthesis and characterization of $NaYb_{1-x}Lu_xS_2$ single crystals
14:30–14:50	CT	**Sreejith Chulliparambil**	Spin-orbital liquids: Anyons, flux crystals and emergent fractionalized fermionic excitations
14:50-15:10	CT	**Sreejith Thamban**	Synthesis and magnetism of unconventional magnets $La_2CuGe_2O_8$ and Mg_6MnO_8
15:10–15:30	**Coffee Break**		
15:30–15:50	**Poster Pitches Session**		
15:50–17:20	**Poster session**		
17:20–17:30	**Award Ceremony & Closing**		

*KL: Keynote Lecture, CT: Contributed Talk

List of Poster Contributions

P1	Sebastian Beckert	Magneto-thermal transport in non-collinear antiferromagnetic thin films
P2	Tamara Holub	Synthesis and characterisation of Rh(IV) oxides with double perovskite structure
P3	Mahdi Behnami	Thermoelectric properties in $TaRhTe_4$ and $TaIrTe_4$ Weyl semimetals
P4	Felix Seewald	Investigation of the magnetic structure of $RE_3Fe_3Sb_7$ (RE=Nd, Pr) by means of ^{57}Fe Mössbauer spectroscopy and μSR
P5	Pedro M. Cônsoli	Fluctuation-induced ferrimagnetism in sublattice-imbalanced antiferromagnets with application to $SrCu_2(BO_3)_2$ under pressure
P6	Charlotte Beneke	Divergence of the Grüneisen ratio at symmetry-enhanced first-order quantum phase transitions
P7	Georgia Fragkopoulou	Impurities in α-$RuCl_3$
P8	Ekaterina Vinokurova	Dilution of the Kitaev candidate α-$RuCl_3$ by non-magnetic elements
P9	Wilhelm Krüger	Modeling the honeycomb magnet $Na_2Co_2TeO_6$: Significance of ring exchange
P10	Abanoub R. N. Hanna	Crystal growth and characterization of unconventional magnets $PbCuTe_2O_6$ & Ba_2CoWO_6

Abstracts of Talks

Keynote Lecture

Quantum many-body physics in moiré superlattices

Mathias S. Scheurer

KL

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When two layers of graphene are stacked and twisted, a moiré pattern forms. Most strikingly, at so-called “magic angles”, the largest of which is around 1 degree, the bands around the Fermi surface become very flat; this enhances the density of states and the impact of electron-electron interactions. Soon after the experimental discovery in 2018 that this enhancement can induce superconductivity and insulating phases, it became clear that twisted bilayer graphene is only one example of an engineered van der Waals moiré system with a complex phase diagram akin to other strongly correlated materials. In this talk, I will provide an introduction to the rich set of possibilities provided by graphene-based moiré superlattices to engineer and study interesting many-body physics at the intersection of strong correlations and topology. I will discuss a few examples from our recent research, involving a combination of analytical, numerical, and experimental projects.

Research Talks

Classification of Weyl points and nodal lines based on magnetic point groups for spin-$\frac{1}{2}$ quasiparticles

Andy Knoll

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Over the past decade, Weyl and nodal-line semimetals have evoked tremendous interest due to their interesting physical properties. In order to predict the existence and locations of protected band touchings, symmetry-based analyses have proven to be of great use. The majority of existing works focuses on nonmagnetic materials. Therefore, we investigate twofold-degenerate band touchings for all 122 magnetic point groups. In particular, we consider two-band models for which the pseudospin degree of freedom transforms like a true spin-1/2. We find that all magnetic point groups that do not contain the product of spatial-inversion and time-reversal symmetries can in principle give rise to topologically protected band touchings. Furthermore, our work shows that 59 out of the 122 magnetic point groups have guaranteed band touchings. By considering the corresponding little group our analysis is applicable to every momentum in the Brillouin zone. Our work provides a useful tool for the identification and design of Weyl and nodal-line semimetals, in particular magnetic ones.

Spin-orbital liquids: Anyons, flux crystals and emergent fractionalized fermionic excitations

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Spin-orbital liquids are quantum disordered states in systems with entangled spin and orbital degrees of freedom. Motivated by Kitaev's sixteenfold way of anyon theories, we constructed a family of microscopic models with exotic topological order characterized by an integer Chern number. Two of these models are particularly relevant since they represent simple, physical and exactly solvable spin-orbital liquid models on a square/honeycomb lattice in two dimensions [1]. We studied the effect of selected Heisenberg-, Kitaev- and Γ-type interactions as well as external magnetic fields on these models and report the presence of a plethora of spin-orbital liquid phases including dispersing Majorana fermions with Fermi surfaces, metamagnetic transitions into non-trivial flux patterns and more [2]. Furthermore, we studied the effect of anti-ferromagnetic Ising and Heisenberg interactions within the spin degrees of freedom resulting in identification of a novel fractionalized Gross Neveu* criticality with emergent fractionalized fermionic excitations [3]. In addition to being excellent starting points for more realistic modelling of experiments, our models are also potentially relevant for Mott insulators with d^1 electronic configurations and strong spin-orbit coupling as well as for twisted bilayer structures of Kitaev materials.

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Microscopic modeling of the Kitaev spin liquid candidates $Na_3Co_2SbO_6$ and $Li_3Co_2SbO_6$ under uniaxial strain

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We study the Kitaev-spin-liquid candidates $Na_3Co_2SbO_6$ [1] and $Li_3Co_2SbO_6$ [2] by using a microscopic DFT-based analysis. Previous theoretical work suggested [3] that $Na_3Co_2SbO_6$ is proximate to the spin liquid phase and can be driven there by apply pressure. Following this conjecture, we simulate the effect of uniaxial strain along the c-axis. For this purpose, the lattice constant c was changed accordingly and the remaining crystal structure was optimized. To get microscopic insights, a Wannier function analysis is performed, which yields local and non-local terms of d and $d-p$ Hamiltonians. From that we determine the crystal field parameters, the spin-orbit coupling constant and the hoppings. A small reduction of the trigonal splitting is found for tensile strain. However, we find that this strain is insufficient to drive the compounds into the spin liquid phase.

The developed theory in [1] considers Co^{2+} interactions in a hexagonal edge-sharing geometry. It takes into account the cubic symmetry with trigonal distortion, making it applicable to the real materials. Using the DFT-estimated parameters, we calculate with this theory the exchange parameters Kitaev K, Heisenberg J and the off-diagonal anisotropy terms Γ, Γ'. In this way, we get into the magnetic behavior of this materials under uniaxial strain.

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Power-law and scaling behaviour in double perovskite system

Bastian Rubrecht

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Quantum spin liquids (QSL), characterized by the absence of long-range magnetic order (LRO) down to zero temperature as well as highly entangled and dynamic spins, are one of the most interesting states predicted to occur in highly frustrated spin systems. Although being theoretically proposed almost half a century ago, experimental realizations are still scarce [1]. Due to the nature of the QSL state, finding solid experimental evidence for its existence is quite challenging. While, in principle, inelastic neutron scattering at dilution fridge temperatures is able to probe the characteristic fractionalized excitations of QSL, this often remains a difficult task due to the required large high-quality single crystals. Thanks to numeric and analytic modelling of different observables, more common techniques like magnetisation or specific heat capacity measurements are frequently used as indicators for QSLs. Here, scaling and power-law behaviour are, besides the absence of LRO, key features for QSLs [2,3,4].

Recently, the search for new QSL compounds has been extended to strongly spin-orbit coupled $4d/5d$ systems, such as Ir-/Rh-based oxides, showing promising results [5], motivating to take a closer look also at $4d$ double perovskites. In our magnetometric and thermodynamic investigations, we found a scaling and power-law behaviour for our Rh-based double perovskite crystals of La_2MgRhO_6. Specific heat capacity studies revealed no sign of LRO down to $0.36\ \mathrm{K}$. A paramagnetic Curie-Weiss behaviour is observed above $100\ \mathrm{K}$, yielding a Curie-Weiss temperature $\theta_{\mathrm{CW}} = 11\ \mathrm{K}$ and an effective magnetic moment of $0.7\mu_{\mathrm{B}}/\mathrm{f.u.}$, which is less than half the expected value for a Rh^{4+} ($J_{\mathrm{eff}} = 1/2$). Pulsed field measurements up to $55\ \mathrm{T}$ showed a linear field dependence for $\mu_0 H > 15\ \mathrm{T}$. At the highest field and a temperature of $1.5\ \mathrm{K}$, the measured magnetic moment is $0.19\mu_{\mathrm{B}}/\mathrm{f.u.}$, which is surprisingly low. Interestingly, we observe a power-law and scaling behaviour of the magnetisation and specific heat capacity in our sample - a typical signature for a QSL state. Here, we discuss the nature of the observed scaling behaviour for our La_2MgRhO_6 sample in context of disorder revealed in our single crystals.

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Synthesis and magnetism of unconventional magnets $La_2CuGe_2O_8$ and Mg_6MnO_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 ($4\ \mathrm{mm} \times 4\ \mathrm{mm} \times 10\ \mathrm{mm}$) of the potential highly geometrically frustrated candidate compound $La_2CuGe_2O_8$ 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 $0.93\ \mathrm{K}$. The ordering temperature is clearly suppressed compared to the Curie-Weiss temperatures which is $-5.7\ \mathrm{K}$, which implies the presence of frustrated antiferromagnetic interactions [2]. INS and neutron powder diffraction analysis are in progress.

Geometrical frustration occurs typically in lattices containing triangular or tetrahedral units where the magnetic ions interact via antiferromagnetic (AF) couplings. Examples in 3-dimensions there are the hyperkagome and pyrochlore lattices which consist of corner-sharing triangles and tetrahedra respectively. The case of edge-sharing tetrahedra has been much less well-studied. This situation is found in the face-centered cubic (FCC) lattice which can also be viewed a series in interpenetrating triangular lattices. The AF correlations between the moments in the edge-sharing tetrahedral network, can form systems showing significant effects of frustration. Previously reported FCC compounds shows a variety of magnetic ground states. For example, spin-3/2 compounds La_2LiRuO_6 and Ba_2YRuO_6 [3] have a long-range antiferromagnetic order and spin 1 compound Ba_2YReO_6 [4] has a short-range order and spin freezing. Spin-1/2 systems such as Ba_2YMoO_6 shows no magnetic ordering [5,6] and Sr_2CaReO_6 shows only short-range ordering [7].

Here we discuss a new frustrated face-centered cubic lattice Mg_6MnO_8 in which Mn^{4+} ions form a network of edge-sharing tetrahedra. Low temperature heat capacity measurements on a polycrystalline sample reveal a second order transition to long-range magnetic order below the Neel temperature of $T_\mathrm{N} = 2.05\ \mathrm{K}$ in zero applied magnetic field. The transition is also evident in DC magnetic susceptibility measurements. Curie-Weiss fit yields an effective moment of $\mu_\mathrm{eff} = 4.63\mu_\mathrm{B}$ which is somewhat larger than the spin only value of $3.87\mu_\mathrm{B}$ for $S = 3/2$ implying the presence or some orbital moment. The Curie-Weiss temperature is $\theta_\mathrm{CW} = -27.9\ \mathrm{K}$ revealing predominantly antiferromagnetic interactions. T_N is considerably smaller than θ_CW (frustration index of $\theta_\mathrm{CW}/T_\mathrm{N} = 13.6$) implying the suppression of magnetic order due to considerable frustration. Finally, the phase diagram is mapped out revealing two field-induced transitions at $\sim 8\ \mathrm{T}$ and $\sim 12.5\ \mathrm{T}$. Magnetic structure calculations and crystal growth of the compound are in progress.

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Anisotropic Nodal-Line-Derived Large Anomalous Hall Conductivity in ZrMnP and HfMnP

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The nontrivial band structure of semimetals has attracted substantial research attention in condensed matter physics and materials science in recent years owing to its intriguing physical properties. Within this class, a group of nontrivial materials known as nodal-line semimetals is particularly important. Nodal-line semimetals exhibit the potential effects of electronic correlation in nonmagnetic materials, whereas they enhance the contribution of the Berry curvature in magnetic materials, resulting in high anomalous Hall conductivity (AHC). In this study, two ferromagnetic compounds, namely ZrMnP and HfMnP, are selected, wherein the abundance of mirror planes in the crystal structure ensures gapped nodal lines at the Fermi energy. These nodal lines result in one of the largest AHC values of $2840\ \Omega^{-1}\mathrm{cm}^{-1}$, with a high anomalous Hall angle of 13.6% in these compounds. First-principles calculations provide a clear and detailed understanding of nodal line-enhanced AHC. The finding suggests a guideline for searching large AHC compounds.

Diluting a triangular-lattice spin liquid: Synthesis and characterization of $NaYb_{1-x}Lu_xS_2$ single crystals

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Yb-based magnets, with a perfect triangular lattice of pseudospin-1/2 Yb^{3+} ions, have emerged as candidates for realizing a quantum spin-liquid state, with $NaYbS_2$ being a prominent example. To investigate the interplay of the electron spins with respect to the magnetic properties in detail, we substituted the Yb^{3+} ions in $NaYbS_2$ with non magnetic Lu^{3+} to dilute the magnetic sublattice.

As the spin-spin interactions are influenced by the geometric confinements of the structure we had a detailed look on the structural parameters before determining the magnetic susceptibility and the electron spin resonance (ESR) properties. We characterized the samples of the solid solution series $NaYb_{1-x}Lu_xS_2$ with $0 \leq x \leq 1$ with respect to their chemical composition, analyzed their structural parameters in single crystal and powder X-ray diffraction experiments and evaluated the structural changes throughout the whole substitution series. In this contribution, we want to show the synthesis and the crystallographic details of the structure as well as giving an insight into the physical properties obtained via ESR spectroscopy and magnetization measurements.

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Investigation of the magnetoelastic properties of α-$RuCl_3$

Andreas Hauspurg

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The honeycomb material α-$RuCl_3$ is of particular interest due to its proximity to a quantum spin liquid (QSL) in the frame of the Kitaev model, where the Kitaev QSL features fractionalized quasiparticle excitations. A promising approach to investigate such excitations is to study the coupling between fractionalized quasiparticles and phonons. My recent studies of the elastic properties of α-$RuCl_3$ show a promising path to unveil the unconventional physics of the debated QSL phase. In this talk, I will present low-temperature results of the sound velocity and attenuation in external magnetic fields and under hydrostatic pressures. At a pressure of $11.3\ \mathrm{kbar}$ the antiferromagnetic order is completely suppressed.

Series expansion studies of the J_1-J_2-Heisenberg bilayer

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The single layer antiferromagnetic J_1-J_2 Heisenberg-model on the square lattice is one of the pillars of frustrated quantum magnetism, with Néel- and collinearly ordered ground states competing for large and small J_1/J_2, and with a quantum disordered phase of still unsettled nature in between. Probing fingerprints of such phases by approaching them out of a well controlled dimer phase is one of the rationals for studying bilayer versions of frustrated spin models. Here, and starting from the limit of decoupled dimers we use the perturbative Continuous Unitary Transformation (pCUT), based on the flow equation method, to perform series expansion in order to analyze the spectrum of the square lattice J_1-J_2-Heisenberg bilayer up to the two-triplon excitations.

Evaluating the ground state energy and the one-particle dispersion up to 7th order in $J_{1,2}$ as well as the two-particle interactions and spectrum up to 5th order, we find emerging (anti-)bound two-particle states. Based on the wavefunctions of these states, we introduce a classification by total spin and real-space symmetry, which we find to be consistent with the J_1-only bilayer on the square lattice [1]. We analyze the phase boundary of the dimer phase with respect to one- and two-particle excitations and find reasonable agreement with recent coupled-cluster calculations [2], while also uncovering prospects for an additional phase introduced by two-particle boundstate condensation.

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Design of High-Temperature Syntheses on the Example of Sn[$PtBi_6I_{12}$]

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Discovered during the search for novel topological insulators [1,2], we discovered new pseudo one-dimensional compounds. The reaction of Bi with Sn, Pt and BiI_3 above $300\ ^\circ\mathrm{C}$ yielded shiny, black, air insensitive crystals of the subiodide Sn[$PtBi_6I_{12}$] as well as the partially substituted ($Bi_{2x}Sn_{1-3x}$)[$PtBi_6I_{12}$], with $x \approx 0.1$. Through extensive investigations into the synthetic pathway with the help of differential scanning calorimetry, the two compounds could be isolated and synthesized independently. The rhombohedral crystal structures consist of alternating cuboctahedral $[PtBi_6I_{12}]^{2-}$ cluster anions and Sn^{2+} or Bi^{3+} cations in octahedral coordination between trigonal faces of two cuboctahedra. These concatenate them into linear chains, which makes Sn[$PtBi_6I_{12}$] an analogue to the compound Pb[$PtBi_6I_{12}$] [3], while ($Bi_{2x}Sn_{1-3x}$)[$PtBi_6I_{12}$] with its vacant positions consists of finite strands. Additionally, the crystals' cube-like morphology originates from six weaker Bi···I inter-cluster bridges per cluster connecting the chains. The heavy elements show strong spin-orbit coupling. If this exceeds the width of the chemical band gap of the compound, a non-trivial topology can be expected.

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Tuning the electronic structure of the trichloride honeycomb lattice by transition metal substitution

Tom Klaproth

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Transition metal trichlorides show peculiar and versatile magnetic properties. Whereas $CrCl_3$ is a layered antiferromagnet with potential applications as an ultrathin two-dimensional magnet, α-$RuCl_3$ may host a spin-liquid state driven by Kitaev interactions. The interest to control their material properties by chemical modifications is immense, both from an application related and from a fundamental point of view. In my talk I present photoemission and electron energy-loss spectroscopy results on $CrCl_3$, $Cr_{0.5}Ru_{0.5}Cl_3$ and α-$RuCl_3$. Transition metal substitution changes the optical properties of the host without compromising its underlying electronic structure. It does so by a Cr–Ru related charge transfer process across the Mott gap effectively opening up a new absorption channel below the principal gap edge of $CrCl_3$. The Cr and Ru valencies as well as the respective valence band density of states remain stable for the mixed $Cr_{0.5}Ru_{0.5}Cl_3$ compound. The study underlines the potential of transition metal substitution as a means of material engineering of trichlorides.

Abstracts of Posters

Magneto-thermal transport in non-collinear antiferromagnetic thin films

Sebastian Beckert

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Understanding the interplay between topological properties and transport phenomena in non-collinear antiferromagnets is important for exploiting their unconventional characteristics in spintronics. In particular, non-collinear antiferromagnets can exhibit phenomena previously known to be exclusive to ferromagnets, such as the anomalous Hall Effect (AHE) or the anomalous Nernst effect (ANE).

We experimentally study the magneto-thermal transport in unconventional antiferromagnetic thin magnetic films with complex band structure, namely Mn_3NiN [1]. In previously studied Mn_3Sn films, all spins are arranged in the sample plane. Therefore, AHE and ANE cannot be measured in a standard Hall bar geometry and a comparison of AHE and ANE is also not straightforward [2]. (001)-oriented Mn_3NiN thin films have their spins arranged in the (111) plane and, therefore, in principle, a component of the Hall vector in both out-of plane and in-plane directions [3]. This makes Mn_3NiN an ideal candidate for a systematic study of magneto-thermal transport phenomena and their anisotropy. We will present measurements of ANE, AHE, magnetoresistance and Seebeck effect in a single device. Based on careful thermal gradient calibration, we can compare the measured amplitudes of the magneto-thermal transport coefficients and discuss them in context of the Mott relation [4].

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Synthesis and characterisation of Rh(IV) oxides with double perovskite structure

Tamara Holub

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Compounds with double perovskite crystal structure currently attract high interest in solid state physics. Because of their compositional flexibility a wide range of compounds with interesting physical properties are known to exist. Double perovskite structure $A_2BB'O_6$ with transition metal Rh^{4+} ($4d^5$ electronic configuration) on the B' site demonstrate a strong magnetic frustration in the crystal lattice. In keeping with related theoretical predictions, these materials should exhibit strong correlations between fluctuating spins [1]. This may lead to quantum spin liquid (QSL) ground state which is our primary interest.

La_2BRhO_6 (B = Zn, Mg) compounds were chosen for further research as potential QSL candidates [2]. Powders were synthesized in monoclinic crystal system $P2_1/n$ space group. For crystal structure investigations X-ray and neutron powder diffraction were performed. The magnetic behaviour of La_2BRhO_6 (B = Zn, Mg) compounds was characterized using SQUID magnetometry and heat capacity measurements. La_2ZnRhO_6 compound has no long range magnetic order down to $1.8\ \mathrm{K}$. At the same time, magnetic measurements on La_2MgRhO_6 show a clear transition at $\sim 7\ \mathrm{K}$.

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Thermoelectric properties in $TaRhTe_4$ and $TaIrTe_4$ Weyl semimetals

Mahdi Behnami

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The magneto-thermo transport measurement can be more sensitive probe of the band structure compared to the magneto resistivity (MR) and Hall measurement [1] and if sufficiently large, it can be also interesting for heat harvesting.

Here we study systematically the thermoelectric properties (Nernst and Seebeck effects). We study Weyl semimetals - $TaRhTe_4$ and $TaIrTe_4$ – and we detect the topological features. Because in our materials [2,3] the Weyl points are above the Fermi level we could not see any topological features by measuring the MR and Hall. We might, on the other hand, observe an anomaly in the Nernst and Seebeck effects.

We quantify a moderate magnitude of the Nernst coefficient, we compare it with other compounds from the same family of materials and we discuss the role of electron mobility on the magnitude of Nernst coefficient.

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Investigation of the magnetic structure of $RE_3Fe_3Sb_7$ (RE=Nd, Pr) by means of ^{57}Fe Mössbauer spectroscopy and μSR

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$RE_3Fe_3Sb_7$ is an intermetallic compound that shows interplay of iron and rare earth magnetism. While the Fe order sets in above room temperature, a second transition can be observed at $50\ \mathrm{K}$ (Nd) or $40\ \mathrm{K}$ (Pr). The Fe atoms form equilateral triangles that are stacked along the c-axis with a $60°$ rotation between layers. Similarly RE atoms form equilateral triangles stacked along the c axis with Sb layers separating the stacks.

^{57}Fe Mössbauer spectra show two magnetically distinct Fe-sites at room temperature exhibiting magnetic hyperfine fields of $B_{\mathrm{Hyp1}} = 14.75(15)\ \mathrm{T}$ and $B_{\mathrm{Hyp2}} = 13.89(15)\ \mathrm{T}$. The absorption intensities are split in a 5:4 area ratio in the spectra. The magnetic hyperfine fields of both sites obtained from the Mössbauer spectra develop with temperature following a $B_{\mathrm{Hyp}} = B_0(1 - (T/T_{\mathrm{C}})^{\alpha})^{\beta}$ behavior where only B_0 differs between both sites. At the second transition both sites collapse on the larger field. By applying an external field of $0.1\ \mathrm{T}$ transversal to the photon beam a considerably turning of the Fe moments is observed in the Mössbauer spectrum at room temperature. We will discuss the implications on the magnetic structure. μSR measurements show a strong change of the local magnetic field at the muon site through the second transition. A dynamic fluctuation peak is visible at $175\ \mathrm{K}$.

Fluctuation-induced ferrimagnetism in sublattice-imbalanced antiferromagnets with application to $SrCu_2(BO_3)_2$ under pressure

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In this poster, we show that a collinear Heisenberg antiferromagnet composed of equal-sized spins develops a uniform magnetization at nonzero temperatures below the Néel temperature once sublattice symmetry is broken at the Hamiltonian level. By using a combination of spin-wave and Landau theories, we first demonstrate how this phenomenon of fluctuation-induced ferrimagnetism manifests in a layered variant of a square-lattice J_1-J_2 model, and then extend our analysis to a case of direct experimental relevance, namely that of $SrCu_2(BO_3)_2$. Known as a near realization of a paradigmatic model of frustrated magnetism, the Shastry-Sutherland model, this material has attracted great attention over the past years as experiments revealed that it undergoes multiple phase transitions driven by hydrostatic pressure. In particular, there are indications that $SrCu_2(BO_3)_2$ exhibits antiferromagnetic order with two inequivalent magnetic sublattices at high pressures. By considering a layered version of the Shastry-Sutherland model, we suggest that this ordered phase of $SrCu_2(BO_3)_2$ is in fact a fluctuation-induced ferrimagnet, and we predict that its uniform magnetization evolves non-monotonically with temperature.

Divergence of the Grüneisen ratio at symmetry-enhanced first-order quantum phase transitions

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The so-called Grüneisen ratio, i.e. the ratio between thermal expansion and specific heat, diverges at a quantum critical point in a power-law manner. This divergence is seen as a characteristic of quantum critical points, i.e. continuous quantum phase transitions. Interestingly, we show that the Grüneisen ratio can also generically diverge at discontinuous *symmetry-enhanced* quantum phase transitions. A symmetry-enhanced phase transition is a phase transition where distinct symmetries in separate phases converge to the same symmetry at the phase boundary. Because of this, discontinuous symmetry-enhanced quantum phase transitions share fundamental features with continuous quantum phase transitions. In particular, spontaneous symmetry breaking at the transition leads to a vanishing mode gap because there must be at least one mode turning to a Goldstone mode. This vanishing energy scale leads to a power-law divergence of the Grüneisen ratio as at a quantum critical point, but with mean-field exponents. We investigate discontinuous quantum phase transitions with an explicit symmetry enhancement in the XZ and XXZ quantum spin model. The phenomenology outlined in this talk may be applicable to a number of correlated-electron materials where unconventional first-order-like transitions have been detected. One example could be $Ce_3Pd_{20}Si_6$.

Impurities in α-$RuCl_3$

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In recent years, α-$RuCl_3$ has been a prime candidate in realizing Kitaev's model on the honeycomb lattice. Experiments such as nuclear magnetic resonance and thermal transport measurements provide strong evidence on the importance of impurities in the material in the presence of a magnetic field. Using a T-matrix calculation we find that when a bond impurity is present, low energy magnetic excitations appear inside the gap of the high-field phase. Finally, we investigate the formation of textures in the case of strong impurities.

Dilution of the Kitaev candidate α-$RuCl_3$ by non-magnetic elements

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During the last several years, α-$RuCl_3$ has been attracting a lot of interest due to its proximity to the Kitaev honeycomb model [1]. It is a van der Waals material where each layer has a honeycomb arrangement of edge-sharing $RuCl_6$ octahedra. Single crystals of α-$RuCl_3$ order antiferromagnetically (with a zigzag arrangement of Ru^{3+} spins) at $7\ \mathrm{K}$ and $14\ \mathrm{K}$ [2]. These different ordering temperatures correspond to various stacking sequences: ABC and AB, respectively. Suppression of these magnetic transitions may lead to new quantum states, and, therefore, is of great interest. Magnetic order in α-$RuCl_3$ can be suppressed by an external magnetic field of $\mu_0 H_c \approx 6.9\ \mathrm{T}$ [3]. Another approach is to dilute the magnetic system of α-$RuCl_3$ by non-magnetic elements. With this aim, we modified the crystal structure of α-$RuCl_3$ along two different routes.

The first route considers the substitution of magnetic Ru^{3+} ($J_{\mathrm{eff}} = 1/2$) atoms by non-magnetic Rh^{3+} atoms. Polycrystalline powders and single crystals of $Ru_{1-x}Rh_xCl_3$ ($x = 0.02 - 0.45$) were grown from a gas phase. The doping rate was controlled by calibrated energy dispersive X-ray spectroscopy. For structural characterization, X-ray diffraction studies were performed. Magnetization data was measured using a SQUID magnetometer. It was found out that $Ru_{1-x}Rh_xCl_3$ is isostructural to α-$RuCl_3$ and dopants are randomly distributed. The suppression of the long-range magnetic order is observed at $x \sim 0.2$ leading to a possible quantum spin liquid state.

The second route represents the electrochemical intercalation of K^+ ions into the van der Waals gaps of α-$RuCl_3$ in order to reduce some magnetic Ru^{3+} to non-magnetic Ru^{2+}. New K_xRuCl_3 ($x = 0.5 - 0.8$) material has formed; its crystal structure was determined using 3D electron diffraction. The Néel temperatures of K_xRuCl_3 crystals decrease down to $2.1\ \mathrm{K}$.

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Modeling the honeycomb magnet $Na_2Co_2TeO_6$: Significance of ring exchange

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The frustrated honeycomb material $Na_2Co_2TeO_6$ is proposed as an approximate Kitaev magnet. The spin-wave spectrum obtained by inelastic neutron scattering shows characteristic low-energy branches which indicate triple-Q magnetic order in this material. Bilinear pseudo-spin models favor zigzag instead of triple-Q order for realistic model parameters. However, ring exchange may be relevant in the description of the magnetic structure if Hubbard t/U is not too small. For a controlled analysis, we start with a dual Heisenberg model where the two phases are degenerate. Adding a ring-exchange term stabilizes the triple-Q order, and the low-energy part of the spin-wave spectrum can be well fitted. The large gap between the low-energy and high-energy parts of the spectrum cannot be reproduced by only nearest-neighbor interactions, so next-nearest-neighbor interactions or broken lattice symmetry have to be taken into account.

Crystal growth and characterization of unconventional magnets $PbCuTe_2O_6$ & Ba_2CoWO_6

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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. Large crystals are essential for further detailed investigation of frustrated quantum magnetism using advanced measuring techniques including inelastic neutron scattering (INS_). Among many interesting frustrated magnets, only few of them were possible to obtain in a single crystalline form due to the melting nature of these compounds. In this talk, large and good-quality single crystals of the compounds $PbCuTe_2O_6$ and Ba_2CoWO_6 were obtained. Single crystals of the three- dimensional quantum spin-liquid candidate $PbCuTe_2O_6$ were grown using both the travelling solvent floating zone (TSFZ) and the top-seeded solution growth (TSSG) techniques. An anomaly around a temperature of $1\ \mathrm{K}$ is revealed in thermodynamic probes of both annealed powder and single crystalline samples. Curiously the position and magnitude of the transition are strongly dependent on the crystallite size and it is almost entirely absent for the smallest crystallites. Ba_2CoWO_6 single crystals were grown using the floating zone technique. The magnetic excitations measured using inelastic neutron scattering revealed the presence of sharp spin waves excitations below $4.5\ \mathrm{meV}$, these excitations have a small gap indicating a weak anisotropy of the Co^{2+} moment. Our measurements also revealed the presence of weak diffuse magnetic signal extending up to $8\ \mathrm{meV}$. This unexpected signal could be due to multi-magnon scattering which suggests the presence of magnetic fluctuations in the ground state possibly due to additional frustrated terms in the Hamiltonian beside the second neighbour interaction.