2021 Retreat of the ct.qmat Quantum Matter Academy

October 11 - 13, 2021
Radisson Blu Hotel in Erfurt

ct.qmat

Complexity and Topology in Quantum Matter

Monday, October 11

- 12:00	Arrival
12:00 - 14:00	Lunch
14:30 - 14:40	Welcome Note from the Organisers
14:40 - 15:00	Introduction to QMA/ct.qmat by Matthias Bode
Session 1: Magnetism & Topology	
15:00 - 15:20	Laura Christina Folkers, TU Dresden [S1.1] *Occupancy Disorder and Magnetism in Tetradymite Based Topological Insulators*
15:20 - 15:40	Christian Northe, JMU Würzburg [S1.2] *Ideal Chern Bands in Magnetic Fields*
15:40 - 16:00	Jonas Schwab, JMU Würzburg [S1.3] *Nematic Quantum Criticality in a Dirac Semimetal*
16:00 - 16:15	Coffee Break
Session 2: Artificial Topology 1 & Flash poster presentation	
16:15 - 16:35	Tobias Hofmann, JMU Würzburg [S2.1] *Non-linear Topolectric Circuits: A new Frontier in Synthetic Metamaterial Design*
16:35 - 16:55	Tobias Helbig, JMU Würzburg [S2.2] *The Reciprocal Skin Effect and its Realization in a Topolectric Circuit*
16:55 - 17:15	Flash Poster Presentation (P1 to P11)
17:15 - 17:30	*Short Break*
17:30 - 19:00	Fire Place Chat with Sol Jacobsen (NTNU) and Tobias Meng (TU Dresden)
19:00 -	Dinner and Ice Breaker (open end)

Tuesday, October 12

7:00 - 8:30	Breakfast
Session 3: Kondo & Magnetism & Flash Poster presentation	
8:30 - 8:50	Felix Friedrich, JMU Würzburg [S3.1] *Revisiting a Classic Kondo-System: Co/Cu(111)*
8:50 - 9:10	Mary Madelynn Nayga, TU Dresden [S3.2] *Strain Tuning of Highly Frustrated Magnets: Order and Disorder in the Distorted Kagome Heisenberg Antiferromagnet*
9:10 - 9:30	Flash Poster Presentation (P12 - P22)
9:30 - 9:45	Coffee Break
Session 4: Novel Theoretical and Numerical Approaches	
9:45 - 10:05	Pablo Basteiro, JMU Würzburg [S4.1] *Quantum Complexity as Hydrodynamics*
10:05 - 10:25	Lorenzo Crippa, TU Dresden [S4.2] *Fourth-Order Exceptional Points in Correlated Quantum Many-Body Systems*
10:25 - 10:45	Alexander Stegmaier, JMU Würzburg [S4.3] *Hyperbolic Lattices in Topolectrical Circuits*
10:45 - 11:00	Coffee Break
Session 5: Artificial Topology 2 & Flash poster presentation	
11:00 - 11:20	Alexander Fritzsche, JMU Würzburg [S5.1] *Two-Dimensional Floquet Topological Insulator with PT-Symmetry*
11:20 - 11:40	Lavi Kumar Upreti, JMU Würzburg [S5.2] *Hyperbolic Hofstadter Butterfly*
11:40 - 12:00	Flash Poster Presentation (P23 - P33)
12:00 - 14:00	Lunch
14:00 - 14:30	Group Photo Session
14:30 - 17:30	Treasure Hunt across Erfurt
17:30 - 19:00	Dinner
19:00 -	Poster Session (open end)

Wednesday, October 13

7:00 - 8:30	Breakfast
Session 6: Magnetism	
8:30 - 8:50	Michel Marcos Jordão Miranda, TU Dresden [S6.1] *The Phase Diagram of a Heisenberg Model: from Disorder to Order and Back Again*
8:50 - 9:10	Sven Luther, Helmholtz-Zentrum Dresden-Rossendorf [S6.2] *NMR and Pulsed-Field Magnetization of Frustrated Triangular-Lattice Delafossites*
9:10 - 9:30	Andreas Hauspurg, Helmholtz-Zentrum Dresden-Rossendorf [S6.3] *Anomalous Elastic Properties Near the Quantum Critical Point in $CoNb_2O_6$*
9:30 - 9:45	Coffee Break
Session 7: Superconductivity	
9:45 - 10:05	Artem Odobesko, JMU Würzburg [S7.1] *STM Functionalized Tips - One Step Beyond the Resolution Limits*
10:05 - 10:25	Viktoriia Kornich, JMU Würzburg [S7.2] *Direct Detection of Odd-Frequency Superconductivity via Time-and Angle-Resolved Photoelectron Fluctuation Spectroscopy*
10:25 - 10:45	Tilman Schwemmer, JMU Würzburg [S7.3] *Nature of Unconventional Pairing in the Kagome Superconductors AV_3Sb_5*
10:45 - 12:00	Election for QMA representatives, Evaluation, Poster Award, Closing
12:00 -	Departure or Lunch

Shortlist of Poster Contributions

P1	Bhargava Balaganchi Anantha Ramu, IFW Dresden
	Non-Hermitian Skin Effect of Dislocations and its Topological Origin
P2	Bernhard Frank, TU Dresden
	Single-Particle Properties and Critical Behavior of a 3d Metal Coupled to Critical 2d Spin-Density Waves
P3	Robin Boshius, JMU Würzburg
	Comparative Growth Study of Ultrathin Bi Films on Clean and Oxygen-Reconstructed Nb(110)
P4	Eduardo Carrillo, TU Dresden
	Discovery, Crystal Growth and Crystal Structure of the Topological Insulator Candidate $Bi_{12}RH_3Ag_6I_9$
P5	Johannes Heßdörfer, JMU Würzburg
	Electronic Structure of Novel Crystalline Materials
P6	Andreas Christ, JMU Würzburg
	Electron and Hole like Transport in Shockley Type Surface Stated Detected by MONA
P7	Armando Consiglio, JMU Würzburg
	Adsorption of Small Molecules on the (110) Surface of the Dirac Semimetal RuO_2
P8	Jonas Erhardt, JMU Würzburg
	Observation of Dirac Fermions in a Triangular Topological Insulator
P9	Florian Goth, JMU Würzburg
	Higher Order Auxiliary Field Quantum Monte Carlo Methods
P10	Patrick Härtl, JMU Würzburg
	Magnetic Domain Structures on Gd(0001)/W(110) Films
P11	Maria Herz, TU Dresden
	Substitution Series in the $Bi_2[PtBi_6I_{12}]_3$ System
P12	Rebeca Ibarra, MPI-CPfS Dresden
	Topological Hall Effect in Thin Films of Noncollinear Magnets
P13	Philipp Kagerer, JMU Würzburg
	Accessing Surface Magnetic and Electronic Properties of $MnBi_2Te_4$ by X-Ray Spectroscopy and Thin-Film Growth

P14	Jiwoong Kim, MPI-CPfS Dresden
	Molecular Beam Epitaxy of Topological Superconductor YPtBi Thin Films
P15	Wilhelm Krüger, TU Dresden
	Nesting Instability of Gapless U(1) Spin Liquids with Spinon Fermi Pockets in Two Dimensions
P16	Markus Leisegang, JMU Würzburg
	Strong Anisotropy in the Ballistic Transport Regime on Pd(110)
P17	Ruben Lier, MPI-PKS Dresden
	Bose-Hubbard Realization of Fracton Defects
P18	Zihong Liu, JMU Würzburg
	Exotic Quantum Criticality in Dirac Systems: Metallic and Deconfined
P19	Sebastian Felipe Mantilla Serrano, MPI-PKS Dresden
	Bosonization of the $Q = 0$ Continuum of Dirac Fermions
P20	Pedro Monteiro Consoli, TU Dresden
	Fluctuation-Induced Ferrimagnetism in Sublattice-Imbalanced Antiferromagnets with Application to $SrCu_2(BO_3)_2$ under Pressure
P21	Artem Odobesko, JMU Würzburg
	STM Functionalized Tips - One Step Beyond the Resolution Limits
P22	Ena Osmic, Helmholtz-Zentrum Dresden-Rossendorf
	Thermopower and Magnetotransport Properties of $Bi_{100-x}Sb_x$ Topological Insulator Thin Films Prepared by Rapid Quenching
P23	Falk Pabst, TU Dresden
	Modification of Magnetic Behavior in $La_xNd_{3-x}Fe_3Sb_7$
P24	Benedikt Placke, MPI-PKS Dresden
	Jamming Dynamics in a Hardcore Spin System
P25	Shouryya Ray, TU Dresden
	Gross-Neveu-SO(3) Quantum Criticality
P26	Christian Niclaas Saggau, IFW Dresden
	Periodic Waveguide Ring Arrays Fabricated in a Microtube Cavity Towards Topological Phase Transition
P27	Jakub Schusser, JMU Würzburg
	Spectroscopic Signatures of Non-trivial Topology in Weyl Semimetals

P28	Valentin Schwarze, Helmholtz-Zentrum Dresden-Rossendorf
	Fermi Surface of the Chiral Topological Semimetal PtGa with Maximal Chern Number
P29	Paula Weber, JMU Würzburg
	SP-STM Study of Magnetic Zig-Zag $2\sqrt{2} \times \sqrt{2}$ Structure on 3 AL Mn/W(001)
P30	Konstantin Weisenberger, JMU Würzburg
	Symmetry Resolved Entanglement in AdS/CFT
P31	Bimla Danu, JMU Würzburg
	Kondo Breakdown in a Spin-1/2 Chain of Adatoms on a Dirac Semimetal
P32	Andrew Ochs, TU Dresden
	Discovery of Axis-Dependent Conduction Polarity in $NaSnAs_{1-x}P_x$ through Computationally-Guided Methods
P33	Robin Schäfer, MPI-PKS Dresden
	The Pyrochlore $S = 1/2$ Heisenberg Antiferromagnet at Finite and Zero Temperature

Talk Abstracts

Occupancy Disorder and Magnetism in Tetradymite based Topological Insulators

S1.1

Laura Christina Folkers, TU Dresden

Magnetic topological insulators (MTIs) are a hot topic of materials science, promising future availability of spintronics with low energy consumption, quantum computing and phenomena like the Quantized Anomalous Hall Effect (QAHE) [1-2]. MTIs are chemically and structurally akin to the original non-magnetic topological insulators. Of those, the tetradymites Bi_2Te_3 and Sb_2Te_3 have recently proven to allow the introduction of a third magnetic element resulting in magnetically active, topologically non-trivial compounds. A magnetic element can be incorporated either via substitution on the Bi/Sb position in $(Bi, Sb)_2Te_3$, or by adding a third element which introduces a new crystallographic site, resulting for example in $MnBi_2Te_4$. $(Bi, Sb)_2Te_3$ itself and all members of its family exhibit the rhombohedral $R\bar{3}m1$ space group (No. 166) [2]. Therein interchanging sheets of Mn, (Bi, Sb) and Te build septuple layers with the central sheet being Mn. Situated between the respective layers is a van der Waals gap.

Our group was the first to successfully grow single crystals, and conduct an in depth study of the physical properties of $MnBi_2Te_4$ [4-5]. Single crystal diffraction experiments reported in that study showed intermixing of Mn and Bi and since then several studies have reported intermixing of the two elements ($MnBi_{2.14}Te_{3.96}$ [6], $Mn_{1.01}Bi_{1.99}Te_4$ and $Mn_{0.98}Bi_{2.05}Te_4$ [7]). While a lot of attention has been given to $MnBi_2Te_4$, $MnSb_2Te_4$ proved to be synthetically achievable too. Similar to $MnBi_2Te_4$, $MnSb_2Te_4$ features intermixing of Mn and Sb ($Mn_{0.852}Sb_{2.296}Te_4$ [8]). For $MnSb_2Te_4$, a recent study by Murakami et al. uncovers the impact of finding a certain amount of the magnetic Mn on the position of the non-magnetic Sb [9]. According to their discoveries, this changes the magnetic order from antiferromagnetic to ferrimagnetic.

These compounds are known to react sensitively to synthesis procedure and

tempering history. Hence, our studies aim at understanding the greater connection between synthesis aspects and the resulting structural and physical properties. More precisely we studied $MnBi_2Te_4$ and $MnSb_2Te_4$ containing various amounts of Mn and other analogues of these systems. In these studies we uncovered, that the magnetism in $MnSb_2Te_4$ is even more sensitive to annealing procedures than previously expected.

[1] Y. Ando, Journal of the Physical Society of Japan, (2013), 82, 102001

[2] I. I. Klimovskikh, M. M. Otrokov, D. Estyunin, et al., Quantum Materials, (2020), 54.

[3] Y. Feutelais, B. Legendre, N. Rodier, V. Agafonov, Materials Research Bulletin, (1993), 28, 591-596

[4] A. Zeugner, F. Nietschke, A. U. B. Wolter, et al., Chemistry of Materials, (2019), 31, 2795-2806.

[5] M. M. Otrokov, I. I. Klimovskikh, H. Bentmann, et al., Nature, (2019), 576, 416-422.

[6] H. Li, S. Liu, C. Liu, et al., Physical Chemistry Chemical Physics, (2020), 22, 556-563.

[7] M.-H. Du, J. Yan, V. R. Cooper, M. Eisenbach, Advanced Functional Materials, (2020), 2006516.

[8] L. Zhou, Z. Tan, D. Yan, et al., Physical Review B, (2020), 102, 85114.

[9] T. Murakami, Y. Nambu, T. Koretsune, et al., Physical Review B, (2019), 100, 195103.

back to timetable ↑

Ideal Chern Bands in Magnetic Fields

S1.2

Christian Northe, JMU Würzburg

Under ideal conditions, Chern insulators (CI) have excitations of fractional charge arising due to the Berry curvature rather than a magnetic field. We initiate the analytic study of ideal CIs which are subject to both effects, Berry curvature and magnetic field. The short term goal presented here is to provide a class of band geometries for ideal CIs with both Ω and B. The long term goal of this program is to understand the interplay of Ω and B in the formation of excitations of fractional charge. Our focus lies on magnetic fields, which are strong enough to affect the band structure, but weaker than the threshold leading to the Hofstadter phase.

back to timetable ↑

Nematic Quantum Criticality in a Dirac Semimetal

S1.3

Jonas Schwab, JMU Würzburg

We investigate models of Dirac fermions coupled to an Ising model in a transverse field. The coupling is such that the Ising transition tiggers nematic symmetry breaking in the Dirac system. The Hamiltonians we consider possess C_{2v} as well as C_{4v} symmetries that are reduced respectively to reflection and C_{2v} in the Ising ordered phase. Using negative sign free quantum Monte Carlo simulations as well as an ϵ-expansion renormalization group analysis, we show that both models exhibit continuous phase transitions. In contrast to generic Gross-Neveu dynamical mass generation transitions, the critical points are characterized by velocity anisotropies such that Lorentz symmetry is not emergent.

back to timetable ↑

Non-linear Topolectric Circuits: A new Frontier in Synthetic Metamaterial Design

S2.1

Tobias Hofmann, JMU Würzburg

Topolectric circuits have proven themselves as a versatile, easily accessible and flexible platform to study topological states in metamaterials. As of yet, the majority of explored models are linear circuits, consisting only of resistors, capacitors, and inductors, despite the family of electric circuit elements being far larger. Circuit networks incorporating non-linear components, such as diodes, transistors or more complex analog multipliers, promise new intriguing phenomena, such as the interplay of non-linear chaos with topology. In this presentation, we will summarize the field's state of the art, which reaches from Floquet states in periodically driven networks to Soliton solutions of non-linear transmission lines. We will elaborate on the chances and challenges non-linearities pose, and argue that they will be paramount for the next step in metamaterial design.

back to timetable ↑

The Reciprocal Skin Effect and its Realization in a Topolectric Circuit

S2.2

Tobias Helbig, JMU Würzburg

The non-Hermitian skin effect constitutes a new paradigm in the research and design of synthetic metamaterials. It fundamentally relies on the combined breaking of Hermiticity and reciprocity. In this talk, we present the novel approach of obtaining extensive eigenmode localization in the presence of reciprocity. In contrast to non-reciprocal implementations of the Skin effect which require an external energy supply, our approach can be implemented by exclusively passive components. We demonstrate this in a passive RLC circuit network. The reciprocal Skin effect suggests itself for realizations in a plethora of metamaterial platforms with limited availability of active components.

back to timetable ↑

Revisiting a Classic Kondo-System: Co/Cu(111)

S3.1

Felix Friedrich, JMU Würzburg

Single cobalt atoms on the (111) surfaces of noble metals were long time considered prototypical systems of the Kondo effect in STM experiments [1]. Spectroscopic measurements on these atoms reveal a Fano-like dip around the Fermi-level, which was explained by two interfering tunneling paths of electrons, one directly into the surface and the second one into a Kondo resonance. However, Bouaziz et al. [2] recently proposed that the observed feature actually originates from spin-flip excitations of the Co atom spin induced by the tunneling electrons. Further, interaction between these spin-flip excitations and conduction electrons was predicted to lead to the formation of a new quasiparticle, called spinaron. We investigated Co atoms on the Cu(111) surface in magnetic fields of up to 12 T and found features that are in disagreement with the former interpretation of the spectroscopic signal as a Kondo resonance. These new experimental results and possible explanations will be discussed.

[1] Science 280, 567 (1998); Nature 403, 512 (2000); PRB 65, 121406 (2002)
[2] Nat. Commun. 11, 6112 (2020)

back to timetable ↑

Strain Tuning of Highly Frustrated Magnets: Order and Disorder in the Distorted Kagome Heisenberg Antiferromagnet

S3.2

Mary Madelynn Nayga, TU Dresden

Strain applied to a condensed-matter system can be used to engineer its excitation spectrum via artificial gauge fields, or it may tune the system through transitions between different phases. Here we demonstrate that strain tuning of the ground state of otherwise highly degenerate frustrated systems can induce novel phases, both ordered and disordered. For the classical Heisenberg antiferromagnet on the kagome lattice, we show that weak triaxial strain reduces the degeneracies of the system, leading to a classical spin liquid with noncoplanar configurations, while stronger strain drives the system into a highly unconventional state which displays signatures of both spin-glass behavior and magnetic long-range order. We provide experimentally testable predictions for the magnetic structure factor, characterize the ground-state degeneracies and the excitation spectrum, and analyze the influence of sample shape and boundaries. Our work opens the way to strain engineering of highly frustrated magnets.

back to timetable ↑

Quantum Complexity as Hydrodynamics

S4.1

Pablo Basteiro, JMU Würzburg

We consider Nielsen's geometric approach to operator complexity for the SU(N) group. We develop a tractable large N limit which leads to regular geometries on the manifold of unitaries. To achieve this, we introduce a particular basis for the $\mathfrak{su}$(N) algebra and define a maximally anisotropic metric with polynomial penalty factors. We implement the Euler-Arnold approach to identify incompressible inviscid hydrodynamics on the two-torus as a novel effective theory for the evaluation of operator complexity of large qudits. The resulting complexity geometry exhibits essential properties of holographic complexity measures, such as ergodicity and conjugate points.

back to timetable ↑

Fourth-Order Exceptional Points in Correlated Quantum Many-Body Systems

S4.2

Lorenzo Crippa, TU Dresden

Non-Hermtian (NH) Hamiltonians effectively describing the physics of dissipative systems have become an important tool with applications ranging from classical meta-materials to quantum many-body systems. Exceptional points, the NH counterpart of spectral degeneracies, are among the paramount phenomena unique to the NH realm. While realizations of second-order exceptional points have been reported in a variety of microscopic models, higher-order ones have largely remained elusive in the many-body context, as they in general require fine tuning in high-dimensional parameter spaces. Here, we propose a microscopic model of correlated fermions in three spatial dimensions and demonstrate the occurrence of interaction-induced fourth-order exceptional points that are protected by chiral symmetry. We demonstrate their stability against symmetry breaking perturbations and investigate their characteristic analytical and topological properties.

back to timetable ↑

Hyperbolic Lattices in Topolectrical Circuits

S4.3

Alexander Stegmaier, JMU Würzburg

Hyperbolic lattices challenge the conventional wisdom of crystallography in various ways. They defy a description by Bloch theory, cannot be compactified by simple periodic boundary conditions and have an extensive amount of boundary sites. Investigating their properties may reveal phenomena and applications that have no direct equivalent in flat lattices. We realize a hyperbolic tiling in an electrical circuit and measure signatures of the inherent negative curvature in its spectral properties and signal propagation. Furthermore, we investigate and develop methods extending concepts such as periodic boundaries and a notion of band theory to hyperbolic lattices.

back to timetable ↑

Two-Dimensional Floquet Topological Insulator with PT-Symmetry

S5.1

Alexander Fritzsche, JMU Würzburg

Gain and loss are characteristic features of open or Non-Hermitian systems and lead, in general, to instable, exponentially increasing and decreasing states. However, these instabilities can be avoided when parity-time (PT) symmetry is added to such arrangements. Because of its unique properties it has been tried to combine PT symmetry with the unrivalled robustness of transport in topological insulators. In this work we propose and experimentally realise a periodically driven topological insulator with two counterpropagating boundary states where gain and loss are distributed not only spatially but also temporally using a photonic platform. Here the periodic driving allows us to circumvent the problems that have so far hindered the combination of PT symmetry and topological insulators thereby allowing us to provide the missing link between these two realms.

back to timetable ↑

Hyperbolic Hofstadter Butterfly

S5.2

Lavi Kumar Upreti, JMU Würzburg

We explore the energy spectrum of a regular hyperbolic lattice in the presence of a constant magnetic field, which is known as the Hofstadter butterfly. In the euclidean case, where this spectrum has an intricate fractal pattern, in the hyperbolic case, such intricacy is smooth out by the underlying curvature of the lattice. Unlike the previous (euclidean) case, where any non-zero magnetic field captures the particle giving rise to the Landau levels, this ceases to be the case in hyperbolic. Interestingly, in the latter case, a critical field exists after only the magnetic field can capture a particle. Hence the Landau levels only appear after such fields. This fact is clearly reflected in the hyperbolic Hofstadter butterfly spectrum.

back to timetable ↑

The Phase Diagram of a Heisenberg Model: from Disorder to Order and Back Again

S6.1

Michel Marcos Jordão Miranda, TU Dresden

In this work we study the effects of bond and site disorder in the classical $J_1 - J_2$ Heisenberg model on a square lattice in the order-by-disorder frustrated regime $2J_2 > |J_1|$. Combining symmetry arguments, numerical energy minimization, and large-scale Monte Carlo simulations, we see that the finite temperature Ising-like transition of the clean system is destroyed in the presence of any finite concentration of impurities. The explanation for this finding comes from a random-field mechanism which generically emerges in systems where disorder locally breaks the same real-space symmetry spontaneously globally broken by the associated order parameter. In this way, the system goes from disorder (frustration) to order (order-by-disorder mechanism) and then back again to disorder (impurities).

back to timetable ↑

NMR and Pulsed-Field Magnetization of Frustrated Triangular-Lattice Delafossites

S6.2

Sven Luther, Helmholtz-Zentrum Dresden-Rossendorf

The Yb-based delafossites $NaYbCh_2$ (Ch = O, S, Se) are triangular-lattice antiferromagnets with a trigonal crystal structure (space group $R\bar{3}m$). In these compounds, spin-orbit coupling and the crystal electric field lead to a pronounced magnetic anisotropy and a pseudospin-1/2 ground state at low temperatures. The chalcogen series provides the possibility for tuning the interlayer distance and the associated exchange couplings by changing the chemical composition. The absence of magnetic long-range order at zero field is suggestive for a quantum spin-liquid ground state. From specific-heat and magnetization experiments, magnetically ordered states were observed for applied fields exceeding 2 T for all three compounds. Measurements of the magnetization up to very high magnetic fields of 30 T allow to determine the saturation fields and polarized moments and, thus, the determination of the in-plane and out-of-plane exchange couplings. Further, our ^{23}Na NMR measurements of $NaYbSe_2$ aim to probe the microscopic details of the field-induced magnetic structure in this compound. Measurements of the field-dependent transition temperature to long-range order via analysis of the $1/T_1$-relaxation rate are in agreement with specific-heat results. For in-plane fields of several tesla, the magnetization indicates an up-up-down spin arrangement, leading to an asymmetric broadening of the NMR spectra. At elevated out-of-plane fields, an umbrella-type configuration of the magnetic moments is predicted and in agreement with a symmetric broadening of the ^{23}Na NMR spectra. Low-field measurements reveal a monotonic low-temperature increase of the $1/T_1$-relaxation rate and spectral broadening, without any signature of long-range order down to 0.3 K.

back to timetable ↑

Anomalous Elastic Properties Near the Quantum Critical Point in $CoNb_2O_6$

S6.3

Andreas Hauspurg, Helmholtz-Zentrum Dresden-Rossendorf

Quantum critical behavior is a central issue in condensed matter physics and can be important for future quantum technologies. At the quantum critical point (QCP) a phase transition, driven by quantum fluctuations, occurs at a temperature of absolute zero. $CoNb_2O_6$ is a model system for the so-called spin-1/2 one-dimensional transverse field Ising model (TFIM) and shows a QCP at 5.4 T. The spin-strain and spin-orbit interactions play an important role in the quantum critical regime of this material. We study $CoNb_2O_6$ close to the QCP by means of ultrasound pulsed-echo technique. Here we present and discuss the anomalous elastic properties near the QCP observed in our experiments.

back to timetable ↑

STM Functionalized Tips - One Step Beyond the Resolution Limits

S7.1

Artem Odobesko, JMU Würzburg

STM and STS is a powerful techniques for local probing of the topography on the atomic level and electron densities of states. Nonetheless, there are limitations on the spatial and energy resolution due to the irregular shape of the tip and the effect of thermal broadening. These limitations can be overcome by functionalizing the STM tip apex with CO molecule to increase the spatial resolution of the tip or tunneling from a superconducting tip to exclude thermal broadening of the Fermi step of a normal metal tip. Here we try to combine both approaches to obtain an extra energy resolution with extra spatial resolution. With the help of such a ultra-functionalized STM tip, we are able to resolve rapidly decaying in space oscillations of Yu-Shiba-Rusinov bound states near magnetic Fe dimer on the bare Nb(110) surface. This allows us, for the first time, to determine the Fermi wavelength of Nb(110) surface. Such ultra-functionalized STM tips take the STM technique to the next level.

back to timetable ↑

Direct Detection of Odd-Frequency Superconductivity via Time- and Angle-resolved Photoelectron Fluctuation Spectroscopy

S7.2

Viktoriia Kornich, JMU Würzburg

We propose a measurement scheme to directly detect odd-frequency superconductivity via time- and angle-resolved photoelectron fluctuation spectroscopy. The scheme includes two consecutive, non-overlapping probe pulses applied to a superconducting sample. The photoemitted electrons are collected in a momentum-resolved fashion. Correlations between signals with opposite momenta are analyzed. Remarkably, these correlations are directly proportional to the absolute square of the time-ordered anomalous Green's function of the superconductor. This setup allows for the direct detection of the "hidden order parameter" of odd-frequency pairing. We illustrate this general scheme by concretely analyzing the signal for the prototypical case of two-band superconductors, which are known to exhibit odd-frequency pairing under certain conditions.

back to timetable ↑

Nature of Unconventional Pairing in the Kagome Superconductors AV_3Sb_5

S7.3

Tilman Schwemmer, JMU Würzburg

The recent discovery of AV_3Sb_5 (A = K, Rb, Cs) has uncovered an intriguing arena for exotic Fermi surface instabilities in a kagome metal. Among them, superconductivity is found in the vicinity of multiple van Hove singularities, exhibiting indications of unconventional pairing. We show that the sublattice interference mechanism is central to understanding the formation of superconductivity in a kagome metal. Starting from an appropriately chosen minimal tight-binding model with multiple with multiple van Hove singularities close to the Fermi level for AV_3Sb_5, we provide a random phase approximation analysis of superconducting instabilities. Non-local Coulomb repulsion, the sublattice profile of the van Hove bands, and the bare interaction strength turn out to be the crucial parameters to determine the preferred pairing symmetry. Implications for potentially topological surface states are discussed, along with a proposal for additional measurements to pin down the nature of superconductivity in AV_3Sb_5.

back to timetable ↑

Poster Abstracts

Non-Hermitian Skin Effect of Dislocations and its Topological Origin

P1

Bhargava Balaganchi Anantha Ramu, IFW Dresden

We demonstrate that dislocations in two-dimensional non-Hermitian systems can give rise to density accumulation or depletion through the localization of an extensive number of states. These effects are shown by numerical simulations in a prototype lattice model and expose a completely new face of non-Hermitian skin effect, by disentangling it from the need for boundaries. We identify a topological invariant responsible for the dislocation skin effect, which takes the form of a Z_2 Hopf index that depends on the Burgers vector characterizing the dislocations. Remarkably, we find that this effect and its corresponding signature for defects in Hermitian systems falls outside of the known topological classification based on bulk-defect correspondence.

back to shortlist ↑

Single-Particle Properties and Critical Behavior of a 3d Metal Coupled to Critical 2d Spin-Density Waves

P2

Bernhard Frank, TU Dresden

We study three-dimensional conduction electrons metal that interact with the fluctuations of an antiferromagnetic order parameter that characterizes the collective behavior of localized magnetic moments located within a single layer of the bulk. Based on a field theoretic model that incorporates the violation of momentum conservation perpendicular to the plane we identify hot and super-hot electrons with anomalous, non-Fermi liquid damping rates. In addition, we determine the critical behavior of the spin sector and give an outlook on electronic transport properties.

back to shortlist ↑

Comparative Growth Study of Ultrathin Bi Films on Clean and Oxygen-Reconstructed Nb(110)

P3

Robin Boshius, JMU Würzburg

We present a detailed study of the growth of Bi films on superconducting Nb(110) substrates in dependence on the Bi coverages and the Nb surface quality. We find that Bi grows in a (110) orientation at low coverage equivalent to about five pseudomorphic monolayers (ML) on clean Nb(110), but then undergoes a structural transition to Bi(111) below about 8 ML. Comparison with two oxygen-reconstructed Nb(110) surfaces, the NbO_x phases I and II, reveals that the film thickness at which the (110)-to-(111) transition takes place depends on the surface quality. Whereas it is observed at lower coverage for the NbO_x phase I, our results indicate that Bi(110) remains stable on NbO_x phase II up to the largest film thickness studied here, i.e., 18 ML. The quality and smoothness of the thin Bi films considerably depends on the cleanliness of the Nb substrate, revealing the most flat and defect-free Bi films grown on the oxygen-free clean Nb(110) surface. The proximity-effect-induced superconducting gap on the Bi surfaces will further be discussed.

back to shortlist ↑

Discovery, Crystal Growth and Crystal Structure of the Topological Insulator Candidate $Bi_{12}Rh_3Ag_6I_9$

P4

Eduardo Carrillo, TU Dresden

A stacking of $[Bi_{12}Rh_3I]^{2+}$ layers, a 2D topological insulator (TI), can be achieved by electrostatic stabilization with an anionic spacer, potentially creating a weak 3D TI. This was first observed for $Bi_{14}Rh_3I_9 = [Bi_{12}Rh_3I]^{2+}[Bi_2I_9]^{2-}$. We are investigating ways to replace the $[Bi_2I_9]^{2-}$ spacer with other layers. By doing so, we hope to introduce new features (e.g., ferromagnetism), but also to learn more about the relationship between the chemical composition and structure on the one hand and the topological properties on the other. Here, we report the synthesis and crystal structure of $Bi_{12}Rh_3Ag_6I_9$, a new compound from the same structural family. It is a periodic stack consisting of the same 2D TI layers $[Bi_{12}Rh_3I]^{2+}$ but now alternating with $[Ag_6I_9]^{2-}$ spacer layers. The spatial separation between the TI layers should be large enough to ensure a (non-trivial) band gap. AgI is one of the most prominent ionic conductors. In a very similar way to AgI, the Ag^+ cations in the $[Ag_6I_9]^{2-}$ spacer layer are distributed over several positions. This unique combination of an ionic conductor and a potential TI material opens up the possibility of electrochemically adjusting the composition to correct for n- or p-doping of the material with high precision. Both single-phase polycrystalline powders and single-crystals are available for further measurements. Electronic structure calculations would also be welcome.

back to shortlist ↑

Electronic Structure of Novel Crystalline Materials

P5

Johannes Heßdörfer, JMU Würzburg

The first synthesized and experimentally realized Weak Topological Insulator was $Bi_{14}Rh_3I_9$. It consists of 2D TI layers with a honeycomb lattice stacked with insulating spacer layers. The 2D TI is formed by rhodium centred bismuth cubes which form a Kagome lattice with iodine atoms in the middle of the lattice. A material with similar structure is $Bi_{13}Pt_3I_7$, it also consists of a 2D TI layer, composed of platinum centred bismuth cubes. Here the spacer layers lead to an alternating coupling and render the material topological trivial. By modifying the spacer layers in this materials the topological properties can be tuned. This led to the search of new compounds with similar structure, the first promising candidates are $Bi_{12}Rh_3Ag_6I_9$, $Bi_{12}Pt_3CuI_5$ and $Bi_{12}Pt_3AgI_5$. First investigations on the structural and electronic properties of this new materials were done by Angle Resolved Photoemission Spectroscopy, X-ray Photoelectron Spectroscopy, Low-Energy Electron Diffraction and Scanning Tunneling Microscopy. This poster will present the first results on the crystalline, atomic and electronic structure of these new compound. The results are promising and encourage further measurements to have a closer look at the electronic structure of the samples, which could confirm if the compound presents a non-trivial topology.

back to shortlist ↑

Electron and Hole like Transport in Shockley Type Surface States Detected by MONA

P6

Andreas Christ, JMU Würzburg

In recent years, we have established the molecular nanoprobe (MONA) technique to detect the transport of hot charge carriers over a distance of a few nanometers [1,2]. In short, MONA uses a charge carrier-driven molecular switching event, such as a tautomerization or rotation, to detect currents injected a few nanometers away. Earlier experiments performed on Ag(111) showed that the surface state characteristic for fcc(111) surfaces facilitates effective charge transport between the charge injection point towards and a single phthalocyanine (HPc) detector molecule [3]. Since, however, the energy threshold for tautomerization switching of HPc exceeds the energy onset of the Ag(111) surface state ($E = -63\,\mathrm{meV}$),detection was limited to electron transport whereas hole transport remained inaccessible. In order to investigate the influence of the band structure on the propagation of hot charge carriers we compare results of MONA experiments performed on Ag(111) with the isoelectronic Cu(111) surface. By focusing on the surface states of Cu(111) and Ag(111) we can compare qualitatively equivalent states which differ quantitatively due to the different energy onset. Our results reveal that due to the lower surface state onset in Cu(111) at $E = -440\,\mathrm{meV}$ hole-like charge transport can also be detected.

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back to shortlist ↑

Adsorption of Small Molecules on the (110) Surface of the Dirac Semimetal RuO_2

P7

Armando Consiglio, JMU Würzburg

A variety of catalytic oxidation and dehydrogenation reactions can be studied on the (110) surface of ruthenium dioxide (RuO_2), whose surface functionality are based on the interplay between Coulomb and kinetic energies, as well as on the interplay of lattice, spin-rotational and time-reversal symmetries. The catalytic qualities are directly related to the properties of its Fermi surface, with antiferromagnetic instabilities driven by a particularly large density of states. Indeed, besides of its outstanding performances and applications, this material gained attention because of its electronic and magnetic properties. The electronic structure induced by the crystal symmetry produces a complex Fermi surface composed of Dirac nodal lines and a consequent flat band surface state (FBSS), the latter having an active role in catalytic charge transfer processes at the oxygen bridge sites. Being tuned by surface doping and electrostatic environment, the FBSS presents an interesting playground for the study of surface chemistry. Also, the strong nesting of the Dirac nodal lines is prone to Fermi surface instabilities, a postulated driving force of the itinerant collinear antiferromagnetism. The proposed work shows the results of a combined theoretical and experimental effort; the aim is at the microscopic understanding of heterogeneous catalysis with a focus on the interplay of the catalyst's de-localized electronic band structure and the localized orbitals of its surface reactants, as well as on its thermodynamic properties.

back to shortlist ↑

Observation of Dirac Fermions in a Triangular Topological Insulator

P8

Jonas Erhardt, JMU Würzburg

Topology in two-dimensional lattices is often connected to a honeycomb-like arrangement of atoms. Contrary to that, we demonstrate the topological non-trivial nature of indenene, a triangular monolayer of indium atoms that hosts massive Dirac fermions at the K/K′-points. As in the case of the large gap topological insulator bismuthene [1,2], the underlying silicon carbide substrate plays a pivotal role for the low-energy physics. Here its electric field along the surface normal causes hybridization between indium p_z and p_+/p_- orbitals, thereby opening a large hybridization gap in the otherwise metallic film. In addition, the substrate creates a competing term to the spin-orbit coupling (SOC) induced gap at K/K′ by breaking the in-plane inversion symmetry (ISB). The ISB lifts the Kramers-degeneracy of the K/K′ bands and promotes orbital angular momentum polarization in a distinct sequence that is unambiguously linked to a SOC vs. ISB induced gap, i.e., the topological character of indenene. In real space, this information is translated to the lateral charge distribution of the unit cell due to interference of adjacent indium wavefunctions, each contributing orbital as well as Bloch-phase. We make use of this remarkable property of the bulk wavefunction to verify the topological non-trivial nature of indenene by mapping the local density of states via scanning tunneling spectroscopy [3].

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back to shortlist ↑

Higher Order Auxiliary Field Quantum Monte Carlo Methods

P9

Florian Goth, JMU Würzburg

The auxiliary field quantum Monte Carlo (AFQMC) method has been a workhorse in the field of strongly correlated electrons for a long time and has found its most recent implementation in the ALF package (`alf.physik.uni-wuerzburg.de`). The utilization of the Trotter decomposition to decouple the interaction from the non-interacting Hamiltonian makes this method inherently second order in terms of the imaginary time slice. We show that due to the use of the Hubbard-Stratonovich transformation (HST) a semigroup structure on the time evolution is imposed that necessitates the introduction of a new family of complex-hermitian splitting methods for the purpose of reaching higher order. We will give examples of these new methods and study their efficiency, as well as perform comparisons with other established second and higher order methods in the realm of the AFQMC method.

back to shortlist ↑

Magnetic Domain Structures on Gd(0001)/W(110) Films

P10

Patrick Härtl, JMU Würzburg

Due their partially filled 4f shell which are coupled by the RKKY interaction, rare earth metals exhibit long-range magnetic order. Depending on the sign of the RKKY coupling and details of the sample geometry many different domain structures have been observed. For example, spin-resolved STM studies of Dy(0001) thin films on W(110) revealed a six-fold symmetric magnetic domain structure [1]. Here we report on similar experiments on Gadolinium (Gd) films epitaxially grown on W(110). Gd is a ferromagnetic metal with a Curie temperature of 293 K. Its half-filled 4f shell results in a spherical charge distribution and therefore a rather small magnetic anisotropy in comparison other rare earth metals [2].

Earlier spatially averaging experiments performed by Berger et. al. [2] suggest that Gd(0001) films on W(110) exhibit a thickness-dependent spin reorientation transition at around 40 nm from in-plane at thin films to out-of-plane for thicker. Our investigation on Gd(0001) films grown on W(110) indeed show a rather rich spin structure in STM/STS studies. We observe spin spiral-like magnetic domains with an in-plane as well as out-of-plane magnetized STM tips. We will discuss the transition of the magnetic structure in dependence of the Gd film thickness.

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back to shortlist ↑

Substitution Series in the $Bi_2[PtBi_6I_{12}]_3$ System

P11

Maria Herz, TU Dresden

The reaction of Bi with Sn, Pt and BiI_3 above 300 °C yielded shiny, black, air insensitive crystals of the novel subiodide $Sn[PtBi_6I_{12}]$. Discovered during the search for novel topological insulators [1], the compound consists of alternating cuboctahedral $[PtBi_6I_{12}]^{2-}$ clusters and Sn^{2+} cations in an octahedral coordination between trigonal faces of two cuboctahedra, which concatenate them into linear chain, which makes it an analogue to the compound $Pb[PtBi_6I_{12}]$ [2]. Additionally, the crystals' cube-like morphology originates from six weaker Bi···I inter-cluster bridges per cluster connecting the chains. This, in combination with the composition of predominantly heavy elements, and hence a strong spin-orbit coupling within the compound, lead to the hope that the information obtained about the band gap could lead to this being fine-tuned and reduced in order to apply to other compounds and obtain topological properties.

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back to shortlist ↑

Topological Hall Effect in Thin Films of Noncollinear Magnets

P12

Rebeca Ibarra, MPI-CPfS Dresden

Topological spin textures in quantum materials are of great interest, along with the associate transport signatures, for next-generation spintronic applications. Spin chirality in metallic materials with noncoplanar spin structure gives rise to a Berry phase-induced topological Hall effect. Recently, the tetragonal (t) Heusler compounds show to host elliptical skyrmions and anti-skyrmions [1], and the hexagonal (h) half-Heusler compound MnPtGa displays noncollinear magnetism [2]. Here, we study the noncollinear spin textures in high-quality epitaxial thin films of the t-Mn_2RhSn and h-MnPtGa compounds. In t-Mn_2RhSn, we observe topological Hall signatures of two distinct chiral spin textures. By single-crystal neutron diffraction in a single thin film we show that the h-MnPtGa undergoes a magnetic phase transition from ferromagnetic to in-plane canted antiferromagnetic. With our thin film method, we can access a novel and fundamental understanding of these compounds not possible with other methods.

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back to shortlist ↑

Accessing Surface Magnetic and Electronic Properties of $MnBi_2Te_4$ by X-Ray Spectroscopy and Thin-Film Growth

P13

Philipp Kagerer, JMU Würzburg

With its discovery as the first antiferromagnetic topological insulator, $MnBi_2Te_4$ has reopened the question of how the interaction between the time reversal symmetry breaking magnetic order and the topological properties can influence the surface electronic structure of a compound [1]. By now several reports on small gap-openings in the surface state of the compound have been published, where effects connected to the magnetic transition have turned out to be very peculiar [2,3]. In this regard a lot of questions are still unanswered experimentally. These include the differences between the magnetic properties of $MnBi_2Te_4$ at its surface vs. its bulk, the potential influence of interfaces up to the question, what role surface magnetism can play in lifting the topological protection of the surface state. Here we will present a study on MBE grown $MnBi_2Te_4$ heterostructures facilitating various soft x-ray and VUV spectroscopy techniques. In recent years we have built up two twin MBE setups in Würzburg and Hamburg for in-situ photoemission experiments and established a flexible growth platform for the growth of $MnBi_2Te_4$ heterostructures on BaF_2 [4]. Facilitating these possibilities we will present insights on the magnetic properties of these materials and try to work out their influence on the electronic structure of the thin films.

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back to shortlist ↑

Molecular Beam Epitaxy of Topological Superconductor YPtBi Thin Films

P14

Jiwoong Kim, MPI-CPfS Dresden

Topological quantum materials have been extensively studied to explore new physics and novel application potentials. Recently, the topologically non-trivial surface state was observed on half-Heusler YPtBi, which led by band inversion like the topological insulator due to strong spin-orbit coupling in non-centrosymmetric crystal structure [1]. The unconventional superconductivity realized in bulk YPtBi is predicted to higher spin quasi-particles paring [2], suggesting this material as topological superconductor. This motivates us to investigate the topologically non-trivial state in YPtBi thin films. We installed a new molecular beam epitaxy setup to grow epitaxial YPtBi thin films by precisely controlled constituent elemental fluxes. The lattice constant of YPtBi, 6.652 Å, is relatively large compared to the available zinc-blende substrates. Therefore, the rock-salt KBr is regarded as one of the most suitable substrate candidates, which exhibits 0.8% lattice mismatch to YPtBi. In this poster presentation, recent progress in research to realize epitaxial YPtBi thin film growth on KBr substrates are shown. This includes preparation of atomically flat KBr terraces by a cleaving tool, EDX analysis to achieve stoichiometric composition of YPtBi, and SEM analysis of the interface.

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back to shortlist ↑

Nesting Instability of Gapless U(1) Spin Liquids with Spinon Fermi Pockets in Two Dimensions

P15

Wilhelm Krüger, TU Dresden

Quantum spin liquids are exotic states of matter that may be realized in frustrated quantum magnets and feature fractionalized excitations and emergent gauge fields. Here, we consider a gapless U(1) spin liquid with spinon Fermi pockets in two spatial dimensions. Such a state appears to be the most promising candidate to describe the exotic field-induced behavior observed in numerical simulations of the antiferromagnetic Kitaev honeycomb model. A similar such state may also be responsible for the recently-reported quantum oscillations of the thermal conductivity in the field-induced quantum paramagnetic phase of α-$RuCl_3$. We consider the regime close to a Lifshitz transition, at which the spinon Fermi pockets shrink to small circles around high-symmetry points in the Brillouin zone. By employing renormalization group and mean-field arguments, we demonstrate that interactions lead to a gap opening in the spinon spectrum at low temperatures, which can be understood as a nesting instability of the spinon Fermi surface. This leads to proliferation of monopole operators of the emergent U(1) gauge field and confinement of spinons. While signatures of fractionalization may be observable at finite temperatures, the gapless U(1) spin liquid state with nested spinon Fermi pockets is ultimately unstable at low temperatures towards a conventional long-range-ordered ground state, such as a valence bond solid. Implications for Kitaev materials in external magnetic fields are discussed.

back to shortlist ↑

Strong Anisotropy in the Ballistic Transport Regime on Pd(110)

P16

Markus Leisegang, JMU Würzburg

Atomic-scale charge transport properties are not only of significant fundamental interest but also highly relevant for numerous technical applications. However, experimental methods that are capable of detecting charge transport at the relevant single-digit nanometer length scale are scarce. We report on molecular nanoprobe experiments [1] on Pd(110), where we use the charge carrier-driven switching of a single cis-2-butene molecule [2] to detect ballistic transport properties over length scales of a few nanometers. Our data demonstrate a striking angular dependence with a dip in the charge transport along the [11$\bar{0}$]-oriented atomic rows and a peak in the transverse [001] direction. The narrow angular width of both features and distance-dependent measurements suggest that the nanometer-scale ballistic transport properties of metallic surfaces are significantly influenced by the atomic structure [3].

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back to shortlist ↑

Bose-Hubbard Realization of Fracton Defects

P17

Ruben Lier, MPI-PKS Dresden

Bose-Hubbard models are simple paradigmatic lattice models used to study dynamics and phases of quantum bosonic matter. We combine the extended Bose-Hubbard model in the hard-core regime with ring-exchange hoppings. By investigating the symmetries and low-energy properties of the Hamiltonian we argue that the model hosts fractonic defect excitations. We back up our claims with exact numerical simulations of defect dynamics exhibiting mobility constraints. Moreover, we confirm the robustness of our results against fracton symmetry breaking perturbations. Finally we argue that this model can be experimentally realized in recently proposed quantum simulator platforms with big time crystals, thus paving a way for the controlled study of many-body dynamics with mobility constraints.

back to shortlist ↑

Exotic Quantum Criticality in Dirac Systems: Metallic and Deconfined

P18

Zihong Liu, JMU Würzburg

Motivated by the physics of spin-orbital liquids, we study a model of interacting Dirac fermions on a bilayer honeycomb lattice at half filling, featuring an explicit global SO(3)×U(1) symmetry. Using large-scale auxiliary-field quantum Monte Carlo (QMC) simulations, we locate two zero-temperature phase transitions as function of increasing interaction strength. First, we observe a continuous transition from the weakly-interacting semimetal to a different semimetallic phase in which the SO(3) symmetry is spontaneously broken and where two out of three Dirac cones acquire a mass gap. The associated quantum critical point can be understood in terms of a Gross-Neveu-SO(3) theory. Second, we subsequently observe a transition towards an insulating phase in which the SO(3) symmetry is restored and the U(1) symmetry is spontaneously broken. While strongly first order at the mean-field level, the QMC data is consistent with a direct and continuous transition. It is thus a candidate for a new type of deconfined quantum critical point that features gapless fermionic degrees of freedom.

back to shortlist ↑

Bosonization of the Q = 0 Continuum of Dirac Fermions

P19

Sebastian Felipe Mantilla Serrano, MPI-PKS Dresden

We develop a bosonization formalism that captures non-perturbatively the interaction effects on the $Q = 0$ continuum of excitations of nodal fermions above one dimension. Our approach is a natural extension of the classic bosonization scheme for higher dimensional Fermi surfaces to include the $Q = 0$ neutral excitations that would be absent in a single-band system. The problem is reduced to solving a boson bilinear Hamiltonian. We establish a rigorous microscopic footing for this approach by showing that the solution of such boson bilinear Hamiltonian is exactly equivalent to performing the infinite sum of Feynman diagrams associated with the Kadanoff-Baym particle-hole propagator that arises from the self-consistent Hartree-Fock approximation to the single particle Green's function. We apply this machinery to compute the interaction corrections to the optical conductivity of 2D Dirac Fermions with Coulomb interactions reproducing the results of perturbative renormalization group at weak coupling and extending them to the strong coupling regime.

back to shortlist ↑

Fluctuation-Induced Ferrimagnetism in Sublattice-Imbalanced Antiferromagnets with Application to $SrCu_2(BO_3)_2$ under Pressure

P20

Pedro Monteiro Consoli, TU Dresden

We show that a collinear Heisenberg antiferromagnet, whose sublattice symmetry is broken at the Hamiltonian level, becomes a fluctuation-induced ferrimagnet at any finite temperature below the Néel temperature. We first demonstrate this in a layered variant of a square-lattice $J_1 - J_2$ model, in which spin-wave and Landau theories are used to determine the behavior of the uniform magnetization at low and elevated temperatures, respectively. We then consider a layered Shastry-Sutherland model, describing a frustrated arrangement of orthogonal dimers. This model displays an antiferromagnetic phase for large intra-dimer couplings. A lattice distortion that breaks the glide symmetry between the two types of dimers leads to broken sublattice symmetry and hence gives rise to ferrimagnetism. Given indications that such a distortion is present in the material $SrCu_2(BO_3)_2$ under high hydrostatic pressure, we suggest the existence of a fluctuation-induced ferrimagnetic phase in pressurized $SrCu_2(BO_3)_2$. We predict a nonmonotonic behavior of its uniform magnetization as a function of temperature.

back to shortlist ↑

STM Functionalized Tips - One Step Beyond the Resolution Limits

P21

Artem Odobesko, JMU Würzburg

STM and STS is a powerful techniques for local probing of the topography on the atomic level and electron densities of states. Nonetheless, there are limitations on the spatial and energy resolution due to the irregular shape of the tip and the effect of thermal broadening. These limitations can be overcome by functionalizing the STM tip apex with CO molecule to increase the spatial resolution of the tip or tunneling from a superconducting tip to exclude thermal broadening of the Fermi step of a normal metal tip. Here we try to combine both approaches to obtain an extra energy resolution with extra spatial resolution. With the help of such a ultra-functionalized STM tip, we are able to resolve rapidly decaying in space oscillations of Yu-Shiba-Rusinov bound states near magnetic Fe dimer on the bare Nb(110) surface. This allows us, for the first time, to determine the Fermi wavelength of Nb(110) surface. Such ultra-functionalized STM tips take the STM technique to the next level.

back to shortlist ↑

Thermopower and Magnetotransport Properties of $Bi_{100-x}Sb_x$ Topological Insulator Thin Films Prepared by Rapid Quenching

P22

Ena Osmic, Helmholtz-Zentrum Dresden-Rossendorf

We have measured the temperature dependence of resistance $R(T)$, thermopower $S(T)$, magnetoresistance (MR) and the Hall effect (HE) of $Bi_{80}Sb_{20}$, $Bi_{85}Sb_{15}$ and $Bi_{90}Sb_{10}$ topological insulator thin films. Samples were prepared by sequential flash-evaporation at room temperature and annealing at $T = 350\,\mathrm{K}$. The $R(T)$ of the three investigated samples shows metallic-like behavior for temperatures less than $T = 75\,\mathrm{K}$, while for higher temperatures, $R(T)$ shows a semiconducting-like behavior. The thermopower $S(T)$ of the three investigated samples is negative in the entire temperature range measured in this work, with a linear behavior from 5 up to $\approx 100\,\mathrm{K}$. The magnetoresistance of all samples is positive with a small temperature dependence. The highest MR ($B = 7\,\mathrm{T}$) was observed in $Bi_{85}Sb_{15}$ with a $\approx 600\%$ and $\approx 125\%$ change at 5 and 300 K, respectively. Clear evidence of weak antilocalization contribution to the MR was observed only in sample $Bi_{85}Sb_{15}$ for temperatures $T < 75\,\mathrm{K}$. Quantum oscillations in the MR originating from the Fermi surface, which has a clear two-dimensional character, were observed in sample $Bi_{85}Sb_{15}$ up to $\approx 21\,\mathrm{K}$. Hall effect results indicate a p-type behavior for sample $Bi_{80}Sb_{20}$, while $Bi_{85}Sb_{15}$ and $Bi_{90}Sb_{10}$ display n-type behavior. Carrier mobility information of sample $Bi_{85}Sb_{15}$ was extracted from low field HE data, showing a remarkably high value of $\mu \approx 2.8 \times 10^4$ $\mathrm{cm}^2/\mathrm{Vs}$ at 5 K, with a small decrease for increasing temperature.

back to shortlist ↑

Modification of Magnetic Behavior in $La_xNd_{3-x}Fe_3Sb_7$

Falk Pabst, TU Dresden

P23

Unsubstituted $RE_3Fe_3Sb_7$ (RE = Nd, Pr) displays a very complex magnetic interaction of the Fe and rare earth sublattice resulting in magnetic compensation and sign reversal f the magnetization at low temperatures. Current investigations aim for a better understanding of this behavior in the parent compounds. Substituting Nd with non-magnetic La allows to modify the rare earth sublattice and subsequently quench the magnetic interaction.

back to shortlist ↑

Jamming Dynamics in a Hardcore Spin System

P24

Benedikt Placke, MPI-PKS Dresden

We study the dynamics of hardcore spin model on the square and triangular lattice, obtained by analogy to hard spheres, where the translational degrees of freedom of the spheres are replaced by orientational degrees of freedom of spins on a lattice and the packing fraction as a control parameter is replaced by an exclusion angle. Analogously to the hard-sphere constraint, where no two sphere centers are allowed to be closer than the sum of their radii, in the hardcore spin model neighboring spins are forced to enclose an angle greater than their exclusion angle. In equilibrium, both models exhibit a Kosterlitz-Thouless transition at an exclusion angle Δ_{KT}. We study phase-ordering kinetics of states prepared using a quench protocol from the paramagnetic into the KT phase inspired by compression of hard spheres. We find a time scale of relaxation towards equilibrium that diverges with a power law with respect to both system size and the deviation from the critical angle $\Delta_J = \pi/2 > \Delta_{\mathrm{KT}}$. We show that this results from a combination of the diffusion-annihilation process describing the relevant phase ordering kinetics of a KT model, with a vanishing defect mobility setting the power law as $\Delta \to \Delta_J$.

back to shortlist ↑

Gross-Neveu-SO(3) Quantum Criticality

P25

Shouryya Ray, TU Dresden

Two-dimensional spin-orbital magnets with strong exchange frustration have recently been predicted to realize a quantum critical point in the Gross-Neveu-SO(3) universality class. Unlike previously studied Gross-Neveu universality classes, this quantum critical point separates a Dirac semimetal from a long-range-ordered phase in which the fermion spectrum is only partially gapped out. Here, we characterize the quantum critical behavior of the Gross-Neveu-SO(3) universality class by employing three complementary field-theoretical techniques beyond their leading orders, and produce best-guess theoretical estimates for critical exponents by averaging over the results of the different techniques.

back to shortlist ↑

Periodic Waveguide Ring Arrays Fabricated in a Microtube Cavity Towards Topological Phase Transition

P26

Christian Niclaas Saggau, IFW Dresden

Topological phenomena have been extensively studied in various systems ranging from solids state materials to metamaterials. Unlike matter, which is formed by atoms, in photonic metamaterials the individual building blocks and the lattices can be flexibly designed and manipulated. Therefore, arrays and meshes of optical components, such as nano-antennas,[1] waveguides[2,3] or optical cavities[4,5] have been employed to simulate topological phenomena. Similarly, to the electrons, unidirectional propagation of light can be observed in edge states of such structures.[6] Here we propose a novel structure of parallelly aligned single-mode ring resonator chains assembled along the surface of a microtubular structure. In contrast to the 2D configuration, in 3D structures optical coupling is not limited to a single point but happens along the whole circumference. Because of the 3D coupling, very high coupling strengths are obtainable manifesting in split-modes that exceed the FSR of the cavity.[7] At points of energetic degeneracy between resonance modes of different orders interference leads to the formation of hybrid-modes that resemble the vibrational excitations of an oscillator chain. Furthermore, the here presented structure is geometrically fundamentally different to its 2D equivalent, as the homotopic identity is constant. By designing periodically coupled ring arrays the here presented system can be used to investigate topological phenomena within the Su-Schrieffer-Heeger (SSH) model. Topological phase transition can be explored by thermal heating or selectively filling up the ring gaps by responsive materials. By introducing optical gain media, topological laser relying on resonant topological edge modes can be expected in the coupled 3D ring array.

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back to shortlist ↑

Spectroscopic Signatures of Non-trivial Topology in Weyl Semimetals

P27

Jakub Schusser, JMU Würzburg

Dirac and Weyl semimetals have become a highly relevant topic in contemporary condensed matter physics. Despite the fact that several experimental approaches have been introduced, none allows for their unambiguous identification in photoemission. By performing angle-resolved photoemission spectroscopy (ARPES) on the bulk samples we show the spectroscopic manifestation of topologial features and Weyl physics beyond the simple photointensity over a broad range of excitation energies from the vacuum ultraviolet (VUV) to the soft X-Ray (SX) regime which allows us to compare the surface and the bulk band structure. Our experimental observations were complemented by state-of-the-art ab initio first principle photoemission calculations based on one-step model of photoemission and density functional theory (DFT). By utilizing the determinant criterion, we confirm the arc character of the spoon features in the constant energy contour close to Fermi level in non-centrosymmetric TaP and TaAs. We further show the drawbacks of the existing spectroscopic techniques used to determine whether given material has non-zero Chern number and discuss an improved approach for identifying Fermi arcs by the means of differential ARPES measurements. Our results represent an important step towards revealing topologically non-trivial materials as well as show the importance of proper final state description.

back to shortlist ↑

Fermi Surface of the Chiral Topological Semimetal PtGa with Maximal Chern Number

P28

Valentin Schwarze, Helmholtz-Zentrum Dresden-Rossendorf

PtGa is a chiral topological semimetal with giant spin-split Fermi arcs with a maximal Chern number of four. We investigated the bulk Fermi surfaces of PtGa with angular-dependent de Haas-van Alphen (dHvA) measurements and band-structure calculations. Strong spin-orbit coupling leads to well separated spin-split bands. Eight bands cross the Fermi energy forming a multitude of Fermi surfaces resulting in intricate dHvA spectra. We were not able to assign all experimentally observed dHvA frequencies to the corresponding calculated extremal orbits, because of their considerable quantity and proximity. Yet, the experiment is in good agreement with the calculations confirming the topological character of PtGa.

back to shortlist ↑

SP-STM Study of Magnetic Zig-Zag $2\sqrt{2} \times \sqrt{2}$ Structure on 3 AL Mn/W(001)

P29

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Spin spirals and dead magnetic layers in the antiferromagnetic transition metal Mn on the heavy bcc(001) surface of W have recently attracted considerable interest [1,2]. In this poster, we present a spin-polarized STM investigation of 2-4 atomic layer (AL) thick Mn films on W(001). For 3 AL Mn on W(001) it has been theoretically proposed that this system grows pseudomorphically as islands while exhibiting an antiferromagnetic state [3]. Our topographic STM data confirm that pseudomorphic growth even prevails up to a Mn film thickness of 4 AL. Spin-resolved data were acquired by scanning with W tips which had been magnetized on Mn layers by in-situ treatment on Mn/W(001). This allowed us to collect topographic and spin-resolved data on the same scanning area. Applying this method, we found a magnetic zig-zag $2\sqrt{2} \times \sqrt{2}$ structure on 3 AL Mn and a strongly bias-dependent labyrinth overlay structure for 4 AL. The sensitivity of each tip was characterized by test measurements on the well-known 2 AL Mn on W(001) [2].

[1] P. Ferriani et al., Phys. Rev. Letters 101, 027201 (2008)
[2] S. Meyer et al., Phys. Rev. Research 2, 012075(R) (2020)
[3] S. Dennler et al., Phys. Rev. B 72, 214413 (2005)

back to shortlist ↑

Symmetry Resolved Entanglement in AdS/CFT

P30

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Quantum entanglement is a key resource in quantum computing, and an important quantity to characterize quantum phases of matter. It is however quite crude, depending only on the central charge of a quantum field theory. We introduce the concept of symmetry resolved entanglement entropy (SREE), which is a fine-grained version of the usual entanglement entropy, resolving the dependence of the entanglement entropy on a conserved charge. SREE can be calculated in a wide range of condensed matter systems like spin chains, free bosons, and free fermions. We calculate SREE in the context of the Anti-de Sitter/Conformal field theory (AdS/CFT) correspondence, for strongly interacting 2D CFTs with U(1) Kac-Moody symmetry. We find equipartition of entanglement between different charge sectors, and in general agreement between both sides of the AdS/CFT correspondence.

back to shortlist ↑

Kondo Breakdown in a Spin-1/2 Chain of Adatoms on a Dirac Semimetal

P31

Bimla Danu, JMU Würzburg

We consider a spin-1/2 Heisenberg chain coupled via a Kondo interaction to two-dimensional Dirac fermions. The Kondo interaction is irrelevant at the decoupled fixed-point, leading to the existence of a Kondo-breakdown phase and a Kondo-breakdown critical point separating such a phase from a heavy Fermi liquid. We reach this conclusion on the basis of a renormalization group analysis, large-N calculations as well as extensive auxiliary-field quantum Monte Carlo simulations. We extract quantities such as the zero-bias tunneling conductance which will be relevant to future experiments involving adatoms on semimetals such as graphene.

back to shortlist ↑

Discovery of Axis-Dependent Conduction Polarity in $NaSnAs_{1-x}P_x$ through Computationally-Guided Methods

P32

Andrew Ochs, MPI-CPfS Dresden

Most electronic materials exhibit a single dominant charge carrier type, either holes (p-type) or electrons (n-type), along all crystallographic directions. However, there are a small number of compounds, mostly metals, that exhibit simultaneous p-type and n-type conduction behavior along different crystallographic directions. We demonstrate the experimental discovery of semiconductors with this axis-dependent conduction polarity can be facilitated by identifying a large anisotropy of either the electron and hole effective masses (m^*), or both, providing the electron and hole masses dominate along different crystallographic directions. In this study, we calculated the layered semiconductors NaSnAs and NaSnP to have a lower electron m^* in-plane than cross-plane, and a very large hole m^* in-plane and small hole m^* cross-plane. We established the growth of large $NaSnAs_{1-x}P_x$ (x = 0, 0.1, 0.2, 0.3, 1) crystals via Sn flux, and measured band gaps ranging from 0.65 eV to 1.04 eV with increasing P content by diffuse reflectance experiments, in agreement with theory. NaSnAs, NaSnP, and their alloys all exhibit p-type thermopowers cross-plane and n-type thermopowers in-plane, confirming that the large anisotropy in the effective mass at the band edges is an excellent indicator for axis-dependent conduction polarity. Overall, this work shows that the discovery of semiconductors with such a phenomenon can be accelerated by computationally evaluating the anisotropic curvatures of the band edges, paving the way for their future discovery and application.

back to shortlist ↑

The Pyrochlore S = 1/2 Heisenberg Antiferromagnet at Finite and Zero Temperature

P33

Robin Schäfer, MPI-PKS Dresden

We use cutting-edge computational methods to investigate the intricate frustrated three-dimensional quantum spin liquid candidate, the pyrochlore $S = 1/2$ antiferromagnet at finite and zero temperature.
Using a systematic cluster expansion based on tetrahedra, including clusters up to 25 lattice sites with nontrivial hexagonal and octagonal loops, we gain access to various thermodynamic properties in the thermodynamic limit at finite temperature. We found a pronounced maximum in the specific heat at $T = 0.57\,J$ that is stable across finite size clusters and converged in the series expansion. At $T \approx 0.25\,J$ (the limit of convergence of our method), the residual entropy per spin is $0.47\,k_{\mathrm{B}}\log(2)$, which is relatively large compared to other frustrated models at this temperature.
We applied SU(2) DMRG to periodic clusters with up to 128 sites to examine the zero temperature properties and determine the ground state energy, $E_0/N_{\mathrm{sites}} = -0.490\,J$. Our most striking finding is a robust spontaneous inversion symmetry breaking, reflected in an energy density difference between the two sublattices of tetrahedra, which is supported by different perturbative treatments. These findings suggest a scenario in which a finite-temperature spin liquid regime gives way to a symmetry-broken state at low temperatures. Furthermore, we study the magnetization process finding a pronounced and apparently robust 1/2-magnetization plateau where the groundstate breaks (real-space) rotational symmetry, exhibiting oppositely polarized spins on alternating kagome and triangular planes. Reminiscent of the kagome ice plateau of the pyrochlore Ising magnet known as spin ice, it arises via a much more subtle 'quantum order by disorder' mechanism.

back to shortlist ↑